

Nonlinear Models with Moderated Parameters: New Methods and Software for Social Science  
Applications

By

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Dissertation

Submitted to the Faculty of the  
Graduate School of Vanderbilt University

in partial fulfillment of the requirements

for the degree of

DOCTOR OF PHILOSOPHY

in

Psychology

May 10, 2024

Nashville, Tennessee

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## ACKNOWLEDGEMENTS

I would like to express my deepest appreciation to my advisor, Dr. Kris Preacher, and my committee members, Drs. Sonya Sterba, Sun-Joo Cho, and Will Doyle, for providing invaluable training throughout my graduate career. Thank you for generously sharing your expertise and advice, supporting me in so many ways throughout my development as a researcher, and affording me the autonomy to pursue the passions and ideas that I was most excited about.

I am endlessly grateful for my partner, Kevin, who has listened to me so much over the past five years that he should have his own Ph.D. Thank you for watching every practice talk, talking with me through every frustration (often circa 2AM), comforting me through every disappointment, and dancing in the living room with me to celebrate every victory, no matter how big or small. (I must also thank Kool & The Gang for making those dance parties happen.) I could go on and on, but you already know how thankful I am for you every day.

I would like to express my love and gratitude to my mom, whose support I have leaned on my entire life. When I took my first really difficult math class as an undergrad, I called my mom and told her I was afraid I would fail. She said, “Honey, someone in that class has to get an A. Why not you?” I’ve carried that encouragement with me throughout everything I’ve done since. Someone is going to get into the program... someone is going to get the grant... someone is going to get the job... why not me? Thank you for your endless love and belief in me.

Thank you to my sister, Erika, and my friends and family in Nashville, Michigan, and beyond. When work feels all-consuming, you remind me of who I am and what really matters. My little network of encouragement and support has sustained me over the last five years, and it means the world to me to be able to support you all right back.

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# CHAPTER I

## INTRODUCTION

Though commonplace in other fields, intrinsically nonlinear models are used rarely in psychology and social science research. One purpose of this dissertation is to establish the utility of nonlinear models for social scientists by demonstrating the enhanced theoretical and substantive contributions that can be made through use of these models. Additionally, assessing the presence of moderation is often of key importance for psychological theory testing. However, methods for testing, plotting, and probing moderation were developed for linear models, and currently, their use remains largely restricted to linear models. Another goal of this dissertation is to develop novel analytical and software tools that enable the specification and examination of moderated parameters within intrinsically nonlinear models. Approaches to model specification, as well as methods for testing, plotting, and probing moderation, will be extended in novel ways for use in nonlinear models; additionally, a Shiny app that unifies this process will be introduced. The goal of the current chapter is to introduce key terms and concepts that will be referenced and intertwined throughout the remainder of the dissertation.

### **Intrinsically Nonlinear Models**

In an intrinsically nonlinear model, the function that relates a predictor ( $x$ ) to an outcome ( $y$ ) is nonlinear in at least one of its parameters. It may be easiest to understand what it means for a model to be “nonlinear in its parameters” by contrasting this to a linear model. When a model is linear in its parameters, each additive term in the model contains only one parameter, and each

parameter (except the intercept) is a multiplicative constant of one or more predictors (Panik, 2014). All other models are nonlinear (Sit & Poulin-Costello, 1994). As an example, the quadratic model (Eq. 1.1) is linear in its parameters, whereas the power model (Eq. 1.2) is nonlinear in its parameters. In the following equations (and throughout the dissertation), letters from the Latin alphabet ( $a$ ,  $b$ ,  $c$ , etc.) will be used to represent nonlinear model parameters, whereas  $\varepsilon$  will denote an error term.

$$y = a + bx + cx^2 + \varepsilon. \quad (1.1)$$

$$y = ax^b + \varepsilon. \quad (1.2)$$

More formally, intrinsically nonlinear models can be defined by their first derivatives. After taking the first derivative of the function with respect to each parameter, a model is intrinsically nonlinear if at least one of these first derivatives contains one or more model parameters (Bates & Watts, 1988; Ratkowsky, 1990).

Models may be described as *nonlinear* according to how parameters appear in the regression equation, or according to the shape of the relation between  $x$  and  $y$  (Panik, 2014). Throughout this dissertation, *nonlinear* will be used to reference models that are nonlinear in at least one parameter in the regression equation, according to the above definition. In other contexts, *nonlinear* is used more broadly to describe relations between  $x$  and  $y$  that do not follow a straight line; for example, the quadratic model is often referred to as a nonlinear model, despite being linear in its parameters. For clarity, *curvilinear* will be used as a broader descriptor for relationships between  $x$  and  $y$  that do not follow a straight line.

The scope of this dissertation will be limited to parametric nonlinear models. These models are defined prior to being fit to the data, in terms of their shape and the parameters that govern that shape (Panik, 2014). Nonparametric nonlinear models take on a shape that is

informed by the data rather than by prespecified functional form; for example, the generalized additive mixed model (GAMM) is largely nonparametric (Lin & Zhang, 1999; Wood, 2017). A more detailed treatment of the contrasts between parametric and nonparametric nonlinear models will be reserved for the discussion.

There exist a wide variety of parametric nonlinear models that can characterize a diverse array of relations between  $x$  and  $y$  (Ratkowsky, 1990; Sit & Poulin-Costello, 1994). There are models that involve lower and/or upper asymptotes, minima, maxima, non-constant rates of change, inflection points, multiple regions/phases of relationships, and more features. Whatever the hypothesized nature of the relation between two variables, there is likely to be an intrinsically nonlinear model that can approximate that relationship. Though each approximates a specific functional form, as a collection, nonlinear models offer much greater flexibility than linear models (Archontoulis & Miguez, 2015). Linear models are very restrictive in terms of the nature of the relationship between  $x$  and  $y$  that can be well-approximated. For example, linear models without polynomial terms assume that as  $x$  increases by one unit, the corresponding change in  $y$  is constant across all possible values of  $x$ . Polynomial models assume a very specific type of curvilinear relation exists between  $x$  and  $y$  (e.g., in the quadratic model, a symmetric parabola). Problematically, it is often not reasonable to expect that psychological constructs will be related in one of the specific ways allowed by linear models. Intrinsically nonlinear models allow us to entertain the possibility of a great many more relationships that are likely to be more realistic.

Often, each parameter in a nonlinear model governs a particular aspect of the curve. This is akin to a linear model whose appearance is controlled by two parameters: the intercept parameter governs the location of the line along the  $y$ -axis, and the slope parameter governs the direction and steepness of the line. Nonlinear models may contain one, two, three, four, or more

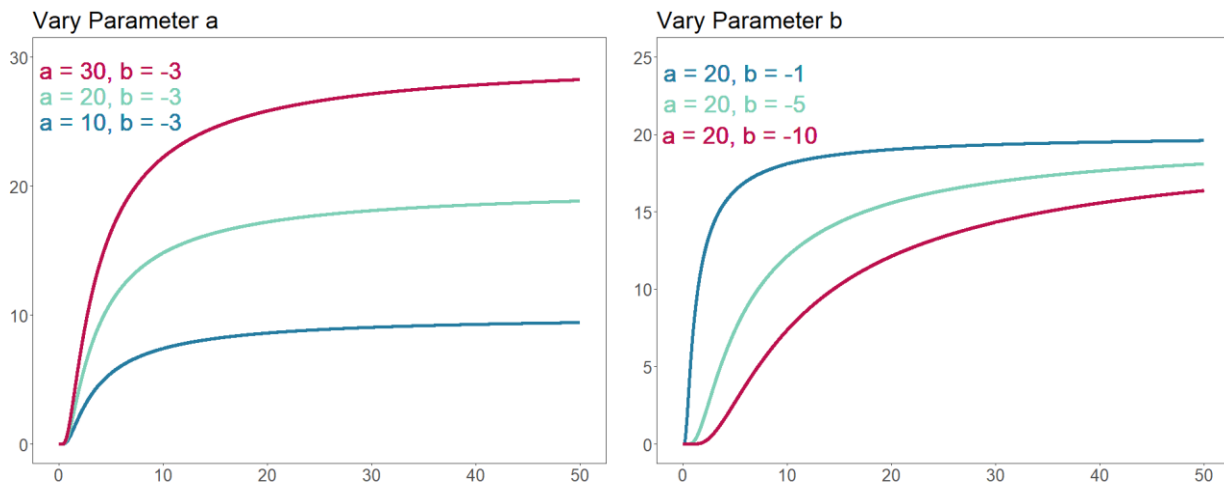
parameters, and each of those parameters often corresponds to a specific attribute of the curve. Beyond intercepts and slopes, a much more diverse variety of curve characteristics can be pinpointed by the parameters that are estimated in a nonlinear model.

As an example, consider a two-parameter exponential model. In this model, the steepness of the slope decreases as  $x$  increases, until the relation between  $x$  and  $y$  eventually levels off to an upper or lower asymptote. One way to express the two-parameter exponential model is:

$$y = a * \exp\left(\frac{b}{x}\right) + \varepsilon, \tag{1.3}$$

where the model is governed by two parameters,  $a$  and  $b$ . Parameter  $a$  governs the vertical location of the asymptote, whereas parameter  $b$  governs the concavity of the curve. When  $b$  is positive, the function decreases toward a lower asymptote (i.e., is concave up), whereas when  $b$  is negative, the function increases toward an upper asymptote (i.e., is concave down). When  $b$  is closer to zero, the curve is steeper and reaches the asymptote earlier. Figure 1.1 depicts how the curve changes as parameter  $a$  is varied and  $b$  is held constant, as well as when parameter  $a$  is held constant and  $b$  is varied.

Figure 1.1. Exponential Curve Examples.



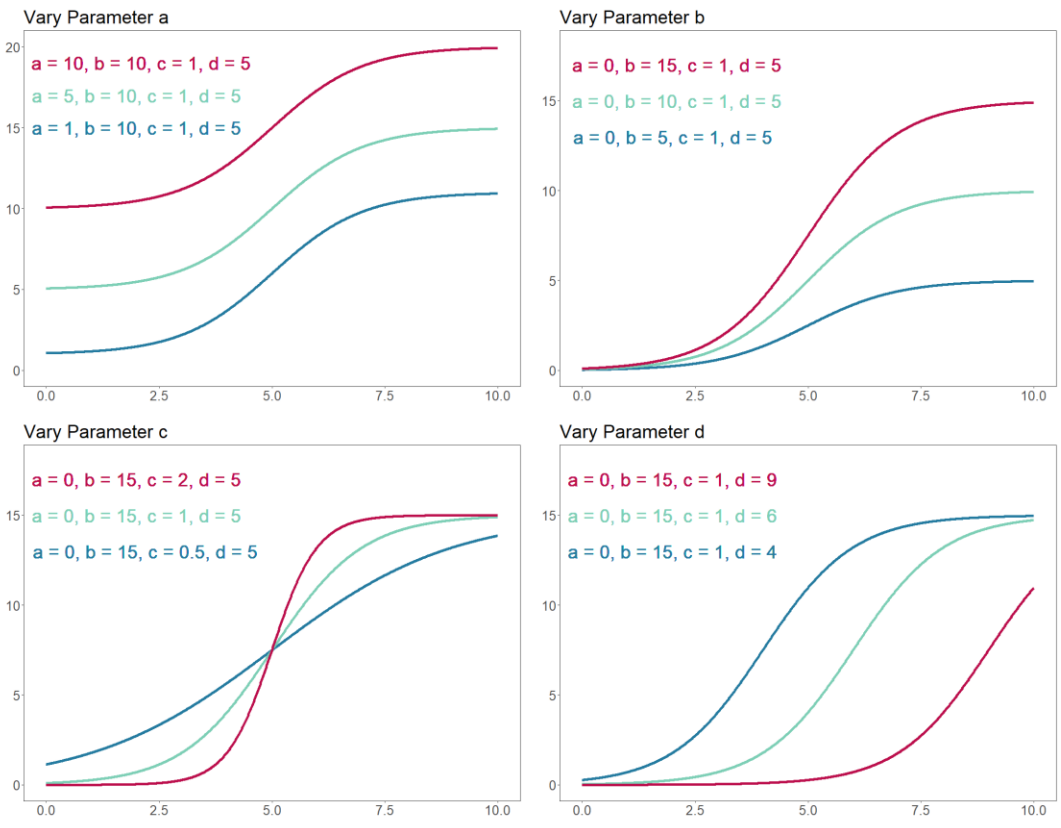


Nonlinear models may contain even more parameters that each correspond with a unique attribute of the curve. As another example, consider the logistic function, which may be controlled by up to four parameters. One version of the four-parameter logistic model is:

$$y = a + b * (1 + \exp(-c(x - d)))^{-1} + \varepsilon. \quad (1.4)$$

Here, parameter  $a$  governs the lower asymptote,  $b$  governs the vertical distance between the lower and upper asymptotes (i.e., total change),  $c$  governs the steepness of the curve (sometimes referred to as “slope” or “rate of approach”), and  $d$  governs the location along the  $x$ -axis at which the slope of the curve is greatest (also referred to as the “inflection point” or “surge point” of the curve). Figure 1.2 displays versions of the logistic curve where each parameter is varied and the others are held constant.

Figure 1.2. Logistic Curve Examples.



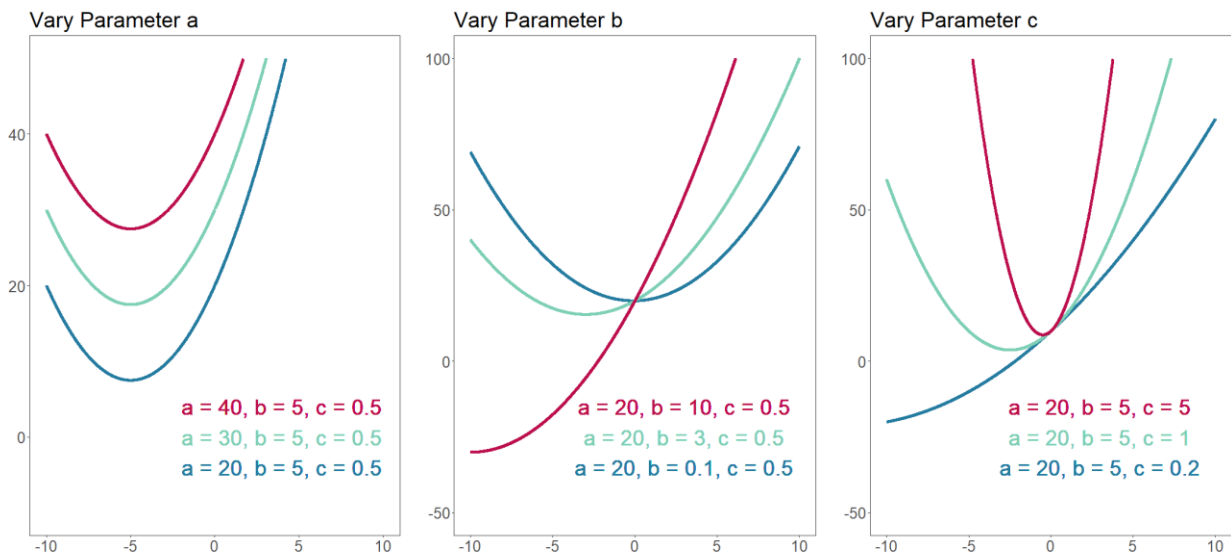
This example highlights the level of detail that can be obtained from nonlinear models when each parameter uniquely corresponds to a specific characteristic of the curve. The clear mapping between each model parameter and each attribute of the curve yields parameters with unambiguous and interpretable meaning. Upon estimating, for example, a logistic model to approximate learning trajectories, we can draw precise conclusions about those trajectories because each parameter influences the shape of the curve in a unique and specific manner (e.g., a larger parameter  $c$  indicates that learning occurs faster, whereas a smaller parameter  $d$  indicates that learning occurs earlier). As will be discussed in later chapters, the benefits of these straightforward mappings are also highly relevant when moderation of parameters is introduced.

By contrasting the exponential and logistic models with the quadratic model, we can further understand the benefits of straightforward mappings between model parameters and important aspects of the curve. The classic version of the quadratic model is given in Eq. 1.1. This curve is governed by three parameters. Parameter  $a$  controls the  $y$ -intercept, parameter  $b$  controls the slope of the line tangent to the parabola where  $x = 0$ , and parameter  $c$  controls the quadratic aspect of the curve, which corresponds to the parabola's overall curvature.

Figure 1.3 illuminates key weaknesses of the classic quadratic model. Although there is a straightforward connection between parameter  $a$  and the location of the  $y$ -intercept, parameters  $b$  and  $c$  govern characteristics of the curve that are unlikely to be substantively important. When parameter  $b$  is varied, the slope of the tangent line at  $x = 0$  changes, and when parameter  $c$  is varied, the curvature of the parabola changes; if using the quadratic function to model, for example, trajectories of happiness across the lifespan, it is unclear how parameters  $b$  and  $c$  could be interpreted in a way that facilitates useful conclusions. Indeed, Cudeck and Harring (2010) note that “the coefficients of polynomial functions do not have a clear-cut and scientifically

meaningful interpretation.” Additionally, parameters  $b$  and  $c$  incidentally govern attributes of the parabola other than those named above, including the location of the parabola’s minimum along the  $x$ -axis. Therefore, our ability to substantively interpret these parameters suffers further, and if parameters  $b$  or  $c$  are found to be moderated, our ability to make meaningful sense of that moderation is limited.

Figure 1.3. Quadratic Curve Examples.



### Nonlinear Mixed-Effects Models

Although nonlinear models remain relatively uncommon in social science, when they *are* implemented, they often take the form of nonlinear mixed-effects (NLME; Pinheiro & Bates, 2000) models in studies of psychological growth or change over time. NLME models are ideal for longitudinal contexts because they can account for the dependence that arises when the same individuals are assessed repeatedly, such that multiple observations (level 1) are nested within each individual (level 2) in a hierarchical data structure. In NLME growth models, variables may

exist at level 1 or level 2. Level-1 variables change across timepoints or assessments (e.g., affect, blood pressure), whereas level-2 variables are static and describe person-level characteristics (e.g., gender, age, socioeconomic status). Additionally, the parameters that govern the growth trajectory can be treated as fixed or random. If treated as fixed, then the parameter is assumed to be the same for all individuals, and if treated as random, then the parameter is allowed to vary across individuals. Random parameters enable the researcher to understand which attributes of the growth trajectory differ across people (Blozis & Harring, 2021; Cudeck & Harring, 2007, 2010; Davidian & Giltinan, 2003; Harring & Blozis, 2014; Pinheiro & Bates, 2000).

As an example, consider the two-parameter exponential model given in Eq. 1.3, which may easily be modified into a NLME model. Suppose we have obtained repeated measurements of vocabulary development among children; each child in our study was assessed multiple times, so our data are hierarchically nested. We also suspect that both model parameters will differ across children. We can specify our NLME model as follows:

$$y_{ti} = a_i * \exp\left(\frac{b_i}{t}\right) + \varepsilon_{ti}, \quad (1.5)$$

where

$$a_i = a_{00} + aResid_i,$$

$$b_i = b_{00} + bResid_i.$$

In Eq. 1.5,  $t$  (time) is the predictor,  $y_{ti}$  is the observation taken for individual  $i$  at time  $t$ ,  $a_i$  is the value of  $a$  for individual  $i$ ,  $b_i$  is the value of  $b$  for individual  $i$ , and  $\varepsilon_{ti}$  is the level-1 residual for individual  $i$  at time  $t$ . Additionally, each individual-specific coefficient ( $a_i, b_i$ ) is made up of two components. The fixed component ( $a_{00}, b_{00}$ ) denotes the mean value of the coefficient for all individuals in the sample. The random component ( $aResid_i, bResid_i$ ) denotes the deviation of

the individual-specific coefficient from the mean value. The (co)variances of the random components ( $aResid_i$ ,  $bResid_i$ ) are estimated, as well as the variance of the level-1 residuals.

In summary, NLME models afford researchers all the key advantages described in the prior section, including clearly interpretable parameters, with the added benefit that nested data structures can be accommodated. Later chapters will review successful use cases of nonlinear models in social science, many of which are NLME models.

### Parameterization

The concept of a model's *parameterization* is also important to define. Most nonlinear functions can be expressed in several equivalent ways (Cudeck & Harring, 2010; Preacher & Hancock, 2015). These expressions may contain different parameters that are each associated with a different attribute of the curve, and therefore, a different interpretation. All these parameterizations yield the same functional form, but the interpretations of the parameters themselves will vary in usefulness depending on the research context. For example, Cudeck and Harring (2010) introduce two potentially useful parameterizations of a three-parameter exponential model. The first is:

$$y = a - (a - b)\exp(-c * x) + \varepsilon, \quad (1.6)$$

where  $a$  corresponds to the upper asymptote,  $b$  is the  $y$ -intercept of the curve, and  $c$  governs the rate of approach toward the upper asymptote. The second parameterization is:

$$y = a - (a - b)2^{-\frac{x}{c}} + \varepsilon. \quad (1.7)$$

Here,  $a$  again corresponds to the upper asymptote and  $b$  again corresponds with the  $y$ -intercept of the curve. However,  $c$  corresponds to the  $x$ -value at which the curve is halfway between the  $y$ -intercept and the upper asymptote. Both parameterizations yield a curve with the same shape, but

parameter  $c$  in Eq. 1.6 corresponds to a different attribute of that curve than parameter  $c$  in Eq. 1.7. Depending on the application, one of these parameterizations may be more useful than the other. For example, if using an exponential model to characterize cognitive skill acquisition, the interpretation of parameter  $c$  may be useful for understanding the general rate at which the skill is acquired over time. When modeling the relation between font size and reading speed, as in Cudeck and Harring (2010), the interpretation of parameter  $c$  was more useful for pinpointing the font size ( $x$ -value) at which reading speed reached 50% of its maximum. In summary, any function can be expressed so that the most important attributes of the curve are represented by a specific parameter. Choosing a parameterization that enables the direct testing of key hypotheses can greatly improve the substantive utility of the model, and as will be demonstrated in later chapters, becomes important when moderation of parameters is examined.

### **Linear Moderation**

It is also important to define linear moderation, as linear (rather than nonlinear) moderation will be the focus of this dissertation. In the context of ordinary least squares (OLS) linear regression, linear moderation occurs when the slope of the focal predictor,  $x$ , changes as a linear function of the moderator,  $z$ . Preacher et al. (2006) use the following notation to represent the regression equation:

$$y = \gamma_0 + \gamma_1x + \gamma_2z + \gamma_3xz + \varepsilon, \tag{1.8}$$

where the  $\gamma$ s are the linear regression weights and  $\varepsilon$  is the error term. From here, we can define the prediction equation, which denotes the expected value of  $y$  conditional on specific values of  $x$  and  $z$ :

$$E[y|(x, z)] = \hat{\gamma}_0 + \hat{\gamma}_1x + \hat{\gamma}_2z + \hat{\gamma}_3xz, \tag{1.9}$$

where the caret symbol (^) denotes the sample estimate of the corresponding linear regression parameter. Rearranging Eq. 1.9, we can obtain the estimated *simple slope* of  $x$  (also referred to as the *conditional slope* or *conditional effect*; Aiken & West, 1991; Darlington, 1990), which represents the effect of  $x$  on  $y$  at a particular value of the moderator:

$$\hat{\omega}_1 = \hat{\gamma}_1 + \hat{\gamma}_3 z. \quad (1.10)$$

Eq. 1.10 shows that  $\hat{\omega}_1$  is a linear function of the moderator. However, linear moderation can be defined more generally such that it also applies to the parameters of nonlinear models.

In general, linear moderation occurs when a parameter varies linearly according to the value of the moderator. In other words, a certain predictor (the moderator) linearly influences a parameter which governs some aspect of the curve linking  $x$  to  $y$ . For example, consider the two-parameter exponential model given in Eq. 1.3. A moderator may linearly influence any of these parameters, or in other words, any attribute of the curve that is governed by these parameters. Suppose we hypothesize that a moderator  $z$  linearly influences parameter  $a$ , which governs the vertical location of the asymptote. To reflect that this parameter is allowed to change linearly according to the value of the moderator, we could specify the moderated model as follows:

$$y = (a_0 + a_1 * z) * \exp\left(\frac{b}{x}\right) + \varepsilon, \quad (1.11)$$

where  $a_0$  denotes the value of parameter  $a$  when the moderator is zero, and  $a_1$  denotes the linear effect of  $z$  on  $a$ . In other words, as the moderator increases by one unit, the vertical location of the asymptote changes by  $a_1$ .

Later chapters will expand on the substantive insight that can be gained by incorporating moderators into nonlinear models. For now, it is important to establish that it is indeed possible to examine linear moderation of any parameter in a nonlinear model, and that each parameter of a nonlinear model often corresponds with a specific characteristic of the curve.

## The Johnson-Neyman Technique

When a parameter is found to be moderated, it is useful to follow up on that result in order to understand the nature of the moderation. Key insights can be gained from visualizing how the moderated parameter changes as the value of the moderator changes. This process is often referred to as “plotting and probing” moderation. A variety of methods exist for visually probing moderation; however, all were developed for linear models, and their use remains largely restricted to the linear modeling framework. In OLS regression, when the slope of the focal predictor is found to be moderated, that result is visually probed to gain insight into how the slope changes across different values of the moderator.

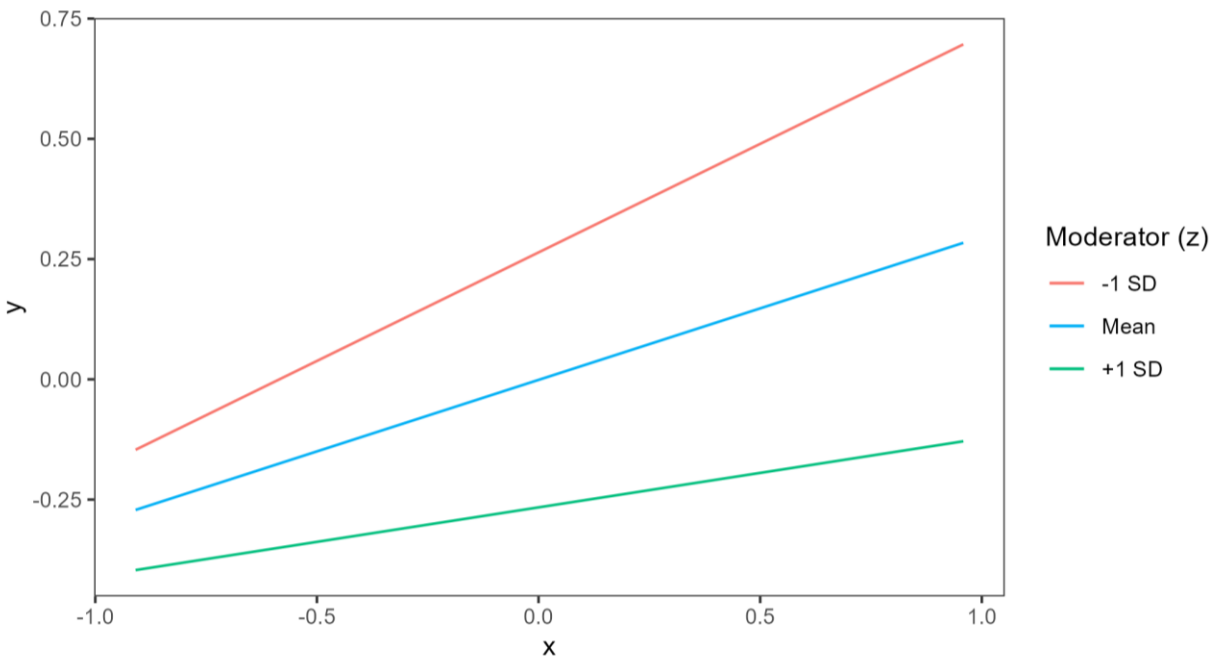
The most popular method for probing moderation is the pick-a-point approach (Aiken & West, 1991). Here, the researcher chooses a few values of the moderator (typically the mean  $\pm 1$  SD) and plots the relation between  $x$  and  $y$  at each of those values. See Figure 1.4 for an example. Using Eq. 1.10, it is straightforward to compute the simple slope of the focal predictor at any chosen value of  $z$ .

The pick-a-point approach remains popular because it is easy to implement and produces intuitive plots that are straightforward to understand and interpret. However, this approach suffers from notable weaknesses. First, the researcher evaluates the conditional slope of  $x$  at only a few values of  $z$ ; these values are inherently arbitrary and are often chosen automatically, which can be problematic. For example, if the three typical values of  $z$  (the mean,  $\pm 1$  SD) are chosen without first examining the data, then it is possible that a chosen  $z$ -value was not observed in the sample or was observed very sparsely. Therefore, extrapolation problems can easily arise (Bodner, 2016). Second, the use of only a few  $z$ -values inherently limits the insight the researcher can gain about  $x$ 's effect across the full observed range of  $z$  (Bauer & Curran, 2005;



McCabe et al., 2018). It is more useful to understand the conditional slope of  $x$ , and our certainty about that conditional slope, at all observed values of the moderator rather than at just a few.

Figure 1.4. Pick-a-Point Plot Example



The Johnson-Neyman (JN) technique (Johnson & Fay, 1950; Johnson & Neyman, 1936) is a general method that evaluates the conditional effect of a focal predictor across all possible values of the moderator. The JN technique improves upon the major weaknesses of the pick-a-point approach, affording two major advantages (Bauer & Curran, 2005). First, results of the JN technique communicate whether the simple slope of  $x$  is significant at every possible value of the moderator. Second, confidence bands communicate how certain we are about the simple slope of  $x$  at all possible values of the moderator, rather than at just a few.

The JN technique was originally developed for categorical-by-continuous moderation. Given two groups (i.e., a group mean difference), the JN technique could compute the values of

the moderator for which the group mean difference was significant. Since then, the technique has been extended so that it also applies to continuous-by-continuous moderation (Bauer & Curran, 2005). The JN technique allows us to answer: given a continuous predictor  $x$  and a continuous moderator  $z$ , for which values of  $z$  is the conditional slope of  $x$  significantly different from zero? The JN technique answers this question by deriving significance boundaries, which demarcate regions of significance. The regions of significance contain the  $z$ -values at which the conditional slope of  $x$  is significant.

Calculating significance boundaries is relatively straightforward with the JN technique. Recall from Eq. 1.10 that in a moderated linear model, the simple slope of  $x$  can be defined as  $\hat{\omega}_1 = \hat{\gamma}_1 + \hat{\gamma}_3 z$ . The standard error of this simple slope will be the square root of its variance, which is given by Aiken and West (1991) as:

$$var(\hat{\omega}_1) = var(\hat{\gamma}_1) + 2zcov(\hat{\gamma}_1, \hat{\gamma}_3) + z^2 var(\hat{\gamma}_3). \quad (1.12)$$

When the pick-a-point approach is used, we choose a few values of  $z$ , compute  $\hat{\omega}_1$  and  $SE(\hat{\omega}_1)$  at each of those values, and assess the significance of  $\hat{\omega}_1$  at each of those values. This is accomplished by the usual  $t$ -test:

$$t = \frac{\hat{\omega}_1}{SE(\hat{\omega}_1)}, \quad (1.13)$$

where both  $\hat{\omega}_1$  and  $SE(\hat{\omega}_1)$  are functions of  $z$ . The obtained  $t$ -statistic is then compared to a critical  $t$ -value ( $t_{crit}$ ) with  $n - p - 1$  degrees of freedom, where  $n$  is sample size and  $p$  is the total number of predictors in the model.

The JN technique essentially reverses the process of the typical significance test. Rather than solving for a  $t$ -statistic and comparing it to  $t_{crit}$  to assess significance, we first choose a  $t_{crit}$  and solve for the values of the moderator that yield it:

$$\pm t_{crit} = \frac{\hat{\omega}_1}{SE(\hat{\omega}_1)}. \quad (1.14)$$

This equation can be solved for values of  $z$  through use of the quadratic formula. The obtained values of the moderator indicate the points at which the simple slope of  $x$  passes from non-significance to significance.

In addition to solving for significance boundaries, the results of the JN technique can be plotted to gain a fuller understanding of the simple slope of  $x$  across all observed values of  $z$ . See Figure 1.5 for an example. In this figure, the moderator is on the  $x$ -axis, and the conditional slope of the focal predictor is on the  $y$ -axis. We can now visualize the simple slope of the focal predictor across all values of the moderator, and the accompanying confidence bands communicate our certainty about that simple slope at each value of the moderator.

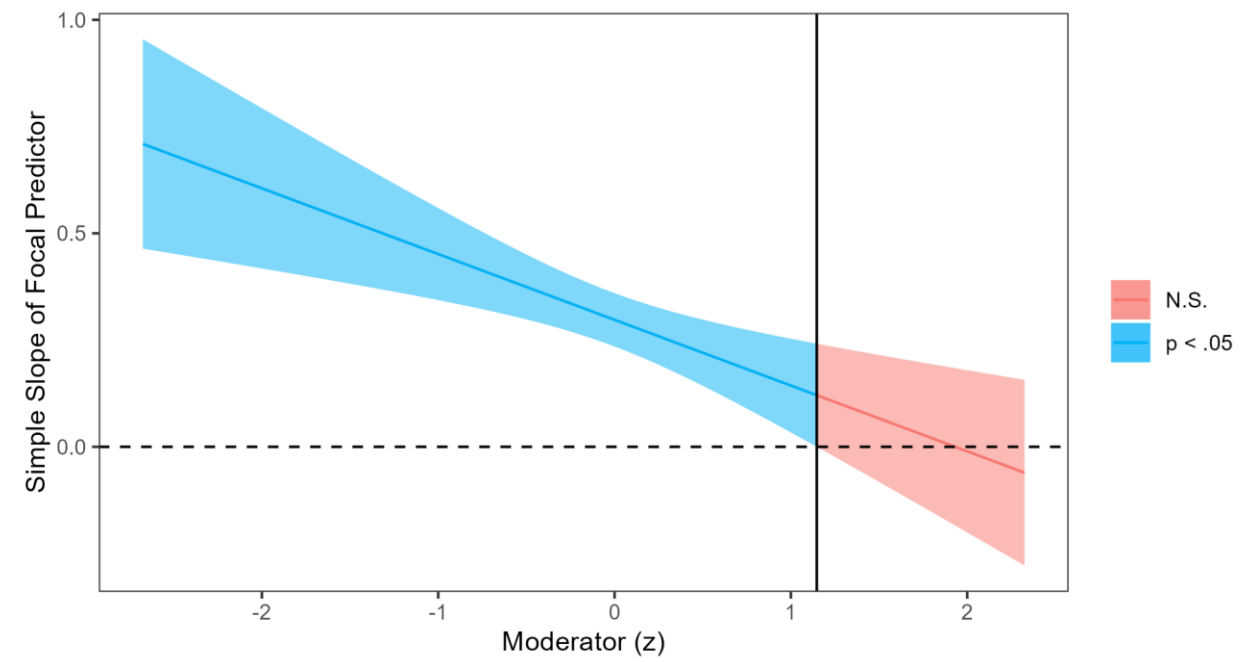
In Fig. 1.5, the vertical line denotes a significance boundary, and the confidence band denotes moderator values at which the simple slope of  $x$  is significantly different from zero (blue) or not (red). Up to two significance boundaries may exist, but one, both, or none of them may fall within the observed range of the moderator. In this example, one significance boundary was within the range of observed data, so one vertical line is shown. When two significance boundaries exist, the simple slope of  $x$  may be significant either between or outside of them.

Overall, the JN technique yields much richer information about the nature of an interaction than the pick-a-point approach. It affords insight into the value of the moderated parameter across every value of the moderator, and pinpoints the precise value(s) of the moderator where that parameter passes from statistical significance to non-significance.

In summary, when a parameter is found to be moderated, there are a variety of methods available for visually understanding the nature of that moderation. Of these methods, the JN technique provides the richest information. At present, the use of the JN technique is restricted to

linear models. One goal of this dissertation will be to derive novel extensions of the JN technique for examination of moderated parameters in nonlinear models.

*Figure 1.5. Johnson-Neyman Plot Example.*



### Summary

This chapter introduced intrinsically nonlinear models and began to delineate some of their benefits, specifically, clear mappings between model parameters and important attributes of the curve. Additionally, linear moderation was introduced alongside methods for visually probing moderation, including the pick-a-point and Johnson-Neyman techniques. These topics have been treated as disparate in most current literature; while some methodologists have discussed the utility of jointly examining curvilinear relations and moderation (e.g., Karaka-Mandic et al., 2012; Li, 2018; Miller et al., 2013; Mize, 2019), these discussions have remained limited to quadratic models, as well as models with linear predictor sets and logit or probit link

functions. Therefore, a central goal of this dissertation is to facilitate the joint use of intrinsically nonlinear models and methods for plotting and probing moderation.

The goal of Chapter 2 is to review both the methodological and applied literature pertaining to nonlinear models for social science. A variety of nonlinear model families will be introduced, and to demonstrate their utility, examples of their use across diverse research areas will be reviewed. Chapter 3 delineates current barriers to the uptake of (moderated) nonlinear models in social science research, in an effort to identify the gaps that need to be filled in order to facilitate use of these models. Theoretical, logistical, and software-based challenges will be reviewed. Chapters 4 and 5 aim to address the theoretical and conceptual challenges faced by social scientists who seek to implement nonlinear models and examine moderation of the parameters within those models. Chapter 4 presents guidelines for selecting a nonlinear functional form, choosing an appropriate parameterization, and specifying the moderated nonlinear model. In Chapter 5, a novel extension of the Johnson-Neyman technique is derived, which enables its application to moderated nonlinear models. Chapter 6 aims to address current logistical and software-based challenges by introducing a novel software tool that was developed in the Shiny web application framework in R. The software tool provides a code-free interface in which each step of nonlinear model specification, testing, evaluation, and visual probing can be easily implemented. Finally, Chapter 7 discusses future directions and opportunities for extension of this work.

## **CHAPTER II**

### **REVIEW OF THE METHODOLOGICAL AND APPLIED LITERATURE**

The aim of this chapter is to provide a thorough review of nonlinear models and their usefulness for social science research. The first section focuses on nonlinear model families and examples of their implementation in social science. In the second section, popular alternatives to nonlinear models are introduced (including polynomial models, piecewise linear models, and latent basis models) and their key drawbacks relative to nonlinear models are discussed.

#### **Nonlinear Models**

To motivate the use of nonlinear models for social science research, it is important to review and demonstrate the many unique advantages that they afford. I begin by summarizing the methodological arguments that have been made in favor of nonlinear models. Next, I will review a variety of nonlinear model families, their key features, and how those features map onto patterns that are often observed or expected in social science research. Throughout, I will present a variety of applied examples wherein nonlinear models were successfully implemented, highlighting the nuanced substantive conclusions that these models afford.

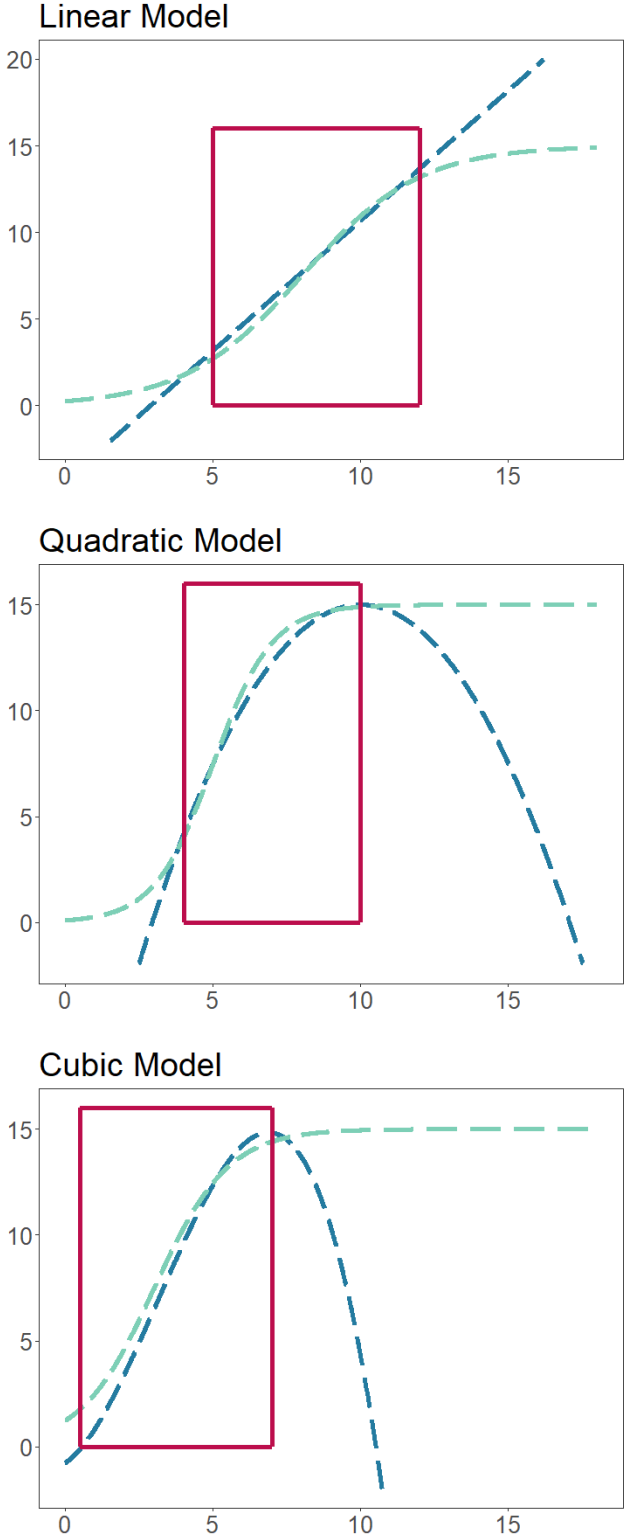
#### **Methodological Arguments and Key Advantages**

Many methodologists have argued in favor of nonlinear models for use in social science research. Most attention has been devoted to the benefits of nonlinear models for the study of psychological change over time; therefore, their advantages within longitudinal contexts are best

understood. A common assertion is that linear models often do not align with hypothesized or observed trajectories. Cudeck (1996) pointed out that the most “natural” way to represent changes in human behavior over time is often with a nonlinear model. In many situations, modeling linear growth is “simply inconsistent” with hypothesized change processes, including those in which growth is expected to occur at different rates across different portions of the trajectory, which are common in psychology (Choi et al., 2009). Indeed, Cudeck and Haring (2007) argue that in most cases, given what is known about growth processes, linear models are “conceptually unsatisfactory.” For most areas of psychological change, nonlinear models often portray a more realistic representation of the process (Grimm et al., 2011), and yield better model-data fit with fewer estimated parameters than linear models (Vonesh & Carter, 1992).

The better match between nonlinear models and expected trends is best highlighted when we consider that linear models (including polynomials) assume that trajectories continue toward positive or negative infinity in both directions. This is a strong assumption that typically does not align with known properties of development (e.g., academic skills are not expected to increase, plateau, then decrease across childhood, as implied by the quadratic model). As such, linear models’ accuracy tends to suffer in the extremes (Choi et al., 2009), and their generalizability beyond the time period of a given study is severely limited (Archontoulis & Miguez, 2015). Linear models may be able to approximate a *portion* of the growth process accurately, but cannot characterize the *entire* range of the trajectory (McCormick et al., 2023). For visualizations of this important limitation, see Figure 2.1. Ultimately, when curvilinear growth processes occur, linear models can at best provide incomplete approximations of these processes, whereas nonlinear models are often better matched to the hypothesized underlying system (Choi et al., 2009; Grimm et al., 2011; Pinheiro & Bates, 2000).

Figure 2.1. Example of Incompatibility Between Hypothesized Curvilinearity and Linear Models.



Note. The hypothesized trajectory is denoted in green, the model-implied trajectory is denoted in blue, and the observed range of the data is denoted in pink.



Methodologists have also emphasized that nonlinear models enable better connections between model parameters and theory, arguing that each parameter should map *as directly as possible* onto the specific hypothesis or theory that is being defined and tested. Therefore, each model parameter should correspond to a specific and substantively important aspect of development (i.e., of the curve under study). Cudeck and Harring (2007) argued that in order to gain novel information about individual change, parameters must have “unambiguous definitions.” Echoing this sentiment, Grimm et al. (2011) note that “a model is of little use when its parameters do not map onto theoretical notions of change or what is known about the developmental system under investigation.” As introduced in Chapter 1, relative to linear and polynomial models, the parameters of nonlinear models often map much more clearly onto specific attributes of the curve (Blozis & Harring, 2021; McCormick, 2023; Pinheiro & Bates, 2000; Ram & Grimm, 2007). As later examples show, these straightforward mappings can be translated to novel insight and enhanced contribution to theory.

In summary, two key arguments underlie methodologists’ support of nonlinear models for characterizing psychological data. First, nonlinear models are typically well matched to the ways in which psychological and behavioral change are hypothesized to occur. Second, nonlinear models are defined by parameters that correspond with substantively meaningful attributes of the curve. Together, these benefits mean that nonlinear models are very well suited for informing theory, directly testing key hypotheses, and identifying interindividual variation in substantively important aspects of development. To date, these arguments have been made in the context of longitudinal social science research; however, later examples will show that the same benefits apply to cross-sectional applications of nonlinear models.

In the following sections, I will provide detailed descriptions of the nonlinear models that have proven most useful for social science and review applied examples wherein those models were successfully implemented. Each section will begin by describing a family of nonlinear models (i.e., a group of models that yield similar-looking curves), the key features of the curves that they yield, and examples of how these features correspond with expected trends in the context of social science research. In addition, where possible, I will review use cases from the applied literature, which demonstrate the many advantages afforded by nonlinear models across a broad variety of research contexts and study designs.

## **Sigmoidal Models**

Nonlinear sigmoidal models yield S-shaped curves, which are characterized by change that is slower near the extremes and more rapid in the middle. All sigmoidal curves contain an inflection point, which is the location along the  $x$ -axis at which the rate of change of the slope (i.e., the first derivative) switches from increasing to decreasing. Popular models in the sigmoidal family are the logistic, Gompertz, and Richards models.

A popular parameterization of the logistic model is:

$$y = a + b * (1 + \exp(-c(x - d)))^{-1} + \varepsilon, \quad (2.1)$$

where  $a$  governs the height of lower asymptote,  $b$  governs the vertical distance between the lower and upper asymptotes,  $c$  governs the rate of change, and  $d$  governs the  $x$ -value at which the inflection point (i.e., fastest rate of change) occurs. An important feature of the logistic curve is that it is symmetric around the inflection point, such that half of the total change in  $y$  occurs before the inflection point and half occurs after.

Similarly, the Gompertz model is often parameterized as:

$$y = a + b * (\exp (-\exp (-c(x - d)))) + \varepsilon, \quad (2.2)$$

where  $a$  is the height of the lower asymptote,  $b$  is the distance between the lower and upper asymptotes,  $c$  governs rate of change, and  $d$  governs the  $x$ -value at which the inflection point occurs. Unlike the logistic curve, the Gompertz curve is not symmetric around the inflection point. Rather, the Gompertz curve is structured such that 37% of the total change in  $y$  occurs below the inflection point, and the rest occurs above it.

Finally, a popular parameterization of the Richards model is:

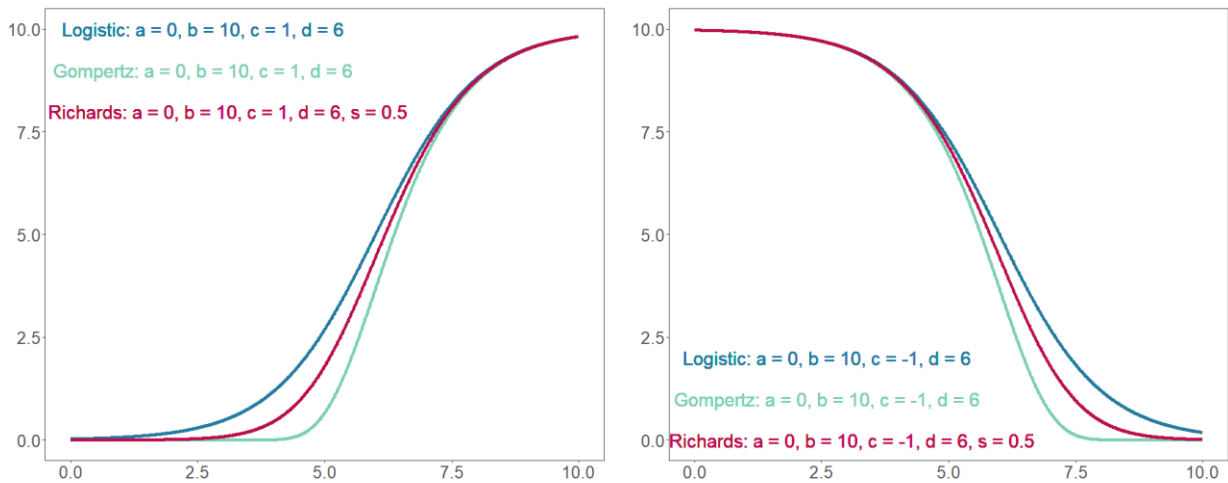
$$y = a + b * \left( \left( 1 + s * (\exp (-c(x - d))) \right)^{1/s} \right)^{-1} + \varepsilon, \quad (2.3)$$

where  $a$  is the lower asymptote,  $b$  is the distance between the lower and upper asymptotes,  $c$  governs rate of change,  $d$  governs the  $x$ -location of the inflection point, and  $s$  governs the amount of asymmetry before and after the inflection point. As  $s$  approaches 1, the curve approaches the logistic curve, such that the curve is symmetric around the inflection point; as  $s$  approaches 0, the curve approaches the Gompertz curve (Boedecker, 2021). Due to the asymmetry parameter, the Richards model is more general than the Gompertz and logistic models.

The logistic, Gompertz, and Richards models introduced here are a very small subset of the many sigmoidal models from which researchers may choose. First, versions of these functions with fewer parameters exist. For example, in the three-parameter versions of the logistic and Gompertz functions, there is no parameter for the lower asymptote because it is constrained to zero (see Sit & Poulin-Costello, 1994). There is a two-parameter version of the logistic function wherein only the lower asymptote and rate of change are estimated (e.g., Rockwood et al., 2008). Additionally, there are many more sigmoidal models that are popular in other fields but have yet to be implemented in social science research, save for a few rare

examples. Other sigmoidal models include the Weibull model (see McNeish et al., 2020; Panik, 2014; Wood et al., 2015) and the Janoschek model (see Panik, 2014; Wood et al., 2015).

Figure 2.2. Examples of Sigmoidal Curves.



There are a few hallmark characteristics of sigmoidal curves that are important to consider. Given the presence of both lower and upper asymptotes, sigmoidal curves are well suited for processes with logical boundaries or “limiting behavior” (Rast et al., 2011). For example, when acquiring a new skill, natural boundaries range from complete absence of the skill to mastery of the skill (Choi et al., 2009). Similarly, the outcome variable of interest may possess natural lower and upper bounds due to the measurement scale being used, such as the minimum and maximum scores on a standardized test. Increasing functions are well suited for processes like learning, whereas decreasing functions are well suited for processes like behavior extinction or memory loss (Choi et al., 2009; Rockwood et al., 2008). There are many other contexts, in both longitudinal and cross-sectional research, where these patterns are expected.

In a sigmoidal curve, the first asymptote reflects the expectation that the variable on the  $x$ -axis must increase somewhat before change in  $y$  begins to occur. In longitudinal research, the first asymptote reflects that a certain amount of time, trials, or practice may be required before noticeable change in the outcome starts. This is frequently expected in studies of learning, task performance, and rehabilitation (Feng et al., 2019). In learning contexts, Choi et al. (2009) note that “the lower plateau implies an initial lag during which time the subject has relatively slow acquisition (perhaps because the subject is not fully prepared for the task, developmentally and/or motivationally)” (p. 622). Additionally, first asymptotes may be expected in cross-sectional research, such as experimental contexts in which a stimulus must be present to some degree before a response is expected.

The second asymptote reflects the expectation that at some point along the  $x$ -axis,  $x$  will no longer affect  $y$ , resulting in a plateau or leveling off which has also been referred to as “change offset” (McNeish et al., 2023). Such a pattern is frequently expected in social science applications. When the second asymptote corresponds with an upper bound, this may reflect that the process or relation under study must reach a logical maximum, such as mastery of a skill, which must be approached because it cannot be exceeded. For Shing et al. (2012) and Zhao et al. (2022), the upper bound was a perfect score on the task being studied. For decreasing logistic functions, the second asymptote may be a known minimum, such as the minimum score on a memory or cognition task. The second asymptote may also reflect expectations of a diminishing effect of  $x$  as  $x$  increases, regardless of the boundaries of  $y$ . In longitudinal contexts this may be described as an equilibrium or a “final” level of  $y$  that will be maintained over the long term. In cross-sectional contexts, hypotheses concerning diminishing returns, plateaus, or leveling off are often consistent with this expectation.

Another key characteristic of sigmoidal functions is what Choi et al. (2009) refer to as the “surge area.” As the curve moves away from the first asymptote, change occurs slowly at first, then accelerates until change is most rapid (i.e., until the inflection point is reached), then decelerates throughout the approach toward the second asymptote. This results in a surge area, or a portion of the  $x$ -axis where the effect of  $x$  on  $y$  is strongest. The surge area often corresponds with expectations of a critical period, such as an age range during which reading skills are gained most rapidly (e.g., Cameron et al. 2015). Vocabulary development is another relevant example, “where children initially acquire new words slowly, beginning at about 1 year of age, then quickly increase the rate of acquisition until later in the preschool years when this rate begins to slow down again” (Burchinal & Appelbaum, 1991, p. 29). Parameters that govern the shape and location of the surge area (e.g., its steepness, the  $x$ -location at which the inflection point occurs,  $x$ -locations that define the boundaries of the surge area) are often of key substantive utility.

For these reasons, numerous applied examples of sigmoidal models can be found in studies of learning, academic achievement trajectories, and skill acquisition. In these applications, key goals are to characterize learning trajectories as accurately as possible, to identify early predictors of later achievement, and to explore sources of interindividual variability in learning trajectories. Sigmoidal models enable identification of relationships between individual characteristics and a variety of attributes of the learning trajectory, which are often better aligned with theoretical expectations and are more relevant for academic interventions. Additionally, sigmoidal models tend to better characterize these growth trajectories, as learning does not occur linearly.

For example, Anthony and Ogg (2020) and Cameron et al. (2015) used Gompertz models to approximate trajectories of science, math, and reading skills throughout elementary school.

Both studies used the parameterization given in Eq. 2.2, and important moderators were found to affect various attributes of the curve. Anthony and Ogg (2020) observed that children with better executive function at baseline had earlier inflection points and greater total growth in their science trajectories, suggesting that these students “hit the ground running” early in elementary school, and “the gaps that open by this time do not close” (p. 1576). Cameron et al. (2015) found that important demographic variables (including gender, race/ethnicity, and socioeconomic status) moderated total growth, location of the inflection point, and rate of growth. In these applications, use of the Gompertz curve allowed for new insight about both the shape and timing of the trajectory of academic skills, including pinpointing the time at which growth is most rapid. This was essential for identifying the “critical period” of learning in each domain (Cameron et al., 2015), and whether that critical period differed across children.

Use cases of sigmoidal models to characterize learning also span beyond school-aged children. Rast et al. (2011) modeled change over time in a verbal learning task among older adults, using a sigmoidal model with the following parameterization:

$$y = a - (a - b) \exp(-(x - 1)c) + \varepsilon, \quad (2.4)$$

where  $a$  is the upper asymptote,  $b$  is the lower asymptote (initial performance), and  $c$  governs rate of approach (learning rate). Each parameter was hypothesized to vary according to cognitive skills measured at pre-test. The authors found that greater cognitive skills at baseline predicted a higher upper asymptote and a faster learning rate.

Sigmoidal models have also proven useful in studies of cognitive growth and decline. Two excellent examples include Womack et al. (2022) and Ricker et al. (2018), each of which implemented Gompertz models as in Eq. 2.2. Findings indicated that important aspects of cognitive growth, which corresponded with parameters of the Gompertz model (e.g., initial

asymptote, growth rate, location of maximum growth, total growth), were moderated by the key child-level variables under study. Moderation of these parameters was in line with theoretical expectations, and findings were well-explained in terms of their implications and substantive relevance. For instance, Womack et al. (2022) found that higher family SES was associated with an earlier inflection point and a slower rate of growth, suggesting that cognitive growth began earlier and continued for a longer period of time among high-SES children. This finding aligned with past work linking higher SES with “positive cognitive developmental outcomes;” however, the moderated Gompertz model allowed for a more nuanced examination of the precise aspects of growth that were positively influenced by high SES. Finally, in an example of a decreasing sigmoidal model, Rockwood et al. (2008) used a two-parameter logistic model to approximate cognitive decline among older adults with dementia, noting that the logistic model characterized expected trends much better than a linear model.

Beyond academic and cognitive change, sigmoidal models have been implemented in a variety of other longitudinal contexts with respect to a diverse array of psychological phenomena. Many examples can be found in the neuroscience literature. Here, NLME Gompertz models have been used to characterize interindividual differences in brain maturation (e.g., Darchia et al., 2022; Sadeghi et al., 2013, 2017; Wright et al., 2014) and logistic models have been used to characterize reward signals in the brain (e.g., Sonnenschein et al., 2003). Gompertz models have also been used to approximate the progression of neuropathy symptoms (e.g., Adams et al., 2015) and brain activity during sleep (e.g., Campbell et al., 2012).

Sigmoidal models have also been applied to cross-sectional data across a variety of social science contexts, where their key benefits (e.g., better connections between parameters and theory, better alignment with hypothesized patterns) have also been realized. For example, some



studies find that participants' ability to correctly identify facial expressions is best characterized by a logistic model. Here, the  $x$ -axis typically corresponds to "signal strength," or the degree to which the face being viewed contains the target emotion (e.g., anger). The  $y$ -axis corresponds to the proportion of trials where the participant correctly identifies the target emotion. Of note, the use of a sigmoidal model – which involves a first asymptote – signals the expectation that the target emotion must be present at least somewhat before participants begin to correctly identify it. In these studies, relevant parameters of the logistic model include rate of change (i.e., the steepness of the curve relating signal strength to correct identification) and "shift point," which has been defined in multiple ways. Zhao et al. (2022) defined shift point as the location along the  $x$ -axis at which the curve began to increase, whereas D'Hondt et al. (2015) were interested in the location along the  $x$ -axis at which the proportion of correct trials crossed 50%. Zhao et al. (2022) found that both slope and shift point were moderated by schizophrenia status, such that people with schizophrenia had a later shift point and a steeper slope. In other words, to begin to correctly identify the target emotion, people with schizophrenia required a greater presence of the target emotion. People with schizophrenia also displayed less uncertainty about the target emotion, such that their correct identifications increased more rapidly from 0% to 100%. D'Hondt et al. (2015) tested whether slope and shift point differed across participants with vs. without alcohol dependence, finding that people with alcohol dependence had a significantly later shift point.

Another interesting area in which sigmoidal models have been applied pertains to hearing and auditory ability (e.g., McCrory & Cooper, 2004; Pogorzelski, 2022; Stelmachowicz et al., 2000). In these applications, the  $x$ -axis contains an indicator of the difficulty of the auditory stimulus being listened to, such as the duration of sound exposure, the audibility of speech, or the

magnitude of the difference between two tones. The y-axis contains an indicator of performance, such as the proportion of trials where the tone with higher pitch is correctly identified or where a word is recognized correctly. These studies find that the relation between difficulty and performance is best characterized by a logistic model. Additionally, tests for moderation allow researchers to identify key interindividual differences in performance, which often have implications for intervention and treatment. For Stelmachowicz et al. (2000), parameters of interest were rate of approach toward the upper asymptote and inflection point (i.e., the audibility level at which 50% correct speech identification was reached). These parameters differed across normal-hearing vs. hearing-impaired children, and findings were discussed in terms of the utility of hearing aids for hearing-impaired children. McCrory and Cooper (2004) observed that general intelligence moderated the inflection point of the logistic curve, such that higher general intelligence was associated with a lower inflection point. In this application, this meant that participants with greater intelligence required less exposure to the stimulus in order to successfully distinguish between two tones. The authors used this result to inform theoretical models concerning intelligence and auditory ability.

In another cross-sectional example, Shing et al. (2012) modeled the effects of practice time (PT) on processing accuracy and working memory performance using a NLME logistic model. The authors provided strong *a priori* justification for their model choice, noting that the shape of the logistic function is well-matched to theoretical expectations of how processing occurs: “the function assumes (a) a minimum amount of PT is required to initiate processing, (b) beyond this minimum amount, PT is translated into carrying out the core cognitive processes necessary for achieving the task, and (c) after a certain maximum amount of PT, there is little to be gained by having more PT available” (p. 452). Multiple parameters of the logistic model were

treated as random and tested for moderation by age group. Age moderated both the rate of change and the upper asymptote, such that younger adults reached a higher asymptote faster.

Finally, some recent theoretical work has hypothesized cross-sectional relations that take on a specific sigmoidal shape. Rigoli and Martinelli (2021) defined a new model of *subjective value* as it relates to eating disorders. In the subjective value literature, it is of interest to model relations between the actual value of an outcome (on the  $x$ -axis, e.g., grades in school) and the subjective or perceived value of that outcome (on the  $y$ -axis, e.g., perceived success in school). The authors propose that this relation should be characterized with a logistic model, wherein multiple parameters are theoretically important. First, the inflection point represents the true value of the outcome (e.g., the actual school grade) at which perceived value goes from being *less* than that actual value (perceived as relative failure) to *greater* than that actual value (perceived as relative success). A high inflection point would signify that most actual outcomes are perceived as relative failure, which has been linked to perfectionism, low self-esteem, and eating disorders. Second, the slope of the curve represents the rate at which actual outcomes switch from being perceived as complete failures to complete successes. A steeper slope may be indicative of dichotomous thinking, a cognitive pattern that has been repeatedly linked to eating disorders. The authors hypothesize that eating disorder status, as well as other relevant variables, likely moderate these parameters. This work enables empirical studies to target specific and nuanced hypotheses about subjective value. Although such examples remain rare, they offer a glimpse into the rich insight to be gained from incorporating sigmoidal (and more generally, nonlinear) models into psychological theories and hypotheses.

In summary, sigmoidal models – including variations of the logistic, Gompertz, and Richards models – have been implemented in numerous areas of social science. Examples of

their utility span across longitudinal, cross-sectional, observational, and experimental designs. The hallmark features of sigmoidal models, including both an upper and lower asymptote, a surge area, and an inflection point, often map straightforwardly onto hypothesized patterns.

## Exponential Models

The exponential family is characterized by curves in which the relationship between  $x$  and  $y$  is strongest initially, then decreases as an asymptote is approached. These curves are sometimes described as an inverted J-shape (e.g., McNeish & Dumas, 2017). Importantly, these curves do not contain an inflection point, as the strength of the relation between  $x$  and  $y$  is always decreasing. Popular models in this family are the three-parameter exponential (3PE) and the Michaelis-Menten (MM) models, though in social science, the 3PE has been used most. Curves in the exponential family may increase toward an upper asymptote (exponential growth) or decrease toward a lower asymptote (exponential decay).

A popular parameterization of the 3PE model (e.g., Ram et al., 2005) is:

$$y = a + b * \exp(-c * x) + \varepsilon, \quad (2.5)$$

where  $a$  is the asymptote,  $b$  is the distance between the  $y$ -intercept and the asymptote, and  $c$  governs the rate of approach toward the asymptote. Other parameterizations of the 3PE have also been used in psychology; for example, Codd and Cudeck (2014) used a parameterization where  $b$  corresponds to the  $y$ -intercept rather than the distance between the  $y$ -intercept and the asymptote.

The MM model has historically been used less than the 3PE in social science research. However, its classic parameterization differs from the 3PE in potentially useful ways, resulting in increased popularity in recent years. A popular parameterization of the MM model is:

$$y = a + \frac{bx}{c+x} + \varepsilon, \quad (2.6)$$

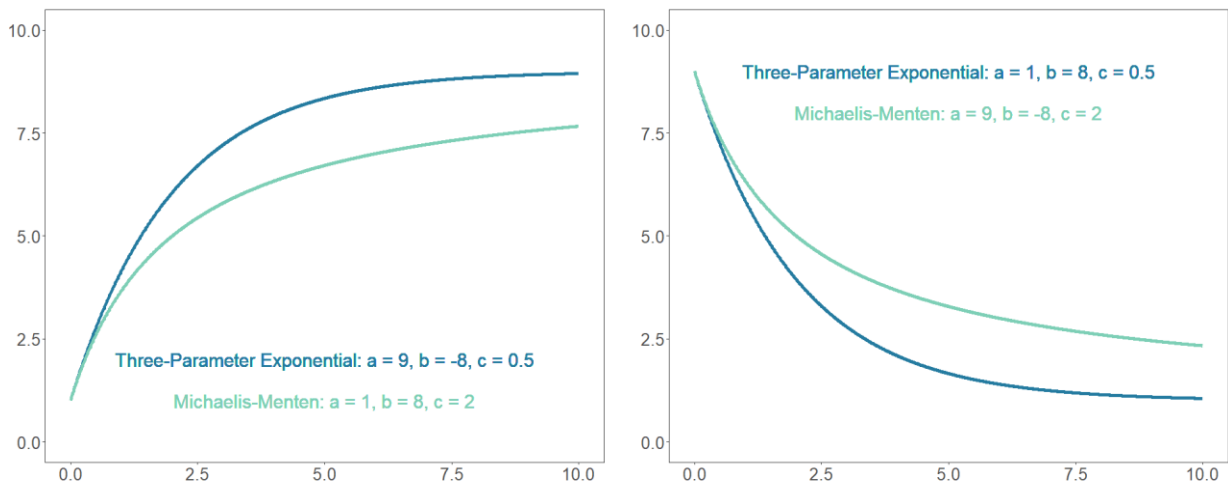
where  $a$  is the  $y$ -intercept,  $b$  is the vertical distance between the  $y$ -intercept and the asymptote, and  $c$  is the  $x$ -value at which half of the change between the intercept and the asymptote has occurred. The interpretation of parameter  $c$  has proven useful in studies of academic achievement trajectories and learning (e.g., Codd & Cudeck, 2014; Johnson & Hancock, 2019; McNeish & Dumas, 2017; McNeish & Matta, 2018).

As is true for the sigmoidal family, there are many other versions of the models mentioned above, such as the two-parameter exponential, which forces the  $y$ -intercept to be zero (see Ratkowsky, 1990) and the generalized MM, which allows for an inflection point (see Lopez et al., 2000; McNeish & Dumas, 2017). There are also a variety of models in the exponential family that are popular in other fields but have been used scarcely in social science research. Examples include the von Bertalanffy model (see McNeish & Dumas, 2017; Panik, 2014; Ratkowsky, 1990; Wood et al., 2015) the McDill-Amateis model (see Panik, 2014), and the power model (see Sit & Poulin-Costello, 1994). Finally, there are some nonlinear models that can take on either an exponential or a sigmoidal shape, including the Schnute model (see Panik, 2014; Wood, 2023) the Morgan-Mercer-Flodin model (see McNeish et al., 2020), and a combined model developed by Wood (2023), which is a weighted combination of the exponential and logistic functions, and the degree to which the curve resembles either is controlled by a weight parameter.

Key differentiators between the exponential family and the sigmoidal family are that models in the exponential family do not involve an inflection point and do not contain a first asymptote. The absence of the first asymptote implies that as  $x$  increases, rapid change in  $y$  begins occurring immediately. Therefore, exponential models are well-suited for processes that “proceed quickly at first and level off to some threshold” (Johnson & Hancock, 2019, p. 698).

This pattern is known to occur in many social science contexts, such as studies of procedural learning, which are learning experiments wherein participants are exposed to a novel task and aim to improve their performance on the task across multiple experimental trials (e.g., Codd & Cudeck, 2014; Cudeck, 1996; Johnson & Hancock, 2019; Ram et al., 2005). For such tasks, it is often expected that performance will improve rapidly beginning with the first trial, and that improvement will be most pronounced over the course of the earliest trials. We can contrast these examples with those from the sigmoidal family, where it was expected that the  $x$ -variable (e.g., time, trials) would increase somewhat before pronounced change in  $y$  began to occur.

Figure 2.3. Examples of Exponential Curves.



There are also cross-sectional scenarios where a model from the exponential family may be most appropriate. In cross-sectional studies, it is often expected that the relation between  $x$  and  $y$  will be strongest at lower levels of  $x$ , and will weaken at the highest levels of  $x$ . Such hypotheses often involve “diminishing returns” or “plateauing associations,” and have arisen across various areas of psychology. For example, the relations between social interaction

quantity and wellbeing (e.g., Kushlev et al., 2018; Ren et al., 2022), interpersonal exchange quality and relationship satisfaction (e.g., Cazzell et al., 2022), as well as cognitive ability and creativity (e.g., Jauk et al., 2013) have been hypothesized to follow such patterns. In each example, theory leads the researchers to expect the presence of a final, but not initial, asymptote, such that the relation between  $x$  and  $y$  weakens as  $x$  increases. Although quadratic or piecewise linear models are typically implemented to characterize these patterns (the disadvantages of which will be discussed later), models from the exponential family are well suited for approximating such trends.

Exponential models have proven useful for modeling psychological change over time in a variety of domains, including psychopathology and addiction research. In one example, Burke et al. (2007) used NLME models to study trajectories of depressive symptoms among adults who experienced the loss of a spouse. Citing past work that suggests recovery is most rapid at first and then slows over time, they implemented a 3PE model with the following parameterization:

$$y = F + (L - F) \exp(-S * t) + \varepsilon, \quad (2.7)$$

where  $t$  (time) is the predictor, parameter  $F$  governs the asymptote (referred to as “final” level of depressive symptoms),  $L$  governs the initial level (referred to as depressive symptoms at time of loss), and  $S$  governs rate of change (referred to as rate of adjustment). All parameters were treated as random (i.e., were allowed to vary across individuals), and estimates were discussed in terms of coping and loss theory as well as implications for intervention. Additionally, pre-loss coping efficacy and marital quality were predictive of lower depression at multiple timepoints (i.e., were significant moderators of  $F$  and  $L$ ). The authors noted that use of a nonlinear model allowed them to avoid “simplifying assumptions” of linear change, and increased their power to detect relationships between moderators and key aspects of the adjustment trajectory.

Aside from procedural learning tasks, there are other learning and skill acquisition contexts in which models from the exponential family have proven useful. For example, Burchinal and Appelbaum (1991) used a decreasing 3PE model to characterize the trajectory of children's speech errors (termed "phonological processes") from ages three to six. The authors chose the 3PE model on a theoretically informed, *a priori* basis, noting that an inflection point was not expected in this trajectory: "The rate of decline in these articulation errors is markedly rapid initially and then gradually slows until all of these processes are eliminated" (p. 31). The authors found that children's speech intelligibility at first and last assessment were correlated with the rate of change parameter in the 3PE model, such that greater speech intelligibility was associated with a more rapid decrease in speech errors.

In some recent applications, the MM model has been used to characterize long-term learning trajectories wherein an inflection point was not observed. For example, McNeish and Dumas (2017) chose a NLME MM model to approximate change in academic ability factor scores over the course of kindergarten to 8<sup>th</sup> grade. Upon plotting factor scores for random subsamples of children, the authors observed that the trajectories did not appear to have an inflection point, and indeed, the MM model yielded a lower BIC than the Gompertz model. Further, by examining interindividual variation in the parameters of the MM model, the authors gained substantively useful insights into how learning trajectories vary across children. "Early bloomers" were identified as children for whom the *y*-intercept was in the top quintile, but midpoint of growth and upper asymptote were in the bottom quintile. "Fast learners" were children whose *y*-intercept was in the bottom quintile, but midpoint and upper asymptote were in the top quintile. Finally, "late bloomers" were children with a *y*-intercept in the bottom quintile, midpoint in the top quintile, and upper asymptote in the middle quintile.



In summary, models from the exponential family are useful for approximating trends wherein the strength of relation between  $x$  and  $y$  decreases as  $x$  increases. Exponential models have enabled researchers to characterize trajectories of learning, skill acquisition, and psychopathology, and the unique parameterizations offered by each model have been leveraged to gain maximally useful insights. Models from the exponential family have yet to be widely applied to cross-sectional social science research; however, there are a variety of contexts in which expected patterns correspond well with an exponential model. These contexts include hypotheses of plateauing associations and diminishing returns.

### **Trigonometric Models**

Prior sections focused on nonlinear models in which the function relating  $x$  to  $y$  is monotonic, meaning the curve is always increasing or always decreasing. However, there may be situations in which non-monotonic models are better suited for the process or relation under study. Trigonometric models may be well suited for these applications, as they yield curves with cyclical increases and decreases. Two popular trigonometric models are the sine and cosine models. A common parameterization of the sine model is:

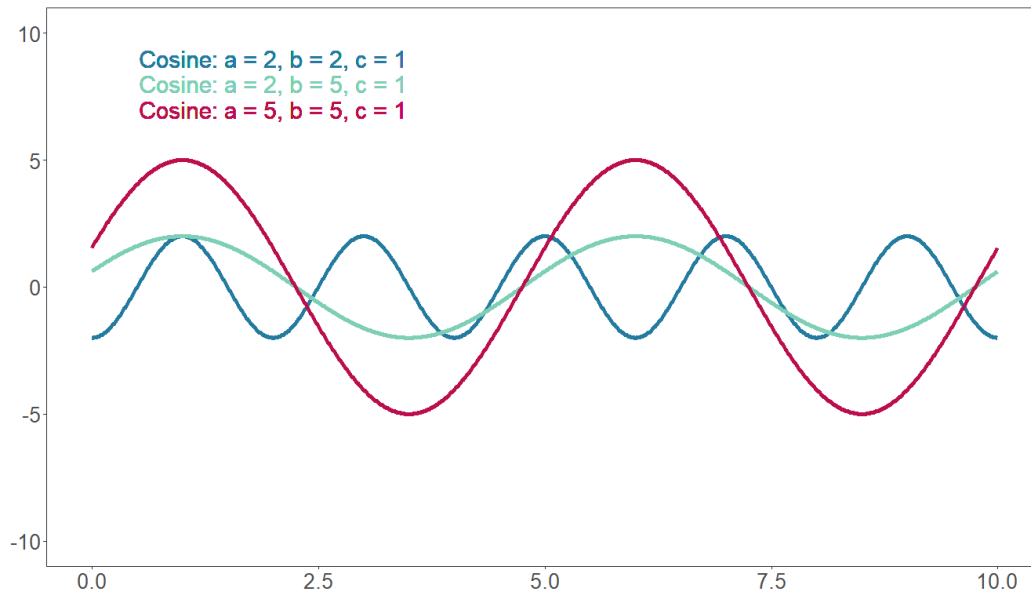
$$y = a * \sin\left(\frac{2\pi}{b}(x - c)\right) + \varepsilon, \quad (2.8)$$

and a popular parameterization of the cosine model is:

$$y = a * \cos\left(\frac{2\pi}{b}(x - c)\right) + \varepsilon. \quad (2.9)$$

In Eqs. 2.8 and 2.9,  $2a$  is the amplitude of the curve, which is the distance between its minimum (troughs) and maximum (peaks),  $b$  is the wavelength of the curve, and  $c$  shifts the curve left and right.

Figure 2.4. Examples of the Cosine Curve.



Trigonometric models have been utilized in social science applications where cyclical patterns were expected. For example, Hipp et al. (2004) used a cosine model to approximate crime rates over time among residential communities. Crime rates were the highest during the summer months and lowest during the winter months, which was well-characterized by the cyclical nature of the cosine model. Additionally, community-level moderators were incorporated to predict the amplitude of the curve (i.e., variability of crime rates throughout the year); greater temperature variability in the community, as well as a greater number of social establishments in the community, were predictive of greater amplitude. Similarly, Kelley et al. (2007) used a NLME cosine model to approximate blood pressure and heart rate changes during the multi-day period between dialysis sessions. Here, more medication was predictive of a lower wave amplitude, i.e., less heart rate variability over the course of the observation period. The authors concluded that individuals who took more medication exhibited a “blunted” wave. Interestingly, both applications incorporated a linear term into the model to account for overall

growth/decline over the course of the study period, in addition to the “periodicity” that was approximated by the cosine portion of the model, highlighting the flexibility of the nonlinear modeling framework.

In summary, trigonometric models are ideal for approximating cyclical relationships, which are often hypothesized in psychology and social science research. The use of trigonometric models remains rare in social science; however, there are a variety of areas in which trigonometric models are likely to be especially useful and informative. Namely, in ecological momentary assessment (EMA) studies, emotions, symptoms, and behaviors are often expected to fluctuate on a daily, weekly, and/or monthly basis (e.g., Beddig et al., 2020; Kuhlmann et al., 2023; Probst et al., 2017; Wilson et al., 2017).

### **Peaked Models**

While trigonometric models are ideal for approximating cyclical relations, there may be applications in which the expected trend is non-monotonic, but not cyclical. Peaked models, such as the inverse quadratic and Bragg models, are well suited for such applications.

The classic parameterization of the inverse quadratic model (e.g., Sit & Poulin-Costello, 1994) contains parameters that are not easily interpretable; therefore, Preacher and Hancock (2015) partially reparameterized the model to contain one interpretable parameter. Building upon their presentation, an even more interpretable parameterization of the inverse quadratic model is:

$$y = \frac{x}{(a^{-1}-2bc)x+c(b^2+x^2)} + \varepsilon, \quad (2.10)$$

where  $a$  is the maximum  $y$ -value,  $b$  is the location along the  $x$ -axis where  $a$  occurs, and  $c$  governs the rate of increase and decrease around the peak.

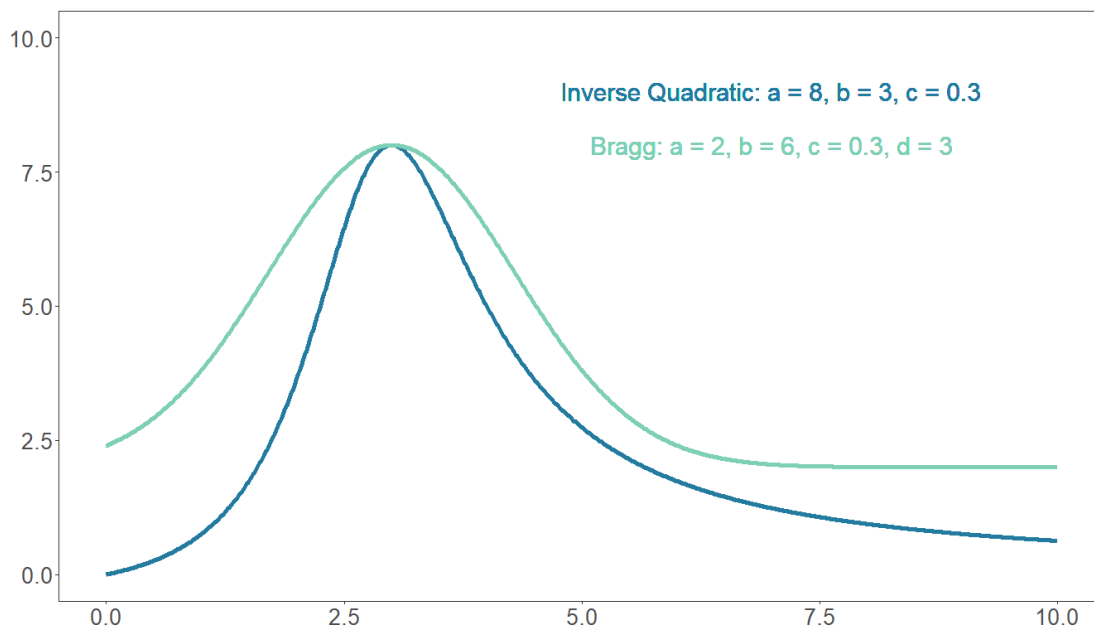
The Bragg model resembles the equation for a normal distribution (Ratkowsky, 1990) and has been presented as:

$$y = a + b * \exp(-c(x - d)^2) + \varepsilon, \quad (2.11)$$

where  $a$  governs the starting and ending  $y$ -value (in the inverse quadratic function, this is constrained to zero),  $b$  is the vertical distance between  $a$  and the maximum  $y$ -value,  $c$  governs the rate of increase/decrease around the peak, and  $d$  governs the location along the  $x$ -axis where the peak occurs.

Like the model families discussed previously, there are a variety of other peaked models that are used in other fields but have yet to be applied to social science research. These models are sometimes referred to as bell-shaped curves. Some examples include the equations for Beta distribution and the Normal distribution (see Archontoulis & Miguez, 2015), the flat parabola (see Ratkowsky, 1990), and the inverse cubic function (see Sit & Poulin-Costello, 1994).

Figure 2.5. Examples of Peaked Curves.



Piecewise linear models or nonparametric models are typically used in applications where a peaked nonlinear model was well matched to the trend under study. In these applications, the observed trend was non-monotonic, and characterized by an increase toward a peak followed by a decrease toward an asymptote. For example, Schlotz et al. (2022) used a latent basis model to characterize cortisol trajectories before, during, and after a stressful task; cortisol levels began at baseline, increased during the task, reached a peak, then gradually decreased back to baseline. Devonshire et al. (2023) used a piecewise linear model to approximate interparental conflict during and after an intervention; here, conflict briefly increased during Phase 1 of the intervention, then decreased throughout Phase 2, and leveled off toward an asymptote following the conclusion of the intervention. Finally, Walters et al. (2022) used a quadratic model to characterize trajectories of alcohol misuse during and after a smartphone intervention; drinking behaviors initially increased before significantly decreasing throughout the latter half of the study period.

In summary, peaked nonlinear models have yet to gain popularity within social science research; however, the functional forms that they yield are ideal for applications in which the expected trend is non-monotonic but not cyclical. Peaked models may be particularly useful for characterizing responses to stressful stimuli and behavioral interventions.

## **Section Summary**

The goal of this section was to provide an in-depth review of nonlinear models and their advantages for social science research. First, I reviewed the key benefits of nonlinear models that have been outlined by methodologists. Second, I described common nonlinear model families, their hallmark characteristics, and how those characteristics map onto trajectories and patterns

that are common to social science. Finally, these points were illuminated via a variety of empirical examples. Although this section focused on the sigmoidal, exponential, trigonometric, and peaked families, it is important to note that there are many more nonlinear models with great potential for psychology and social science. In future applications, scientists need not restrict their focus to models reviewed here.

### **Alternatives to Nonlinear Models**

In addition to reviewing the utility of nonlinear models for social science, it is also useful to review the drawbacks of linear models – and other alternative methods that are often used – when curvilinear patterns are hypothesized or observed. In each of the following sections, common alternative methods (including polynomial models, latent basis models, piecewise linear models, and variable transformations) will be introduced, and their drawbacks compared to nonlinear models will be reviewed. Additionally, I will review empirical examples wherein the alternative method was used in place of a nonlinear model. In these examples, the conclusions that *were* drawn will be contrasted with the potential insights that *could* have been gained through use of a nonlinear model, highlighting the limitations of each alternative method. This chapter is not the result of an exhaustive or systematic review of the applied literature, but rather, focuses on selected empirical examples from diverse research areas.

### **Polynomial Models**

Polynomial models, including the quadratic and cubic models, are pervasive in social science research. When curvilinear patterns are observed or expected, the polynomial model is the most common method for characterizing these patterns (Cudeck & Harring, 2010;

McCormick, 2023; Simonsohn, 2018). Because polynomial models are linear in their parameters, their use was originally motivated by the relative computational ease with which they could be fit, as opposed to the challenges that often arose with nonlinear models (Blozis & Cudeck, 1999; McNeish et al., 2023). However, this obstacle is much less salient given present-day computing power, and many methodologists now argue that the common use of polynomial models as “catch-all” tests for curvilinearity is problematic (e.g., Choi et al., 2009; Grimm et al., 2011). The disadvantages of relying on polynomial models have largely been argued in the context of longitudinal research, and are reviewed next.

### ***Limitations***

First, polynomial functions are not monotonic, and therefore imply that the growth trajectory will at some point reverse direction and approach positive/negative infinity at both extremes. This feature yields major incongruence between theoretically-expected and model-implied trajectories (Cudeck & Harring, 2007, 2010; Grimm & Ram, 2009). For example, academic skills are not expected to increase, reach a maximum, and later decrease across childhood; rather, it is known that growth decelerates and eventually stops when an upper asymptote is reached. Similarly, following treatment, psychopathology symptoms are not expected to decrease, reach a minimum, and then increase back to positive infinity. Additionally, because polynomial models force a directional change where not realistic, the location of the inflection point(s) tends to be highly influenced by observations at the tails of the  $x$ -range (Fjell et al., 2010; McCormick et al., 2023).

Second, given the fundamental incongruence between trajectories implied by polynomial models and expected trajectories, it follows that polynomial models can approximate only a small portion of the entire hypothesized trajectory (Blozis, 2004; Choi et al., 2009; McCormick

et al., 2023; McNeish et al., 2023; Pinheiro & Bates, 2000). See Figures 2.1 and 2.2 for a review of this limitation. The polynomial model acts as a descriptor of growth patterns within the observed range of the data, but precludes inferences or generalizations beyond this range.

Third, the classic parameterizations of polynomial models suffer from poor parameter interpretability. As noted in Chapter 1, mappings between the parameters and key characteristics of the curve are often unclear. As a result, the substantive conclusions that can be drawn from polynomial models are typically limited, and moderation of polynomial terms is difficult to interpret (Cudeck & Harring, 2010; Grimm et al., 2011; McCormick, 2023; McNeish et al., 2023). Later examples will further demonstrate this drawback.

Fourth, polynomial models inherently impose specific theoretical assumptions that often go unacknowledged. For example, Ram and Grimm (2007) explain that the quadratic model imposes strict assumptions regarding how change occurs: at each successive measurement occasion, change occurs by (1) a fixed amount – the linear term – and (2) another amount that changes from occasion to occasion in a predetermined fashion, but without a clear definition or interpretation – the quadratic term. Individuals may differ *only* in terms of these aspects of change; any other interindividual differences are treated as error by the model. These inherent assumptions are exceedingly difficult to justify or connect to a psychological theory.

Finally, polynomial models are susceptible to false positive results when the true data-generating pattern is asymptotic. In a simulation study by Simonsohn (2018), quadratic models were fit to data exhibiting the following trends: (1) an initial strong positive slope followed by a plateau, consistent with functions from the exponential family, and (2) a logistic function. For each of these trends, the quadratic model yielded exceedingly high false-positive rates that often reached 100%. It was therefore concluded that the quadratic model is especially prone to false



positive results when the true function flattens out or exhibits asymptotic behavior. While the quadratic model is highly likely to fit better than the linear model in these scenarios, it is not an accurate characterization of the data-generating process.

### ***Longitudinal Examples***

The drawbacks of polynomial models are easy to observe in a variety of longitudinal examples from diverse literatures, including education, psychopathology, substance use, and cognitive science. First, consider a study by Lee (2010), who modeled reading and math achievement from 4<sup>th</sup> to 12<sup>th</sup> grade using quadratic growth mixture models. In this study, a key hypothesis was that eighth grade was a “major turning point in the growth trajectory.” Therefore, the analytic approach was to center time (the predictor) at eighth grade, so that the linear parameter corresponded with instantaneous rate of change at eighth grade. The major drawback of this approach is that it *assumes*, rather than *tests*, that eighth grade is indeed a turning point in the growth trajectory. In contrast, many sigmoidal models contain parameters for (1) the location of the inflection point and (2) instantaneous rate of change at the inflection point. These models would allow us to directly estimate whether there is indeed a turning point in the growth trajectory at eighth grade, and if so, the growth rate during eighth grade. In this example, a nonlinear model would have enabled direct testing of key study hypotheses, whereas the quadratic model did not.

In other examples, we can observe that the nonsensical trajectories implied by polynomial models typically do not align with the expectations, interpretations, or substantive conclusions of the researchers. In longitudinal psychopathology research, study goals often involve characterizing the trajectory of psychopathology symptoms over a key developmental timespan, identifying moderators of the shape and timing of that trajectory (e.g., LoParo et al.,

2024; Morgan et al., 2022; Romano et al., 2022), or tracking symptom trajectories following an intervention (e.g., Kang et al., 2022; Walters et al., 2022). A commonly observed pattern is for symptoms to decrease rapidly at first and eventually level off, resulting in a curvilinear trajectory. However, in all the examples referenced here, analyses were limited to quadratic models, and trajectories' substantive interpretations were not supported by the model. For example, in their study of psychotic symptoms, Morgan et al. (2022) identified a latent class wherein symptoms decreased rapidly then plateaued. This class was interpreted as the "remitting" class. Importantly, the quadratic model does not imply that the trajectory will level off (i.e., remain stable at a lower asymptote), and therefore is not consistent with the "remitting" label. Rather, the quadratic model forces a directional change, implying that the trajectory will decrease, reach a minimum, then increase back to positive infinity in a symmetric manner. The quadratic model characterizes only a portion of the assumed pattern, resulting in unsubstantiated conclusions regarding the *entire* course of the trajectory. A nonlinear model allowing for asymptotic behavior would have much better supported the interpretation of this trajectory.

These examples also highlight that – due to limited interpretability of their parameters – polynomial models severely limit the level of detail that can be obtained through parameter estimates. Comparing linear and quadratic/cubic models essentially tests whether the trajectory is linear or curvilinear, and any further conclusions are largely descriptive and subjective (e.g., they arise from visual inspection of model-implied trajectories). Contrast this to nonlinear models, which afford more quantifiable information about the trajectory (McNeish et al., 2023). For example, in Morgan et al.'s (2022) "remitting class," a nonlinear model would enable us to estimate key quantities such as the age at which the lower asymptote of psychotic symptoms is typically reached, the age at which decreases in psychotic symptoms tend to begin, the age at

which this decrease the most rapid, and/or any other specific aspects of the trajectory that are substantively useful. Much more detailed quantitative information about these trajectories could be obtained via the parameter estimates of nonlinear models.

### *Cross-Sectional Examples*

These same drawbacks apply to cross-sectional research. When curvilinear relations are hypothesized or observed, the most common approach is to fit a quadratic model. However, due to the strict assumptions about the shape of curvilinearity that are imposed by the quadratic model, there are many examples of clear mismatches between quadratic model-implied patterns and the curvilinear patterns that are theorized. Therefore, reliance on the quadratic model tends to result in an inability to test key study hypotheses.

For example, Cazzell et al. (2022) explored the relation between the quality of interpersonal exchanges and marital satisfaction among couples. They found the quadratic term to be significant, seemingly confirming their hypothesis of “plateauing associations” between exchange quality and relationship satisfaction. Akin to longitudinal applications, the quadratic model was able to approximate a portion of the expected pattern, but generalizations regarding the entire shape of the relation (i.e., that the effect of interpersonal exchange quality continuously diminishes as exchange quality increases) were unsubstantiated by the quadratic model. A nonlinear model allowing for asymptotic behavior would align much better with the researchers’ expectations, and empirical evidence in favor of such a model would offer much stronger evidence in favor of the plateauing associations hypothesis.

Ren et al. (2022) faced a similar problem in their study of social interaction frequency and wellbeing. At the highest frequencies, their goal was to assess whether the positive effects of social interaction would be reduced (an asymptotic trend) or reversed (a trend characterized by

increase, plateau, and decrease). Their statistical approach was to fit a piecewise linear model (to approximate the asymptotic trend) and quadratic model (to approximate the reversed-direction trend). Problematically, the symmetric parabola enforced by the quadratic model did not match well to the reversed-direction trend, which was theorized to be asymmetric and contain a plateau. The authors acknowledged this limitation, noting: “this approach assumes a quadratic relationship that forces the parabola to bend at a single turning point and be symmetric around said point. This assumption prevents us from evaluating the two competing hypotheses regarding the shape of the curve.” In this example, a polynomial model could not achieve a match between model-implied and theoretically-expected patterns. By confining themselves to linear models, the authors were unable to directly test their hypotheses and their contribution to theory was limited in kind.

### ***Moderation***

When polynomial models are used to characterize curvilinear relationships, moderators of the quadratic or cubic term are often found to be significant. By incorporating moderators of these terms, authors can merely assess whether the overall shape or curvature of the trend differs according to the moderator. Therefore, most conclusions are largely subjective, as they arise from visually inspecting model-implied relations for different values of the moderator. This analytic approach precludes researchers from drawing more precise conclusions about moderation, thereby inhibiting their ability to test hypotheses and inform theory. Indeed, many methodologists have argued that when curvilinear relations are present and moderation is of key substantive interest, the greatest advantage of the nonlinear model is its clear-cut and interpretable parameters (Burke et al., 2007; Choi et al., 2009; Harring & Blozis, 2014; Preacher & Hancock, 2012, 2015; Ram & Grimm 2007).

Due to the pervasiveness of polynomial models in social science research, examples of moderated quadratic or cubic terms are common and span diverse areas of study (e.g., cortisol trajectories, Zhan et al., 2023; posttraumatic stress trajectories, Dar & Iqbal, 2020). As a running example, we will consider a study by Kim et al. (2023). Here, the quadratic model was used to characterize trajectories of happiness across the lifespan, which followed an inverted U-shape. Agreeableness and neuroticism moderated the quadratic term. To probe this result, the authors used post-hoc analyses including the pick-a-point approach (to visualize the parabola at different levels of agreeableness) and the JN technique (to plot values of the quadratic term at different levels of agreeableness). Ultimately, the authors' conclusions were limited to largely qualitative information about how agreeableness and neuroticism affected the overall curvature of the trajectory. A nonlinear model would have allowed for moderation of parameters that map more directly onto distinct attributes of the curve, such as maximum happiness levels, rate of change to/from the maximum throughout the lifespan, and starting/ending happiness levels.

Relatedly, examining moderation of the quadratic term does not yield substantively useful model-implied values, because the value of the quadratic term carries little interpretability. In Kim et al. (2023), the JN plot showed that when agreeableness was at its mean, the quadratic term was equal to about 0.001, whereas when agreeableness was high, the quadratic term was equal to about 0.003. Substantively, these numbers mean little. Suppose the authors instead used a nonlinear model containing a parameter that governed, for example, the age at which maximum happiness was reached. Moderation of this term – and subsequent probing – could have yielded substantively useful *quantitative* results such as the age at which more vs. less agreeable people reach peak happiness. Such model-implied values are practically meaningful, and likely would have better informed theory and future studies.

### *U-Shaped Hypotheses*

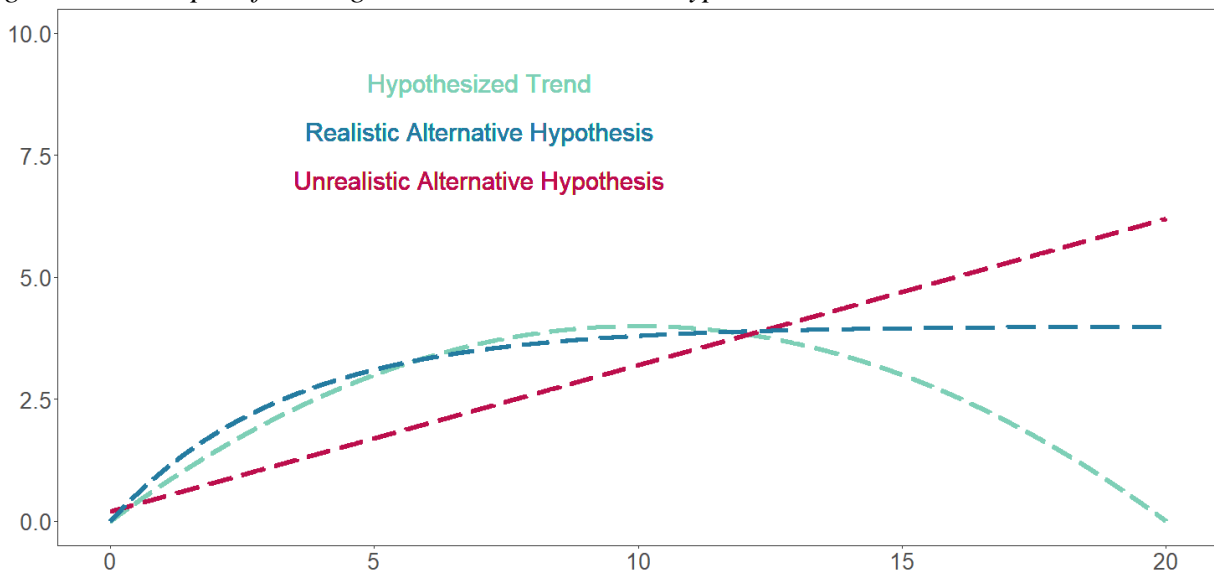
In some contexts, there *is* theoretical reason to believe that the trajectory or relation under study is best characterized by a polynomial model. Such hypotheses have arisen with respect to the trajectory of episodic memory across the lifespan (e.g., Tacconat et al., 2023), relations between employee qualifications and employers' motivating behaviors (e.g., Jiang et al., 2022), relations between conscientiousness and task performance (e.g., Harris-Watson et al., 2022), and relations between SES and depressive symptoms (e.g. Korous et al., 2023), each of which are theorized to follow an inverted U-shape. As a running demonstrative example, I will discuss an application from the industrial/organizational literature. Here, psychologists have theorized that workplace diversity exhibits a “too-much-of-a-good thing (TMGT)” effect, such that the relation between workplace diversity and workplace success/thriving will show an inverted U-shape (Pierce & Aguinis, 2013). When such hypotheses arise, the typical approach is to simply compare fits of the linear and quadratic models. Wu et al. (2023) implemented this approach as they explored relations between age diversity and team effectiveness. Seemingly “confirming” the TMGT effect, they compared the linear and quadratic models and found the quadratic term was statistically significant.

I argue that in the presence of U-shaped hypotheses, there are still advantages to considering nonlinear candidate models, and it is insufficient to only compare the quadratic model against the linear model. First, the linear model is likely akin to a “straw man hypothesis” that will almost certainly be rejected, such that this rejection does not provide strong evidence in favor of the U-shaped hypothesis. If the quadratic model fits better than the linear model, there may be a variety of data-generating relationships underlying this result. Recall that Simonsohn (2018) observed exceedingly high false-positive rates for the quadratic model when data

exhibited a sigmoidal or exponential relationship. This suggests that although the quadratic model fits better than linear, this does not necessarily confirm the presence of an inverted U-shape in the data.

Demonstrating the superiority of the quadratic model *compared to other models characterized by curvilinearity*, rather than the linear model alone, would provide much stronger support in favor of the hypothesized trajectory. For example, comparing the quadratic model against the 3PE or MM model allows the research to pinpoint whether – at high levels of diversity – team success decreases or simply levels off. Such a specific question cannot be answered by comparing the linear and quadratic models. Testing a variety of models against each other, each of which characterizes a feasible curvilinear relationship, would be much more informative for theory. For an example, see Figure 2.6. Even if a polynomial model is ultimately chosen as the best model, critically comparing that model against several nonlinear candidate models garners much greater support for the chosen model (Cudeck & Harring, 2007).

Figure 2.6 Example of Testing a Feasible Alternative Hypothesis with a Nonlinear Model.



In summary, when theory leads us to expect a U-shaped relation between key constructs, comparing the quadratic model to a linear model provides only weak support in favor of that theory. To more rigorously assess the presence – and nature – of a curvilinear relationship, implementing nonlinear models and comparing a diverse set of functional forms will provide stronger evidence in support of a given theory.

### **Latent Basis Models**

Upon observing curvilinear growth patterns, many studies use latent basis models as a means of approximating those patterns. In latent basis models (a variant of latent growth curve models), some factor loadings are constrained and others are freely estimated (McArdle, 2009), which means that no specific shape is imposed on the model-implied trajectory. This approach offers greater flexibility than polynomial models in terms of the functional forms that can be approximated, but also possesses important drawbacks.

First, latent basis models do not require the researcher to form *a priori* expectations about the shape of the trajectory; rather, the shape of the curve is fully informed by the data. This feature has been described as advantageous if the researcher has no prior expectations about the shape of the curve or is uninterested in testing for specific types of nonlinear growth trajectories (e.g., McNeish & Matta, 2018); however, other methodologists have criticized the latent basis model for being “atheoretical” (Grimm et al., 2011). I argue that the non-confirmatory nature of the latent basis model is, overall, a drawback. Latent basis models do not possess the primary advantage of the parametric nonlinear model, which is strong connection between model parameters and theory; therefore, latent basis models do not facilitate strong hypothesis- or theory-testing. Indeed, McCormick et al. (2023) argue, “the idea that these data-driven



approaches can replace more theoretically informed forms of trajectories is likely ill-conceived both practically and theoretically... They are most often not useful as explanatory models and instead are most useful as descriptive or purely predictive models” (p. 13). In other words, latent basis models limit the researcher to merely describing curvilinear patterns, rather than testing *a priori* hypotheses about curvilinear patterns.

Second, latent basis models suffer from poor parameter interpretability (McCormick et al., 2023). Depending on how the model is specified, the estimated parameters that govern the shape of the trajectory may correspond with (1) the proportion of total change that has occurred at a given timepoint, or with (2) the amount of change that has occurred at a given time point, proportional to the change that occurred between the first two timepoints. These interpretations are often not substantively useful, and therefore, any moderation of these parameters is unlikely to be meaningful.

Third, latent basis models do not permit generalizability outside of the observation period, as they provide only a descriptive picture of the observed data (Grimm et al., 2011). Fourth, latent basis models often require more estimated parameters than a nonlinear model that would approximate the data equally well (Grimm et al., 2011). Finally, latent basis models tend to overfit the local features of a data set (McCormick et al., 2023).

These drawbacks are highlighted in the following examples from educational research. In both applications, key study hypotheses involved whether student-level variables moderated academic skill trajectories. Chen et al. (2014) used latent basis mixture models in their study of math and science achievement trajectories for children held back in first grade. Two latent classes were identified, and differences in their trajectories were probed visually; one class was descriptively termed the “low intercept, high growth” group, whereas the other was termed the

“high intercept, slow growth” group. To incorporate moderation, various student-level variables (e.g., learning skills, self-regulation, prosocial behavior) were added as predictors of class membership. Lesaux et al. (2007) took a similar approach to approximate reading skill trajectories for native and non-native English elementary students. Latent basis growth curve models were fit separately for each group (native vs. non-native English speakers), and to investigate group similarities and differences in the growth trajectory, increasingly strict invariance constraints were imposed. In both examples, model parameters did not directly correspond with specific attributes of the growth trajectory. Therefore, it was not possible to directly test for moderation by student-level variables. The use of moderated nonlinear models would have allowed these researchers to pinpoint whether specific characteristics of academic growth trajectories (e.g., overall improvement, time/age at which growth was fastest, overall rate of improvement over time) were moderated by the key student characteristics under study (e.g., learning skills, native English-speaking status). Though latent basis models may do better than polynomials in terms of characterizing curvilinear trajectories, they still preclude many inferences and direct tests of key hypotheses.

### **Piecewise Models**

In the presence of a curvilinear pattern or a nonconstant strength of the relation between  $x$  and  $y$ , another common approach is to implement piecewise models. In most piecewise models, a different linear slope of  $x$  is estimated across different segments of  $x$ ; however, other types of relations, such as quadratic or cubic, can also be incorporated into any segment (e.g., Feng et al., 2019; Haring et al., 2021; McNeish et al., 2023). The values of  $x$  that demarcate the segments are referred to as *knot points*, and may be pre-specified by the researcher or freely estimated.

Piecewise models have been argued to be advantageous in some contexts, such as if the location of the knot point is theoretically important (Kohli & Harring, 2013). However, compared to parametric nonlinear models, piecewise models possess notable drawbacks.

First, it is often not realistic to impose an instantaneous change in slope at each knot point. Cudeck and Harring (2010) note that often, “a more plausible assumption is that the transition between phases is gradual and smooth” (p. 303). The abrupt change in the relation between  $x$  and  $y$  is a strong assumption that is often not well-aligned with psychological theory (Ram & Grimm, 2007). To highlight this point, Briet et al. (2023) discuss an example from the intelligence literature. Here, it is hypothesized that the relation between intelligence and creativity weakens as intelligence levels increase; however, most theories do not posit a specific breakpoint at which the relation abruptly changes. Use of the piecewise linear model is not justified in the absence of such a theory.

Second, because piecewise models are linear, they imply that the trajectory will increase/decrease toward infinity in either direction. This feature results in “increasingly questionable” accuracy toward the extremes of the observed data (Choi et al., 2009), as well as lack of generalizability beyond this observed range. Third, Burke et al. (2007) note that piecewise linear models require the researcher to make the “simplifying assumption” of local linearity throughout the change process, which may not be realistic. Fourth, as the following examples will demonstrate, piecewise linear models typically involve more estimated parameters than nonlinear models that would approximate the observed trajectory equally well (McNeish et al., 2023). Often, these parameters do not correspond with the most important attributes of the trajectory under study, precluding hypothesis tests and direct incorporation of moderators.

Finally, analytic approaches that empirically test for the presence of a knot point have been shown to yield exceedingly high false positive rates under many data conditions (Breit et al., 2023). Segmented regression analyses (SRA) are often used to either confirm or disconfirm whether a piecewise linear relation is present, and if so, where along the  $x$ -axis the knot point is located. In many areas of social science, SRA is used if it is suspected that the strength of the relation between  $x$  and  $y$  changes across different levels of  $x$ , but it is unknown whether the relation can be modeled with a piecewise linear model. In a simulation study, Briet et al. (2023) found that when the data generating relation was quadratic or exponential, a popular SRA method yielded false positive rates of 58 – 83%. In these conditions, SRA incorrectly indicated the presence of a knot point. As a result, these authors strongly recommended against empirically testing for piecewise linear relations, and instead suggested the use of nonlinear models.

The drawbacks of piecewise models are demonstrable in a variety of empirical applications from diverse research areas and study designs. For example, in their study of reading score trajectories from kindergarten to 3<sup>rd</sup> grade, Aikens and Barbarin (2008) observed non-constant rates of change upon plotting their data. The growth rate was slow across the earliest timepoints, fastest throughout 1<sup>st</sup> grade, then slow again over the latest timepoints (indeed, consistent with the shape of a sigmoidal model). To accommodate the pattern, they used a piecewise linear model with three segments; the knot points were chosen by the researchers, such that the segments corresponded roughly to the three periods that appeared to display different growth rates. Of key substantive interest was whether student demographics, family characteristics, and neighborhood characteristics moderated initial reading levels and reading growth rates. These variables were incorporated as moderators of the intercept and slope segments, resulting in a very complex model with approximately 50 estimated parameters.

Indeed, these moderation tests could have been incorporated more directly through use of a nonlinear model, where initial reading levels, growth rates, and final reading levels can be estimated as model parameters. Interindividual differences in these important aspects of the reading trajectory could have been probed with far fewer parameters.

In another example, Devonshire et al. (2023) tracked interparental conflict behavior during and after a family intervention, where they observed non-monotonic trajectories with varying rates of change. Conflict behaviors increased between pretest and posttest, decreased between the posttest and 12-month follow-up measurement occasions, and leveled off between the 12-month and 3-year measurement occasions (consistent with the shape provided by peaked nonlinear models). The authors fit a 3-segment piecewise linear model (though noted that the ideal location of the knot points was “not obvious”), then incorporated intervention condition as a moderator of the intercept and each of the three slopes. Specifically, this analytic method allowed the authors to assess whether the intervention moderated (1) initial levels of interparental conflict, (2) the rate at which conflict increased during the intervention, (3) the rate at which conflict decreased following the intervention, and (4) the rate at which conflict changed throughout the following three years. Through use of a peaked nonlinear model, the authors could have assessed moderation of more substantively useful aspects of the conflict trajectory, while implementing an equal or smaller number of tests. For example, consider the Bragg model given in Eq. 2.11, where in this example, the parameters would govern: (1) the starting and ending levels of interparental conflict, (2) the maximum level of conflict reached at the peak, (3) the rate of increase and decrease around that peak, and (4) the time at which the peak was reached. By testing for moderation of these parameters, the authors likely would have gained more useful insight into how their intervention affected interparental conflict. For example, were

maximum conflict levels lower or higher for parents in the intervention? Was that maximum level reached earlier or later? Perhaps most importantly, did parents in the intervention group display lower or higher asymptotic levels of conflict? These questions could not be directly answered via the piecewise linear model.

### **Variable Transformations**

When curvilinear relationships are observed among variables in their original metric, some researchers rely on transformations to achieve linear relations. For example, in their study of reading and math trajectories, Shin et al. (2013) observed growth rates that decelerated over time. Therefore, they implemented a linear model where the log-transformation of time was the predictor. The authors argued that this approach yielded better interpretability than a quadratic model because only one model parameter (rather than two) governed the change rate. However, it was difficult to interpret growth in terms of meaningful units of time. Indeed, Cohen et al. (2003) note that transformations should yield “conceptually meaningful units,” and when transformations result in *less* interpretable parameter estimates, it may be unwise to implement them. This approach also suffers from the other identified drawbacks of linear models, such as nonsensical model-implied trajectories outside the study period.

### **Summary**

The goal of this chapter was to motivate the use of nonlinear models within social science by reviewing their many benefits in the presence of curvilinear relations. By exploring examples that successfully implemented nonlinear models, and contrasting these with examples that were restricted to alternative approaches, it is easy to see the advantages that nonlinear models

provide. Better congruence between model-implied and theoretically expected trends, more interpretable parameters, and more detailed insight into moderation are some of the primary benefits highlighted here. These benefits apply to longitudinal, cross-sectional, experimental, and observational research across diverse subjects of study within the social sciences.

## CHAPTER III

### BARRIERS TO THE UPTAKE OF NONLINEAR MODELS IN SOCIAL SCIENCE

Despite their many benefits, intrinsically nonlinear models are implemented far less frequently than linear models across the social sciences. There are many likely reasons for this disparity. For example, limitations in education and training are important to consider. Upon conducting an exhaustive review of psychology graduate programs, Aiken et al. (2008) concluded that comprehensive methodological training was not required and/or not offered in most programs. Similarly, Flake et al. (2020) note that most psychology graduate students do not receive formal methodological training beyond the first-year statistics sequence. It is reasonable to expect that these few required statistics courses remain restricted to linear models in terms of course material. This has likely resulted in a general lack of awareness of nonlinear models and their usefulness among psychological scientists. Indeed, Baldwin (2017) notes that without better statistical training, “researchers can get stuck in a rut of one or two methods and never... develop perspective that comes from using new and alternative methods” (p. 13). With little-to-no exposure to nonlinear modeling and its advantages, psychology researchers are likely to maintain the status quo of relying on linear approaches.

Historically, researchers were largely restricted to the linear framework – even when curvilinear patterns were observed – due to limitations in computing power (Blozis & Cudeck, 1999; McNeish et al., 2023). Indeed, linear models are computationally easier for software to fit than nonlinear models, which require iterative estimation (Ratkowsky, 1990). Even though present-day computing power largely mitigates this obstacle, linear models remain pervasive.



Overall, there is a general lack of precedent for applying nonlinear models to psychological research questions. Researchers therefore face challenges in mapping models onto theory, dealing with practical issues that often arise from iterative estimation, and carrying out the modeling process with software. In this chapter, these challenges are expanded upon in turn.

### **Theoretical Challenges**

The first major challenges that social scientists face when implementing nonlinear models concern model-theory connections. First, the researcher is required to choose a nonlinear model from among the very large number that exist. This is a major departure from the linear modeling framework, where fewer models are possible. Indeed, some methodologists have noted that for social scientists, selecting a nonlinear model may be the most difficult step of the entire modeling process (e.g., Blozis & Harring, 2021; Cudeck & Harring, 2010). Cudeck and Harring (2007) regard this step as “the major scientific issue when using nonlinear models” (p. 625).

Making the choice even more difficult, many resources on nonlinear modeling assume that the researcher will already know which function is most appropriate for their data. For example, Ritz and Streibig (2008) note: “it is implicitly assumed that the data analyst has some prior knowledge about which kind of function  $f$  should be used” (p. 2). Similarly, Motulsky and Christopolous (2004) state: “in many cases, picking a model will be easy, as you will likely be choosing a model that is conventionally used in your field” (p. 62). This assumption is often made because most nonlinear functions were derived with respect to a specific biological process. Textbook examples, therefore, tend to concern certain biological phenomena with a well-known accompanying nonlinear equation; for example, many kinetics processes are known to follow the Michaelis-Menten equation, and dose-response processes can typically be modeled

by a logistic function (Davidian & Giltinan, 1995; Motulsky & Christopolous, 2004; Ritz & Streibig, 2008). Similarly, the Preece-Baines and Jenss-Bayley equations were developed specifically to model humans' physical growth over time (Grimm et al., 2011; Jenss & Bayley, 1937; Preece & Baines, 1978), and the Gompertz curve was developed to model tumor growth (Laird, 1964). Unfortunately, most nonlinear functions were not developed with the intention of modeling change over time of a psychological construct, or relationships between multiple psychological constructs. Therefore, such obvious pairings between a given topic of study and a corresponding nonlinear model are typically not available. It is often less clear how psychologists should choose an appropriate nonlinear model.

Social scientists also face the challenge of choosing a useful parameterization. Indeed, a primary benefit afforded by the nonlinear model is that its parameters are interpretable and can be connected in useful ways to the theory under study (Cudeck & Haring, 2010; Ram & Grimm, 2007). However, to accomplish this connection, "active conceptualization" is required on the part of the researcher (Grimm et al., 2011) to pinpoint the precise attributes of the curve that are substantively important, and to ensure the model contains parameters that correspond with each of those attributes. This process of explicit model-theory mapping may feel foreign to researchers who are familiar only with linear models. Within the linear modeling framework, estimated attributes of the curve are largely restricted to baseline levels (intercepts), linear growth rates, and strengths of linear relationships. Therefore, these quantities typically must be the basis of key study hypotheses. In nonlinear models, an extremely diverse array of quantities can be represented by model parameters, which opens up the possibility of more nuanced and specific theories and hypotheses that can be tested via the model. Therefore, more critical thought is required from the researcher to make connections between parameters and theory.

These challenges are exacerbated when moderation is introduced. In nonlinear contexts it may be more difficult to map specific moderations onto theory (Cudeck & Harring, 2010). When past theories have largely been informed by linear-by-linear interactions, there is less basis to inform expectations of how specific parameters of a nonlinear model may be moderated. For example, though there is vast prior research concerning aptitude-by-treatment interactions, most of this research has involved linear models (Preacher & Sterba, 2019). Therefore, forming hypotheses about moderation of specific aspects of nonlinear learning processes may be difficult due to limited prior research.

Finally, nonlinear models require the researcher to rely more on theory and expectation – and less on empirical evidence – when deciding which predictors, moderators, and covariates to include in the model. In the absence of theory to inform *a priori* expectations about the “best” model, within the linear modeling framework it is easy to explore which predictor(s) ought to be included in a model. Procedures such as forward, backward, and stepwise regression have been written about extensively and are readily available in major software packages, and therefore, are frequently used to empirically determine the optimal predictor set for a given outcome. Analogs of these procedures do not exist for nonlinear models (Ratkowsky, 1990). The expectation that the researcher will begin the modeling process with knowledge of not only the correct model, but also the optimal predictor(s) to include, is likely attributable to the original applications for which nonlinear models were developed. For example, in controlled experimental studies of plant growth, the choice of which predictor(s) to include is likely to be obvious. These choices are far less straightforward for psychologists considering competing theories, uncontrolled observational research designs, latent variables, myriad potential covariates, and less precedent

on which to base nonlinear analyses. Therefore, arriving at the “best” model specification may be a challenging process in nonlinear regression (Cudeck & Harring, 2010).

### **Practical Challenges**

Psychologists also face a greater variety of logistical challenges when fitting nonlinear models. First, convergence problems arise regularly, often due to misspecification. However, many aspects of misspecification may cause nonconvergence, and it is often difficult to identify the specific source of convergence problems. Choosing a functional form that does not approximate the observed data well, or including too few or too many random effects in a NLME model, is a common cause of nonconvergence (Pinheiro & Bates, 2000; Ratkowsky, 1990). Similarly, if the functional form of the model is too complex for the data, nonconvergence rates tend to be high (Savalei & Kolenikov, 2008; Wood, 2023). Nonconvergence is also more frequent when the model has a larger number of parameters to be estimated, and therefore becomes more likely as more terms (e.g., moderators) are introduced (Gallant, 1987; Sit & Poulin-Costello, 1994). Aside from misspecification, another cause of nonconvergence is an inadequate number of observations across all regions of the design space (Bates & Watts, 1988). Although sparse observations in certain regions of the data space can lead to questionable inferences and lack of generalizability in moderated linear models (Bodner, 2016), it typically will not preclude the estimation of parameters. Ultimately, if the model does not converge, then assessments of model fit, model selection, and model interpretation cannot be undertaken (Motulsky & Christopolous, 2004). Non-estimability is common to the nonlinear framework because all nonlinear models, whether they include random effects or not, rely on iterative estimation procedures (described in Appendix A).

Second, when implementing nonlinear models, it is important to supply start values for each parameter. The choice of start values is nontrivial, because if start values are too dissimilar to the best-fitting parameter values, convergence is less likely. Reasonable start values should yield a curve that corresponds to the observed data somewhat closely. To quickly generate adequate start values, the researcher would need to possess in-depth knowledge of how each parameter changes the appearance of the nonlinear curve; for example, in the logistic model, what does the curve look like when the parameter governing rate of approach is equal to 0.5 versus 1? Psychology researchers typically do not possess this knowledge *a priori*. In such situations, it is recommended that the researcher plot the function, with various values chosen for each parameter, to gain an understanding of how the parameters govern the curve and therefore arrive at reasonable start values that match the observed data (Bates & Watts, 1988; Ratkowsky, 1990); however, this process is likely to be arduous and time-consuming for the typical researcher using extant software. Selecting good start values becomes even more important as models become more complex (Burke et al., 2007), so this step is salient when moderators are involved. Although the implications of start values have never been discussed with respect to moderated nonlinear models specifically, it is likely especially important – and difficult – to choose good start values for these models due to their increased complexity.

A third challenge that becomes salient in nonlinear regression is that certain parameters may need to be constrained to a constant (i.e., not estimated) in order to achieve convergence. This is more true as the number of estimated parameters increases, and is therefore likely to become relevant in moderated nonlinear models. In moderated linear models, although such constraints may be applicable, there is no consequence if the researcher does not incorporate them into the model.

Similarly, when working with NLME models, the researcher must decide whether each parameter should be treated as random or fixed. McCormick (2023) notes that for most nonlinear models, there is no clear hierarchy or ordering of parameters that may aid researchers as they decide what to treat as random vs. fixed. We can contrast this with linear models, where parameters often fall into an intuitive hierarchy. For example, consider a cubic polynomial model – where all parameters are specified as random – that does not converge. The typical first step is to specify the cubic term as fixed, and if the model still does not converge, to then specify the quadratic term as fixed, and so on. There is an intuitive “top down” approach that can be taken when searching for a linear mixed model that converges. When NLME models do not converge, the process by which to constrain parameters becomes less clear.

In summary, nonlinear models are estimated through iterative procedures, which means that they commonly fail to converge. Convergence problems arise more frequently as models possess more parameters, and therefore, moderated models may face these problems frequently. Such practical challenges almost never arise for linear models, and therefore, they serve as further barriers to the uptake of nonlinear regression models in psychology.

### **Software Challenges**

In addition to the theoretical and practical challenges that psychology researchers face when choosing and fitting a nonlinear model, there are also new obstacles presented when carrying out this process with software. Regardless of the software being used, platforms for nonlinear modeling are different and more complex than those used for linear modeling; the researcher must become familiar with new functions, formulas, and procedures. These procedures are often notably more complicated than those available for linear models, as

nonlinear models are not offered as standard options in many major software packages. Indeed, McCormick (2023) notes that due to the complicated nature of current software utilities for nonlinear modeling, nonlinear models remain largely restricted to advanced methodological applications.

The first roadblock encountered by researchers using R, SAS, or SPSS is that the nonlinear model formula must be manually entered. Depending on the model, this step alone may be arduous and become error prone as the model increases in complexity. A simple example is the two-parameter power model, with no moderation:  $y = a * (x * \exp(b))$ . In contrast, suppose the researcher wishes to implement a four-parameter logistic model with each parameter moderated. The corresponding formula could be:

$$y = (a_0 + a_1 * z) + (b_0 + b_1 * z) / (1 + \exp(-(c_0 + c_1 * z) * (x - (d_0 + d_1 * z)))) .$$

For the typical social scientist, manually coding the model formula quickly becomes difficult. If the researcher is fitting a NLME model, then specification of fixed and random effects introduces further complexities in the required code (Pinheiro et al., 2023).

Additionally, if and when convergence failures occur, it is up to the researcher to manually address this problem. The most commonly recommended strategies include choosing a nonlinear model with a less complex functional form or fewer parameters, entering different start values, centering and/or scaling variables, reparameterizing the model, adjusting the convergence criterion, and/or increasing the maximum number of iterations that the estimation algorithm will attempt before it stops (Bates & Watts, 1988; Gallant, 1987; Motulsky & Christopoulos, 2004; Preacher & Hancock, 2015; Ratkowsky, 1990; Wood, 2023). For NLME models, further strategies include changing the number of random effects in the model, rescaling the predictors to have more similar ranges, reparameterizing the random effects covariance matrix via a Cholesky composition, or the more advanced option of decomposing the random effects

covariance matrix via factor analysis (Bates et al., 2014; Cheng et al., 2010; Hedeker & Gibbons, 1996; Kohli et al., 2019; McNeish et al., 2020; McNeish & Bauer, 2022). In the most dire of circumstances, some methodologists have even recommended using a “brute force” approach of searching over a grid of all possible combinations of parameter estimates (Archontoulis & Miguez, 2015). Some of these strategies are available in popular software packages such as SAS and R. However, many R functions designed to carry out these strategies are not geared toward social scientists, and instead, are couched within packages written for biologists or agricultural researchers. This may result in increased difficulty for psychology researchers to carry out these procedures when convergence fails.

When model parameters are hypothesized to be moderated, the limitations of current software become even more apparent. At present, there is no unified resource, function, package, or tool that enables researchers to easily incorporate moderation into their nonlinear model specification, or to subsequently plot and probe moderation of nonlinear model parameters. It would be up to the researcher to write code to do this from scratch. This significantly hinders researchers’ ability to understand the nature of moderation in nonlinear regression models, and is likely a primary reason why moderation is not explored more frequently in such models.

Extant R packages for plotting and probing moderation cannot accommodate nonlinear models. Functions that were developed specifically for probing interactions, such as those in the *interactions* (Long, 2019) and *reghelper* (Hughes & Beiner, 2023) packages, accept a model object that has already been created. However, the model objects that are supported by these functions are those that are linear in the parameters, such as *lm*, *glm*, *aov*, *lme*, and *merMod* objects. When nonlinear models are fit in R, different kinds of model objects are created, which cannot be inputted into extant utilities for plotting and probing. Additionally, extant software



options for fitting nonlinear models are accompanied by few or no plotting capabilities. Although SAS procedures like NLIN and NLMIXED enable the incorporation of moderated parameters, there are no straightforward options for plotting or probing the output of such an analysis. The same is true for *nls* objects (nonlinear regression models, created in base R) and *nlme* objects (NLME models, created with the *nlme* package; Pinheiro et al., 2023) in R. In summary, popular software packages do not offer straightforward functionality for plotting, probing, and/or visualizing the results of a moderated nonlinear model. It would be up to the researcher to manually create code from scratch to carry out the desired computations and plots.

There is a clear need for unified software utilities that easily allow for plotting and probing of moderation within nonlinear models. At minimum, there ought to be simple ways to plot the curve linking  $x$  to  $y$  across different values of the moderator (i.e., the pick-a-point plot), whether that moderator is categorical or continuous. At best, the JN technique would be incorporated into plotting functionality, but extensions of the JN technique to nonlinear models currently do not exist.

Beyond plotting capabilities, a maximally useful piece of software could go further to unify the entire process of fitting, testing, evaluating, and plotting/probing a moderated nonlinear model. Prototypes of such tools exist for linear regression. For example, McCabe et al. (2018) developed a Shiny interface called *interActive* which provides a code-free environment for the researcher to carry out each step of the modeling process. Steps for data upload, specifying and testing the significance of two-way interactions, adding covariates, and plotting and probing are all available. However, these utilities only accommodate intrinsically linear models.

## Summary

Researchers in psychology and other social sciences face a variety of barriers that make the implementation of nonlinear models challenging. First, it is difficult for social scientists to choose a nonlinear model with strong theoretical motivation, often due to a lack of precedent and/or models that were developed with respect to a biological process. For similar reasons, it can also be challenging to parameterize the chosen model such that each parameter corresponds with a substantively important attribute of the curve. Second, researchers face new logistical challenges that follow from iterative estimation methods, including choosing good start values, constraining parameters when appropriate, and implementing strategies to overcome nonconvergence. Third, researchers must contend with scattered and incomplete software utilities for fitting nonlinear models and including moderated parameters.

The subsequent chapters of this dissertation aim to equip readers with knowledge and tools to overcome many of the largest barriers identified here. Chapters 4 and 5 address theoretical challenges, whereas Chapter 6 addresses software-based challenges.

## CHAPTER IV

### SELECTING, PARAMETERIZING, AND SPECIFYING MODERATED NONLINEAR MODELS

In Chapter 3, I reviewed the most salient conceptual challenges that arise when social scientists seek to implement nonlinear models. The purpose of this chapter is to summarize methodological recommendations, as well as provide new guidelines, to supply researchers with resources for overcoming these challenges. The primary steps discussed here are selecting a nonlinear model, choosing a useful parameterization, conceptualizing moderation and incorporating it into the nonlinear model specification, and adding covariates.

#### Choosing a Nonlinear Model

Methodologists have noted that choosing a nonlinear model may be the most important, yet most daunting, stage of the nonlinear modeling process (Blozis & Haring, 2021; Choi et al., 2009). For reasons noted in Chapter 3, social scientists face exacerbated challenges at this stage because most nonlinear functions were derived with respect to a specific biological phenomenon. The purpose of this section is to provide a review of the options for social scientists at this stage of the modeling process. Here, I synthesize potential approaches to model selection that have been suggested by social science methodologists, collect prototypical examples of each approach to provide a basis from which to draw for future analyses, and propose guidelines for thinking about this decision.

I begin by reviewing general considerations for choosing a nonlinear model. First, it is important to acknowledge that in social science applications, there is almost never an objectively

“correct” choice. Often, the best we can do is find a model that is better than others in some way (Cudeck & Harring, 2010; Myung & Pitt, 1998; Wood et al., 2015). There are likely to be multiple nonlinear models that fit the data similarly well, making the best choice unclear. Indeed, Cudeck and Harring (2010) note that in the same situation and with the same data set, different researchers would likely end up with different nonlinear models. Therefore, rather than focusing on choosing the “correct” model, it is more feasible to simply focus on transparency about how the model was chosen. An emphasis on transparency is not uncommon in statistics; in data analysis situations where subjective decisions are required, such as choosing priors in Bayesian estimation, methodologists frequently advocate for detailed explanation of how those decisions are made (Flake et al., 2020). Indeed, this theme carries over to nonlinear modeling (Cudeck & Harring, 2010).

Second, Cudeck and Harring (2007, 2010) present three general criteria with which to evaluate nonlinear models in social science applications – *fit*, *appropriateness*, and *interpretability* – which are helpful to keep in mind while thinking through model choice. Regarding *fit*, the chosen model should follow the data reasonably closely. Fit may be evaluated by plotting the fitted curve over a scatterplot of the observed data, and/or assessing fit statistics and empirical indicators of model-data fit. Regarding *appropriateness*, the chosen model should make sense conceptually and correspond with expected patterns in the data, given the scientific context of the study. For example, if prior research or theory leads the researcher to believe that the observed pattern will level off or plateau, then the chosen model should include an asymptote. This criterion can be evaluated only by substantive expertise, and is inherently subjective, again pointing to the idea that different researchers will have different opinions about an ideal model. Finally, for *interpretability*, the parameters of the chosen model should have

clear meaning and correspond with the aspects of the curve that are most important for the given application. Parameter interpretability is a key advantage of nonlinear models, so this criterion is sometimes argued to be the most important (Grimm et al., 2011; Preacher & Hancock, 2015).

While keeping these general criteria in mind, there are many potential approaches to choosing a nonlinear model and their corresponding rationales differ greatly. Next, I will outline three potential approaches that have been proposed and implemented in social science contexts, which vary in the degree to which they rely on theory vs. observed data. Examples will be provided for each approach, and their benefits and drawbacks will be discussed.

### **Theory-Driven Approach**

The ideal approach for selecting a nonlinear model is to make the choice based on substantive expertise and expectations about how to best inform, update, or test theory. The theory-driven approach is largely confirmatory; the researcher begins the statistical analysis process by enumerating *a priori* expectations and hypotheses to be tested. The purpose of the statistical model is to provide evidence for or against these *a priori* hypotheses, and results must then be reconciled with existing theory (Meehl, 1978). Therefore, this approach places strong emphasis on model-theory connections, and relying on substantive expertise – rather than the observed data – to make decisions about the model.

Psychological theories are often expressed verbally and are imprecise. Translating a vague verbal theory into a formal theory, which can be represented by a mathematical model, forces the researcher to be precise about the patterns and structures that they expect to observe. Formation of specific, formal theories (i.e., mapping theories to mathematical models) facilitates replicability (Chen et al., 2024; Haslbeck et al., 2022). Additionally, formal theories are specific

enough to be falsifiable, which is paramount for determining whether the theory falls short of explaining psychological phenomena (Haslbeck et al., 2022; Meehl, 1978, 1986).

Therefore, strong theoretical justification for the chosen model is likely to result in a scientifically valid, practical, and substantively meaningful model (Archontoulis & Miguez, 2015; Cudeck & Harring, 2007; Grimm et al., 2011; Motulsky & Christopoulos, 2004; Ram & Grimm, 2007). Indeed, MacCallum (2003) notes that because all models are wrong, “At best, they can provide an approximation of the real world that has some substantive meaning and some utility” (p. 114-115). Whether the chosen model provides substantive meaning and utility is largely informed by the expertise of the researcher, and corresponds closely with the *appropriateness* and *interpretability* criteria. For *appropriateness*, Ram and Grimm (2007, p. 304) note that “models should be selected so that they match with one’s beliefs (i.e., theory) about how change is structured,” and for *interpretability*, the function’s parameters should yield meaningful, useful, and interesting substantive information (Cudeck & Harring, 2007). Prioritizing these criteria enables the researcher to ensure that the model is a direct and specific reflection of the theory being tested. There are many social science contexts in which it is possible to choose a nonlinear model on fully theoretical grounds.

First, the researcher may be approximating relations between variables for which the model was originally intended. Functions are typically derived such that their parameters yield substantively useful information about the intended process, so this scenario is likely to yield a model that affords meaningful scientific conclusions. For example, the Jenss-Bayley function (Jenss & Bayley, 1937) was derived specifically to model human growth over the first six years of life. Preacher and Hancock (2012) used this model to investigate whether breastfeeding over the life span was associated with growth deficits at various timepoints throughout childhood.

Similarly, the Preece-Baines function (Preece & Baines, 1978) was created to model growth in human height over the course of childhood, puberty, and adulthood. Grimm et al. (2011) noted that this function has useful parameters that map onto developmental theory, and therefore, used a Preece-Baines model to test for relationships between growth patterns and pubertal timing. In summary, there are some social science applications in which a nonlinear model can be used for its original purpose, especially if the application involves physical growth or change. If feasible, this approach yields strong model-theory connections.

Second, there may be a psychological theory that suggests a specific nonlinear model is the most appropriate for a given study. One example (see Chapter 2) is the subjective value theory proposed by Rigoli and Martinelli (2021). These authors posited that relations between actual and subjective value should be characterized with the logistic model (i.e., articulated a formal theory), provided rationale for this argument, and detailed how between-person variability in each parameter of the logistic model would map onto theory. Ideally, future studies will test this model empirically, and citing this foundation as rationale for the logistic model will result in a theoretically well-supported analysis. Indeed, in their discussion of growth curve models, Ram and Grimm (2007) note the need for “precise articulation of the types of changes we expect” (p. 304); when that articulation is provided, the nonlinear model that best maps onto our expectations often becomes clear. Ideally, emergence of such formal theories will facilitate greater use of theoretically motivated nonlinear models. Theories that cite a specific nonlinear model are currently rare in social science, but if they exist, provide ideal justification for choosing a nonlinear model in empirical work.

Third, past findings and theory may not explicitly point to a specific model, but may enable the researcher to infer that a model is best suited for their application. For example, in

their study of adjustment following the loss of a spouse, Burke et al. (2007) cited past work that suggests “adjustment should happen more rapidly at first, when the individual is furthest from equilibrium, and should slow over time as the individual nears his or her equilibrium level of adjustment” (p. 406). Given this expected pattern, the authors chose a decreasing exponential model. Although theory did not explicitly connect the adjustment process to the exponential model, the researchers inferred that this model was a good match to theoretically expected patterns. Additionally, the chosen model contained parameters that were substantively useful. Taken together, this approach resulted in a chosen nonlinear model with strong scientific justification. It is possible that a different nonlinear model would have fit the data equally well or slightly better. However, the chosen model corresponded well with theoretical expectation (*acceptability*) and contained meaningful parameters (*interpretability*); because these key criteria were met, it was not necessary to compare multiple models.

Fourth, there may be an accumulation of prior findings to establish a precedent for use of a given model. A large cache of consistent evidence in favor of a model, particularly if theoretical contributions have been made through use of that model, can yield strong justification. For example, many studies of academic and cognitive development (e.g., Anthony & Ogg, 2020; Cameron et al., 2015; Ricker et al., 2018; Womack et al., 2022), find that the Gompertz model exhibits better goodness-of-fit to the data than other linear and nonlinear models. It has been speculated that the Gompertz curve aligns particularly well with learning processes because most total growth occurs after the inflection point. Cameron et al. (2015) posit that the inflection point signifies the shift from *acquisition of foundational skills* to *slow and steady learning*, and that this shift is theoretically expected to occur early in the learning process for both reading and math. Therefore, consistent findings that the Gompertz model fits well to



learning data are in line with theory. Additionally, past studies have demonstrated that the parameters of the Gompertz model correspond with substantively important aspects of learning, which has enabled rich theoretical contributions in this area. Taken together, evidence points to strong theoretical rationale for use of the Gompertz model to approximate learning trajectories.

Similarly, several studies have demonstrated the benefits of the logistic function for approximating pubertal development throughout childhood and adolescence (e.g., Beltz et al., 2014; Marceau et al., 2011; Marceau et al., 2015). In these studies, the logistic model has yielded rich insight due to the substantive relevance of each model parameter. The rate-of-growth parameter corresponds with *pubertal tempo*, or the speed at which pubertal development occurs over the course of observation, and parameter that governs location of the inflection point corresponds with *pubertal timing*, or the age at which the individual is halfway through pubertal development. Pubertal timing and tempo are key quantities that have been found to be associated with a variety of predictors and outcomes over the lifespan; therefore, model parameters that directly correspond with these aspects of development have yielded novel insight. In future studies, drawing on this accumulation of past findings to provide theoretical justification for the logistic model will be a strong approach.

To summarize, there are many scenarios in which the researcher can take a theory-driven approach to choosing a nonlinear model. There may be a nonlinear function that was derived for the same purpose as the study, there may be psychological theory that suggests a certain model is ideal, or there may be a strong accumulation of evidence supporting the theoretical utility of a certain model for a given application. In all these cases, the *appropriateness* criterion is inherently met, and the *interpretability* criterion is usually inherent, as well. Additionally, the theory-driven approach facilitates the enumeration of specific, falsifiable, formal theories on an *a*

*priori* basis. For a more detailed review of the benefits of this approach, and more generally, the advantages of theory formalization, see Haslbeck et al. (2022).

However, it has also been argued that there are drawbacks to a theory-driven approach. Perhaps most importantly, the theoretically motivated model may not fit well to the data. Some methodologists have suggested that strong substantive justification and interpretable parameters may overshadow suboptimal model-data fit, contending that it is acceptable to prioritize *appropriateness* and *interpretability* over *fit* (e.g., Cudeck & Harring, 2007). On the other hand, Wood et al. (2015) take a largely opposite stance, arguing that model-data fit should be prioritized over theoretical motivation. The authors posit that rather than confirming a pre-existing theory, identifying a model with weaker theoretical motivation but better model-data fit may better serve the process of theory updating. These ideas are important to address, but at the same time, it is essential to note that good *fit* without *appropriateness* and *interpretability* yields a substantively useless model (Grimm et al., 2011; Ram & Grimm, 2007). Overall, I argue that the benefits of a theory-driven approach outweigh the potential drawbacks.

### **Mix of Theory- and Data-Driven Approaches**

Although it is ideal to choose a nonlinear model based on theoretical rationale, there is often not enough theory or research to support this approach. The next-best approach is to use a mix of theoretical and empirical justification for the chosen model. This may involve using theory and past findings to inform a small set of candidate models, then using data-driven information to select one model from among the candidates. Comparing model selection criteria like AIC and BIC, inspecting graphs of each candidate model with the observed data, and/or evaluating diagnostic plots are all frequently recommended. Indeed, many social science

methodologists have argued that it is acceptable to choose a model on both theoretical and empirical grounds (e.g., Grimm et al., 2011). If the model's parameters are interpretable and useful, and the model makes sense conceptually, then it is appropriate to select a model on the grounds that it performs well with the observed data (Cudeck & Harring, 2007, 2010).

In these situations, substantive knowledge can often help the researcher formulate expectations about the general shape of the curve. This general shape may lead the researcher to a family of nonlinear models; multiple models from that family can then be fit to the observed data, and the "best" model is chosen empirically. For example, in their study of science achievement trajectories, Anthony and Ogg (2020) compared the fit of logistic, Gompertz, and Richards models. The authors stated: "Based on prior research, we anticipated that a sigmoidal 's-shaped' nonlinear curve would provide the best fit for science growth" (p. 1569). In this context, substantive knowledge helped the researchers direct their attention to the sigmoidal family, then AIC and BIC were used to select one model.

In another example, McNeish and Dumas (2017) took a mixed approach to selecting a nonlinear model to approximate trajectories of academic ability, by "choosing a small number of models that align well with our theoretical modeling goals and then compar[ing] the empirical fit of these models" (p. 71). The authors began by plotting their data to visually inspect trends; they noted that there did not appear to be a lower asymptote or inflection point, and the rate of growth was strongest initially and decreased with the passage of time. These observations steered them toward the exponential family, and therefore, the Michaelis-Menten (MM) model and the von Bertalanffy model were chosen as the candidate set. (The Gompertz model was also included in the candidate set to account for the possibility that an inflection point existed in the data but was not visually apparent). The MM model yielded the lowest BIC, and importantly, yielded the most

substantively interpretable parameters given the context of the study. Therefore, the MM model was chosen based on *fit*, while also considering *appropriateness* and *interpretability*.

These examples demonstrate that, when relying on a mix of theoretical and empirical justification to create a candidate set and select a nonlinear model, the weight placed on theory vs. empirical evidence may vary notably. Anthony and Ogg (2020) relied solely on past findings to arrive at a small set of candidate models, whereas McNeish and Dumas (2017) relied largely on graphical evidence to create a candidate set. The prior process is more representative of a confirmatory approach, whereas the latter process is more representative of an exploratory approach to model selection.

When employing a mixed approach to nonlinear model selection, there is little consensus regarding how to prioritize theory vs. empirical evidence. Although Cudeck and Harring (2007) note that “graphical displays are irreplaceable in judging whether a function is appropriate” (p. 625) and suggest plotting sample data alongside each curve in the candidate set, they also strongly encourage prioritizing *appropriateness* and *interpretability* when selecting a nonlinear model. Other methodologists have more firmly argued that better model-theory connections are the primary benefit afforded by nonlinear models, and therefore should be the primary motivation for their use, as opposed to better model-data fit (e.g., Preacher & Hancock, 2015; Ram & Grimm, 2007). Additionally, arguments in favor of a confirmatory approach would suggest that *any* reliance on sample data to select a model would compromise the *a priori* quality that theories and hypotheses should possess. Ultimately, the weight placed on theory vs. empirical evidence may be determined by (1) the availability of theory and prior findings to inform expectations about the shape of the curve, and (2) the researcher’s willingness to rely on sample data to inform model choice.

In summary, the mixed approach enables the researcher to choose a nonlinear model that is substantively useful, while also integrating empirical evidence regarding model-data fit. Therefore, this approach enables the incorporation of the *appropriateness*, *interpretability*, and *fit* criteria, and the researcher may strike whatever balance of the three that is warranted. Somewhere in the process of creating the candidate model set and/or selecting the “best” model, theory and interpretation are considered, which greatly increases the likelihood of selecting a substantively useful model. However, there are also disadvantages to this approach. First, conclusions may be the result of capitalizations on chance or overfitting to the sample data. Second, many classic model selection indices and indicators of model performance are unreliable when applied to nonlinear models, which will be discussed further in the next section.

### **Data-Driven Approach**

When taking a data-driven approach to choosing a nonlinear model, the researcher typically defines a large pool of candidate models and relies heavily on model selection criteria and/or goodness-of-fit statistics to choose the “best” model from among the candidates. To preface this discussion, I note that the candidate pool may include nonparametric or semiparametric models; however, the scope of this dissertation is restricted to parametric models. Therefore, this section will focus on parametric models, used in scenarios where little-to-no theory or prior knowledge is considered throughout the process of creating the candidate pool and choosing the “best” model. For example, in many applications, researchers compare the fit of a diverse array of conceptually distinct parametric models, including linear, quadratic, cubic, piecewise linear, sigmoidal, and exponential, and choose the “best” model based on selection criteria and/or goodness-of-fit statistics (e.g., Darchia et al., 2022; Ricker et al., 2018; Womack

et al., 2022; Wright et al., 2014). Most of the arguments presented in this section would also apply if nonparametric and/or semiparametric models were included in the candidate pool, but nonparametric and semiparametric models suffer from the additional drawback of uninterpretable parameters.

Choosing a nonlinear model based on empirical evidence constitutes an exploratory, rather than confirmatory, approach. Typically, when there is sufficient theory to inform expectations about the patterns that will be observed, a confirmatory approach can be taken such that a formal theory may be articulated and a corresponding model may be chosen before the data are analyzed or even collected (Haslbeck et al., 2022). In contrast, the data-driven approach largely eliminates the need for the researcher to enumerate theory-driven hypotheses in an *a priori* manner. Relatedly, the nonlinear model that fits best to the data may not make sense conceptually, so the *appropriateness* and *interpretability* criteria may easily be unmet. Of course, it is important that the chosen nonlinear model corresponds reasonably well with the observed data, consistent with the *fit* criterion, but meeting the *fit* criterion without meeting the *appropriateness* and *interpretability* criteria is likely to result in a model that is not very useful (Archontoulis & Miguez, 2015; Cudeck & Harring, 2010; Grimm et al., 2011).

In addition to the conceptual and theoretical issues that may easily arise, another drawback of the data-driven approach is that empirical indicators of model performance (most of which were developed for linear models) often do not perform well when applied to nonlinear models. For example, sole use of empirical model selection criteria is not always a reliable way to select the best nonlinear model for the data at hand. Information criteria like AIC and BIC balance goodness-of-fit to the data with model complexity, which is accounted for by the number of estimated parameters in the model; however, especially for nonlinear models, the number of

model parameters does not always reflect the complexity of the functional form (Preacher & Yaremych, 2023). Therefore, model selection criteria may not perform optimally when applied to nonlinear models.

Three studies have systematically investigated the performance of model selection criteria for choosing a nonlinear model, and all have observed that AIC and BIC are fallible under many realistic data conditions. In a study of model selection criteria for NLME models, Christensen (2019) found that AIC, AICC, BIC, CAIC, and HQIC became less likely to correctly select the nonlinear data-generating model when the “distinctiveness” of the curve was lower. For example, when the data-generating function was logistic, but the distinctiveness of that logistic curve was low, correct selection rates were no higher than 3% across all data conditions. Rohloff et al. (2022) found that information criteria including AIC and BIC were susceptible to overfitting (i.e., choosing a nonlinear model that was more complex than the data-generating function) when sample size was small and residual variance of  $y$  was large. Wood et al. (2015) found that BIC was less likely to correctly identify the data-generating nonlinear model when measurement reliability was low and sample size was small. Overall, sole reliance on model selection criteria may not always result in the “best” model choice, as their performance is highly variable based on characteristics of the nonlinear model and the data.

Other metrics that are often used to select and compare models are  $R^2$  and adjusted  $R^2$ . However, it has been repeatedly argued that these are poor indicators of performance for nonlinear models (Archontoulis & Miguez, 2015; Ratkowsky, 1990; Wallach, 2006).  $R^2$  is informed by the total sum of squares ( $y$ 's deviations from its mean) and the regression sum of squares ( $y$ 's deviations from the regression line). Therefore,  $R^2$  effectively compares the intercept-only model to the regression model, and it is assumed that the intercept-only model is

nested within the regression model. It follows that  $R^2$  makes sense only for models that involve a constant or intercept term. Nonlinear models frequently do not contain an intercept term, so the logic of  $R^2$  does not apply to these nonlinear models, leading to conclusions that “ $R^2$  does not have any obvious meaning for a nonlinear regression model” (Ratkowsky, 1990, p. 44).

Although adjusted  $R^2$  attempts to account for model complexity by incorporating the number of parameters in the model, this is not always indicative of functional form complexity for nonlinear models, and the same logical issues arise. In summary, reliance on  $R^2$  or adjusted  $R^2$  for selecting a nonlinear model is unlikely to be a meaningful or useful approach.

Another data-driven way to choose from among a set of candidate nonlinear models is to graph each function with the observed data, then visually inspect how well each model follows the data. Cudeck and Haring (2007) recommend this approach over the use of model selection criteria. However, this approach may be difficult in the presence of “messy” data that do not follow any curve closely. In social science, it is common to observe high residual variance, such that much of the variability in  $y$  is left unexplained by the chosen model (Rohloff et al., 2022). In these cases, visual inspection will usually not yield a clear conclusion about which model best characterizes the data. This approach also suffers from the same drawbacks as model selection criteria, namely, a lack of emphasis on the researcher’s prior knowledge and theory.

Despite the drawbacks discussed here, some methodologists have argued in favor of a data-driven approach to model selection. For example, Wood et al. (2015) encourage comparing broad “classes” of statistical models, including linear, latent basis, and parametric nonlinear, then selecting from among the classes based on empirical values like BIC. These authors argue that an exploratory approach does *more* to inform the research area (compared to a confirmatory approach) by addressing whether alternative explanations underlying the data are plausible, and



by potentially identifying better-fitting models to pursue in future research. To counter the argument that a data-driven model selection process risks overcapitalization on chance, the authors posit that identifying unexpected patterns is how psychological theory moves forward. At the same time, most methodologists to have addressed this topic argue in favor of prioritizing *appropriateness* and *interpretability*, or at least balancing them with considerations of *fit*.

In summary, due to conceptual issues and the fallibility of empirical model selection indices, taking a solely data-driven approach to model selection may easily lead to a model choice that is not theoretically motivated. By instead drawing on past findings, theory, and substantive expectations – even to narrow down the candidate set to models that are conceptually appropriate – the chosen model is much more likely to facilitate meaningful theory testing. Therefore, I argue that it is preferable to choose a nonlinear model in a way that at least somewhat, but preferably fully, relies on theory.

### **Choosing a Parameterization**

#### **Identifying Substantively Important Attributes of the Curve**

Choosing a useful parameterization is essential for meeting the *interpretability* criterion. The central goal of parameterization is for the chosen model to contain parameters that correspond with the most substantively meaningful and theoretically important attributes of the curve (Cudeck & Harring, 2007; Ram & Grimm, 2007). Therefore, the ideal parameterization of a given nonlinear function is likely specific to a particular research context and/or a particular study. Preacher and Hancock (2012, 2015) note there are many reasons why it is ideal for the most important attributes of the curve to correspond directly with a model parameter. First, it is

often easier to directly estimate the quantity of interest as part of the model, rather than via post hoc calculations. Second, an estimated parameter yields both point and interval estimates, which allow us to test hypotheses (via significance tests) and determine how precisely these key quantities have been estimated. Third, in NLME models, parameters can be treated as random to reflect expected interindividual differences in certain attributes of the curve. Fourth, any parameter can be constrained to a constant if this makes conceptual sense for the corresponding attribute of the curve.

The final benefit of useful parameterization is that moderators can be incorporated directly for each parameter, which allows the researcher to identify whether the corresponding attribute of the curve varies according to any relevant variable. Preacher and Hancock (2015) argue this to be the most important benefit. Cudeck and Harring (2010) note that when moderation is incorporated, the moderated parameter essentially becomes a dependent variable that is predicted by the moderator (more on this in the following section); therefore, in order for the moderation to be interpretable, it is essential for the parameter to have a clear definition.

Any nonlinear model can be parameterized in an infinite number of ways. The process of translating a given model from one parameterization to another is called *reparameterization*. The mathematical details of reparameterization are beyond the scope of this dissertation, but steps for carrying out this process are described by Preacher and Hancock (2012, 2015). The general process involves (1) isolating the "target aspect" of the curve, (2) expressing it in terms of other model parameters, (3) substituting that expression back into the original equation, and (4) simplifying. This process may involve simple algebra or calculus. Ultimately, deciding which attributes of the curve are most substantively important will require critical thought from the researcher (Grimm et al., 2011). Here, my goal is to catalyze this process by providing examples

of useful reparameterizations. These examples demonstrate the flexibility of reparameterization, as well as the diverse hypotheses that can be tested via thoughtfully reparameterized models.

For instance, in longitudinal applications, recent methodological work has focused on reparameterizations that enable the researcher to determine the specific time (i.e., location along the  $x$ -axis) at which a certain criterion (i.e.,  $y$ -value) is reached. In one example, Johnson and Hancock (2019) reparameterized the MM model such that it contains a *time-to-criterion* (T2C) parameter. The T2C is a flexible parameter that indicates the location along the  $x$ -axis at which any criterion  $y$ -value is reached. The criterion  $y$ -value is pre-specified by the researcher, and is flexible according to the research context; it could be set to a certain test score that indicates competency, or a certain level of performance on an experimental task.

In a similar example, Choi et al. (2009) implemented a logistic model and derived parameters that they referred to as *jerk points*, which are the locations along the  $x$ -axis that demarcate the asymptotes from the surge area in a sigmoidal curve. Indeed, the  $x$ -locations at which change begins and ends are often substantively important in many areas of social science, including learning and development. McNeish et al. (2023) note that “researchers often are not only interested in the ultimate level that people reach but also in how fast they get there” (p. 402). Reparameterizing a nonlinear model – particularly a sigmoidal model – is one approach to estimating such key quantities.

Thinking about reparameterizations in an alternative way, McCormick (2023) notes that there may be contexts in which it is useful to reparameterize a model such that a parameter corresponds to the value of  $y$  at a theoretically important value of  $x$ . As examples of this type of research question, the author cites the number of words acquired by 20 months of age (Huttenlocher et al., 1991) and levels of drug/alcohol use upon entry to a university (Derefinko et

al., 2016). The chosen value of  $x$  may reflect a developmental milestone or a timepoint that is otherwise meaningful. In a similar example, Preacher and Hancock (2012) reparameterized a Jenss-Bayley model that tracked infant weight ( $y$ -axis) over the course of zero to two years of age ( $x$ -axis). Here, they created a parameter that corresponded to model-implied weight at any chosen  $x$ -value. This parameter enabled the authors to estimate and examine individual differences in weight at any timepoint throughout the trajectory.

In summary, even if previously nonexistent, it is possible to create a parameterization of any nonlinear model such that the most important attributes of the curve -- for a given study -- are each represented by a unique parameter. In some applications, important attributes of the curve may correspond with  $x$ -values at which a certain level of  $y$  is reached,  $y$ -values at important locations along the  $x$ -axis, and/or locations along the  $x$ -axis at which change begins and ends. However, many more attributes of the curve can be isolated and estimated via reparameterization. There is great flexibility in this regard, and researchers need not remain confined to parameterizations that have been used in previous research.

### **Implementing Constraints**

Another aspect of parameterization is deciding whether certain parameters should be constrained. In some contexts, it may be appropriate to constrain a parameter to a constant (e.g., zero), meaning the parameter is not estimated at all. Constraining a parameter implies that the corresponding attribute of the curve is “known and common” to all individuals (Choi et al., 2009). Parameter constraints are often intuitive and arise from knowledge of the variables under study. For example, Marceau and colleagues (2011, 2015) used NLME logistic models to approximate pubertal development, wherein the lower asymptote was constrained for all

individuals (as the minimum score on the pubertal developmental scale) and the upper asymptote was constrained for all individuals (as the maximum score on the pubertal development scale). It is often reasonable to constrain lower and/or upper asymptotes if the y-variable under study has a known minimum or maximum that is expected to be realized for all individuals. If a parameter is constrained to a constant, it does not need to be estimated, which simplifies the model and facilitates convergence.

### **Special Considerations for NLME Models**

In NLME models, additional constraints must be considered, as the researcher must decide whether each parameter should be treated as random (i.e., variable across individuals) or fixed (i.e., the same for all individuals). This is an important decision, because inaccurate specification of the random effects can lead to biased standard errors of the fixed effect estimates (Cho et al., 2022; McNeish & Bauer, 2022). There are a variety of approaches that have been recommended for choosing which parameters to treat as random vs. fixed. Ideally, the decision would be made on substantive grounds. If interindividual variability is theoretically expected for certain attributes of the curve, then the corresponding parameters should be specified as random (Cudeck, 1996; Grimm et al., 2011; Grimm & Ram, 2009; McNeish & Bauer, 2022; Preacher & Hancock, 2012).

In the absence of substantive justification for treating parameters as random vs. fixed, one popular approach is to begin with a “maximal” random effects structure – which typically means specifying all parameters as random – and then progressively removing random terms if the model does not converge (e.g., McNeish et al., 2020; McNeish & Bauer, 2022; Pinheiro & Bates, 2000). However, the optimal order by which to remove random terms is often unclear

(McCormick et al., 2023). Several approaches have been suggested by methodologists. Haring and Blozis (2014) note that convergence problems are most often caused by random coefficients that enter the model nonlinearly (e.g., parameters that appear within exponents), rather than random coefficients that enter the model linearly (e.g., parameters that appear outside of fractions and exponents). Therefore, if a model with maximal random effects does not converge, a straightforward approach is to locate the parameters that enter the function nonlinearly and treat them as fixed. Alternatively, removal of random effects could be based on substantive justification. If the interindividual variability of a certain parameter is of great theoretical or practical importance, then the random effects associated with the less substantively important parameters could be removed first (e.g., McNeish et al., 2020). Although the top-down approach remains popular in practice, McNeish and Bauer (2022) note that constraining a parameter to be fixed due to convergence difficulties – rather than the expectation that there is no interindividual variability in that parameter – is neither substantively justified nor desirable.

Other, largely data-driven, approaches to choosing a random effects structure have also been proposed. For example, Feng et al. (2019) suggest the use of nested model comparisons like the likelihood ratio test (LRT) to decide on a random effects structure; in addition to LRTs, Cho et al. (2022) recommend comparing goodness-of-fit criteria like RMSE, AIC, and BIC.

Graphical approaches, such as plotting the curve separately for each individual to inspect which attributes may differ across persons, have also been illustrated (e.g., Cho et al., 2022; Pinheiro & Bates, 2000). In summary, the degree to which the researcher relies on theory vs. empirical evidence may vary widely when specifying a random effects structure for a NLME model. Like other aspects of model parameterization, it is ideal to rely primarily on theory when specifying

this piece of the NLME model. Regardless of the chosen justification for the inclusion vs. removal of random terms, it is ideal to be transparent about how these decisions were made.

### **Incorporating Moderators**

In social science, tests for moderation are often regarded as the most useful step of the entire modeling process. Moderation analysis has been described as “the very heart of theory testing in the social sciences” (Cohen et al., 2003, p. 255), as it enables us to assess where, when, and for whom certain processes and relations may occur (Hayes & Preacher, 2013). In the context of nonlinear models, Choi et al. (2009) note that knowledge about moderation is “invaluable” in determining for whom an intervention might be most useful or when it should be implemented. Similarly, Cudeck and Harring (2010) argue that “the search for effective covariates is in many ways the most valuable part of a successful application.” Therefore, it is important to approach the incorporation of moderators with intentionality. The goal of this section is to describe different approaches by which moderators may be incorporated into nonlinear models, as well as the benefits and drawbacks of each approach.

When incorporating moderation into nonlinear models, interesting conceptual considerations arise that are not applicable to the linear framework. In a nonlinear model, parameters may correspond with many attributes of the curve. Any of these parameters – and relatedly, any attribute of the curve – may be hypothesized to be moderated. Therefore, in nonlinear models we can think of moderation much more broadly than we do in the linear framework. In linear models, the *linear effect of the focal predictor* is typically hypothesized to change at a fixed rate across different values of the moderator. In nonlinear models, *any attribute of the curve corresponding to a model parameter* may be hypothesized to change across different

values of the moderator. Because such a large variety of curve attributes may be moderated, it becomes important to carefully consider the rationale for either including or excluding a moderator of each parameter. Next, I will review two opposing approaches that may be taken when deciding how to specify a moderated nonlinear model, which I will term the *omnibus approach* and the *selective approach*.

### **Omnibus Approach**

When implementing the omnibus approach, if a variable is expected to moderate *any* model parameter, then it is included as a moderator of *all* model parameters. For example, consider a four-parameter Gompertz model (Eq. 2.2) where time is on the  $x$ -axis and reading skills are on the  $y$ -axis. Suppose that we have created a reading intervention. We hypothesize that the intervention will moderate parameter  $d$  (the timing of most rapid growth) and parameter  $b$  (total growth); for children who receive the intervention, the most rapid reading improvement will occur earlier and total reading improvement will be greater. According to the omnibus approach, we should also incorporate our intervention as a moderator of the other two model parameters, which govern the lower asymptote and rate of learning, even though we have no theoretical basis to expect that the intervention will moderate these attributes of the trajectory.

Under the omnibus approach, our model will be:

$$y = (a_0 + a_1Int) + (b_0 + b_1Int) * \left( \exp \left( -\exp \left( -(c_0 + c_1Int)(x - (d_0 + d_1Int)) \right) \right) \right) + \varepsilon, \quad (4.1)$$

where parameter  $a$  has been replaced with  $(a_0 + a_1Int)$ , parameter  $b$  has been replaced with

$(b_0 + b_1Int)$ , and so on. This equation reflects that each parameter is linearly moderated by  $Int$ .

The most substantively important parameters are highlighted in red:  $b_1$  is the effect of  $Int$  on total growth, and  $d_1$  is the effect of  $Int$  on the time of fastest growth.



The omnibus approach is consistent with how moderators are incorporated in linear regression. Consider a simple linear regression equation with focal predictor  $x$ :

$$y = \gamma_0 + \gamma_1 x + \varepsilon. \quad (4.2)$$

When we incorporate a moderator  $z$  into Eq. 4.2, this is represented by an interaction term involving  $xz$ . However, it is standard practice to also include the “main effect” of the moderator:

$$y = \gamma_0 + \gamma_1 x + \gamma_2 z + \gamma_3 xz + \varepsilon. \quad (4.3)$$

Inclusion of the “main effect” of  $z$  means that, in addition to the linear effect of  $x$  being moderated, the intercept is also moderated. Rearranging Eq. 4.3, we see that both the slope of  $x$  and the intercept change linearly as a function of  $z$ :

$$y = (\gamma_0 + \gamma_2 z) + (\gamma_1 + \gamma_3 z)x + \varepsilon. \quad (4.4)$$

Therefore, all attributes of the line are moderated by  $z$ , even though in many cases, moderation of the linear effect of  $x$  is the theoretically motivated component of the model.

The omnibus approach is common in linear regression because it is backed by strong methodological support. If the  $x$  and  $z$  terms were omitted from Eq. 4.3 and only the interaction term was included, then any first-order effects of  $x$  and  $z$  that were correlated with the  $xz$  term would be incorrectly attributed to the interaction (Cohen et al., 2003). The same principle applies in more complicated linear models involving moderation; for example, when three-way interactions are involved, methodologists strongly recommended that all lower-order interactions also be included in the model (Aiken & West, 1991; Cohen, 1978; Cohen et al., 2003). Including all lower-order terms serves to linearly partial out the lower-order effects from the interaction; therefore, the interaction term accounts for variance in  $y$  that is above and beyond any variance in  $y$  that is accounted for by the lower-order terms, yielding an interpretable interaction effect.

Social science methodologists have argued that when an interaction term is included, it is acceptable to omit lower-order terms from the model *only if* there is strong theory that dictates the effects of the lower-order terms must be zero (Aiken & West, 1991; Fisher, 1988; Kmenta, 1986). Indeed, omitting the main effect of  $z$  from Eq. 4.3 imposes the assumption that the main effect of  $z$  ( $\gamma_2$ ) is zero. Put another way, omitting the main effect of  $z$  means we assume that the intercept is not moderated by  $z$ . Therefore, if the intercept is moderated by  $z$  even slightly, then the model is misspecified, and that effect will be incorrectly absorbed by the effect of the interaction term ( $\gamma_3$ ). To avoid this potential misspecification, it is recommended to always include lower-order terms, consistent with the omnibus approach.

Similar arguments could be made in favor of the omnibus approach for nonlinear models involving moderation. Returning to our earlier example, we suspect that parameters  $b$  and  $d$  of the Gompertz model are moderated by our intervention. However, it is certainly possible that the intervention will also – at least slightly – moderate parameters  $a$  and  $c$  of the model, even if the intervention was not designed for this purpose. Including the intervention as a moderator of all model parameters, as shown in Eq. 4.1, accounts for this possibility. Therefore, if the intervention incidentally moderates any unexpected attributes of the curve, the model will not be misspecified. This is a major advantage of the omnibus approach.

In linear regression, the benefits of the omnibus approach far outweigh the costs. OLS regression estimates are obtained from closed-form solutions; iterative estimation is not necessary and convergence problems almost never arise, regardless of the complexity of the model. Therefore, the computational burden of including multiple lower-order terms is nearly nonexistent. Even if the omnibus approach yields a model that is more complex than necessary (e.g., some lower-order terms *could* have been omitted but were not), this is of little consequence

in linear regression. The primary consequence of an overly complex model is likely to be interpretational difficulties (Cohen et al., 2003). However, in nonlinear models involving moderation, potential costs of the omnibus approach are much more salient. Nonlinear model estimates are obtained iteratively, meaning that convergence problems arise frequently. Convergence becomes less likely when models are too complex (Bates & Watts, 1988; Gallant, 1987; Pinheiro & Bates, 2000; Sit & Poulin-Costello, 1994; Ratkowsky, 1990). Therefore, the omnibus approach may easily result in a nonlinear model wherein the number of parameters makes estimation unfeasible, which is a major disadvantage.

### Selective Approach

Given the drawbacks of the omnibus approach for nonlinear models, it may be useful to consider taking a *selective approach* to adding moderators. Using the selective approach, the model is specified such that the moderator influences *only* the parameters for which there is theoretical reason to expect moderation. Returning to our Gompertz example, our intervention was designed to moderate parameters  $b$  and  $d$ . Therefore, we would specify our model as:

$$y = a + (b_0 + b_1 Int) * \left( \exp \left( -\exp \left( -c(x - (d_0 + d_1 Int)) \right) \right) \right) + \varepsilon, \quad (4.5)$$

where  $Int$  moderates only parameters  $b$  and  $d$ .

The selective approach does not correspond with how moderators are incorporated in linear regression. Indeed, there are important drawbacks to the model given in Eq. 4.5, which arise from imposing the assumption that the effect of  $Int$  on parameters  $a$  and  $c$  is zero. First, this implies that any interindividual differences in parameters  $a$  and  $c$  should be considered error, which is a strong and potentially unrealistic assumption (Ram & Grimm, 2007). Second, if  $Int$  incidentally moderates parameters  $a$  or  $c$ , even though this is not hypothesized or expected, then

the model will be misspecified and estimates may be biased. Akin to the problems that arise in moderated linear models without lower-order terms, the unspecified moderation of parameters  $a$  or  $c$  may be incorrectly absorbed by the moderation terms involving parameters  $b$  and  $d$ , leading to erroneous conclusions.

There are also important advantages to the selective approach. First, and perhaps most importantly, the selective approach facilitates fully theoretically-motivated model specification. The Gompertz model in Eq. 4.1 – created according to the omnibus approach – does not accurately reflect our expectations grounded in substantive expertise. In contrast, the model in Eq. 4.5 – created according to the selective approach – closely aligns with our hypotheses regarding the intervention and how it will affect reading development. The selective approach enables us to articulate precisely which aspects of the curve we hypothesize to be moderated, and to then specify the model such that only those hypotheses are tested with our analysis. Therefore, the selective approach is likely to result in a more substantively justified model, as opposed to the omnibus approach. Second, compared to the omnibus approach, the selective approach facilitates specification of a more parsimonious model. With fewer parameters to be estimated, convergence of the nonlinear model becomes more likely.

## **Summary**

When specifying a moderated nonlinear model, interesting conceptual and logistical considerations arise that are unique to the nonlinear framework. Many attributes of the curve may be moderated, necessitating careful consideration about how the moderation of each parameter may map onto theory, and convergence failures become a salient issue, necessitating

intentional inclusion and/or exclusion of moderators. Here, I presented two potential avenues for incorporating moderators, termed the omnibus and selective approaches.

At present, it is unclear whether the omnibus or selective approach is the better way to incorporate moderators into a nonlinear model. Simulation studies may be helpful for developing methodological recommendations about which approach is optimal, and whether the optimal approach may differ according to study context and data conditions. For example, if a researcher implements the selective approach and an important moderator is omitted, what are the consequences of that omission? Are estimates biased, and if so, what is the magnitude of that bias? Which parameter estimates tend to be biased? Do results change depending on the magnitude of the omitted moderation effect, the functional form of the curve, and/or sample size? Similarly, if the researcher implements the omnibus approach and creates a model that is more complex than necessary (i.e., is more complex than the data-generating function), how is the likelihood of convergence affected? Do results change depending on the functional form and/or sample size? These questions will be interesting avenues for future research.

### **Incorporating Covariates**

A final conceptual issue to address is the incorporation of covariates or control variables. This aspect of model specification has received little attention in the broader nonlinear modeling literature, as it is largely unique to social science. As an example, for nonlinear models fit to data from controlled experiments in the biological or plant sciences, the incorporation of covariates is not typically necessary. In social science applications, it is typical to control for the effects of many covariates in an effort to isolate the effect of the focal predictor (e.g., controlling for child

age, gender, and SES while testing for the effect of an educational intervention). This section expands on the specification of nonlinear models involving covariates.

When thinking about how to incorporate covariates, it is again helpful to reference the process that is followed within the linear framework. Begin with a simple linear regression model, containing a focal predictor  $x$  and three covariates  $w_1 - w_3$ :

$$y = \gamma_0 + \gamma_1 x + \gamma_2 w_1 + \gamma_3 w_2 + \gamma_4 w_3 + \varepsilon. \quad (4.6)$$

Rearranging this equation illuminates that in fact, covariates are moderators of the intercept. The intercept changes linearly as a function of each covariate:

$$y = (\gamma_0 + \gamma_2 w_1 + \gamma_3 w_2 + \gamma_4 w_3) + \gamma_1 x + \varepsilon. \quad (4.7)$$

Therefore, in linear regression, we can think of covariates as additional moderators (i.e., predictors) of the intercept. By including covariates in this way, the estimated slope of the focal predictor is above and beyond the effects of the covariates (Cohen et al., 2003). Therefore, the inclusion of covariates as moderators of the intercept effectively “controls for” their effects.

Can this approach to incorporating covariates – i.e., including covariates as moderators of  $y$ 's intercept – be extended to nonlinear models? In most cases, it appears not. A variety of problems would follow from this approach. First, nonlinear models often do not contain a parameter that corresponds directly to the  $y$ -intercept. Therefore, incorporation of an intercept moderator is not always possible (unless the researcher is willing to reparameterize the model such that it contains an intercept parameter). Second, even if it is possible to directly incorporate a moderator of the intercept, the intercept parameter (and/or moderation of it) may not be substantively useful or important. Third, it is unclear whether including a covariate as a moderator of the intercept would constitute “controlling for it” in the sense familiar from the

linear framework; in multiple linear regression, the effects of the predictors can be neatly partialled out from one another, whereas this is not necessarily the case for nonlinear regression.

Alternatively, it may be tempting to alter a nonlinear model by adding a new linear term for each covariate; this approach would mimic the model specification process followed within the linear framework. For example, consider the cosine model (Eq. 2.9), which has no parameter for the  $y$ -intercept. Adding a linear term for each of three covariates,  $w_1 - w_3$ , would yield:

$$y = a * \sin\left(\frac{2\pi}{b}(x - c)\right) + f_1 w_1 + f_2 w_2 + f_3 w_3 + \varepsilon, \quad (4.8)$$

where  $f_1 - f_3$  are linear effects of the covariates  $w_1 - w_3$ . This approach is also problematic. First, it adds parameters to the model that were not there before, which fundamentally alters the shape of the curve. Second, it constrains the covariates' effects on all other parameters to be zero, implying there is theoretical reason to believe that each covariate exerts *only* a linear effect on the outcome variable. In summary, familiar approaches to incorporating covariates – though commonplace in linear modeling – are likely to create problems if applied to nonlinear models.

To successfully incorporate covariates into a nonlinear model, the model should reflect that we expect the covariates to have some influence over the shape of the curve. The curve has – ideally – been selected *a priori*, so inclusion of covariates should not fundamentally alter the functional form. For example, the inclusion of a covariate should not cause the curve to change from exponential to sigmoidal, or to change from a sine wave to a linearly increasing sine wave. To avoid fundamentally altering the functional form, we should include covariates as predictors of the original model parameters, rather than introducing new terms containing the covariates as we do in linear regression. The original model parameters (e.g., in Eq. 4.8, parameters  $a$ ,  $b$ , and  $c$ ) govern all the theoretically important attributes of the curve, so if a covariate has any notable influence over the curve, it should be realized in its effect on each of those model parameters.

As an example, Cameron et al. (2015) fit Gompertz models that approximated growth of reading and math skills over time. Gender, parental education, family SES, and race/ethnicity were included as covariates for each model parameter. This model specification was:

$$y = (a_0 + a_1 \textit{Gender} + a_2 \textit{ParentalEd} + a_3 \textit{SES} + a_4 \textit{Race}) + (b_0 + b_1 \textit{Gender} + b_2 \textit{ParentalEd} + b_3 \textit{SES} + b_4 \textit{Race}) * \exp\left(-\exp\left(-(c_0 + c_1 \textit{Gender} + c_2 \textit{ParentalEd} + c_3 \textit{SES} + c_4 \textit{Race})(x - (d_0 + d_1 \textit{Gender} + d_2 \textit{ParentalEd} + d_3 \textit{SES} + d_4 \textit{Race}))\right)\right) + \varepsilon, \quad (4.9)$$

where  $a_0$  is the value of parameter  $a$  when all covariates are zero,  $a_1$  is the linear effect of *Gender* on parameter  $a$ ,  $a_2$  is the linear effect of *ParentalEd* on parameter  $a$ ,  $a_3$  is the linear effect of *SES* on parameter  $a$ , and  $a_4$  is the linear effect of *Race* on parameter  $a$ . Other parameters are interpreted analogously. This model specification ensures that the effect of each variable on each parameter is above and beyond the effects of the other variables, effectively isolating the influence of each predictor on each attribute of the curve.

Eq. 4.9 shows that mathematically, moderators and covariates are the same in nonlinear models. Therefore, the distinction between “moderators” and “covariates” is purely substantive. Whether a variable is considered a moderator or a covariate may depend on whether its influence on the shape of the curve is theoretically important or not. Additionally, this means that when we incorporate covariates into a nonlinear model, we may again make use of either the omnibus approach or the selective approach.

Following the omnibus approach, if we expect a covariate to affect *any* model parameter, then we include it as a predictor of *all* model parameters. While this approach enables us to avoid potential model misspecifications, it can quickly yield a very complex model – especially if there are multiple covariates – that makes estimation infeasible. In contrast, the selective approach



requires the researcher to consider whether theory suggests the covariate will influence some attributes of the curve but not others. This approach is likely to yield a theoretically well-justified model, but risks misspecification and bias if an important effect of a covariate is omitted. Finally, if the model contains “focal” or theoretically important moderators, we may opt for neither of the above approaches, and instead incorporate covariates as additional predictors of any parameters that are already predicted by a “focal” moderator. This approach will ensure that the effects of any focal moderators are above and beyond the effects of any control variables that also influence certain attributes of the curve. Again, it is unclear which of these approaches to incorporating covariates is “optimal,” and whether the optimal approach may change depending on the data, the model, and/or the research context.

### **Moderators and Covariates in NLME Models**

Nonlinear mixed-effects (NLME) models present unique conceptual challenges regarding the incorporation of moderators and covariates. It is often of key substantive importance to introduce moderators to explain interindividual variation in the growth trajectory. The general process of NLME modeling is to first determine which attributes of the curve vary across people (i.e., which parameters should be treated as random), and then incorporate moderators to explain that variation (Blozis & Harring, 2021; Cudeck & Harring, 2007, 2010; Davidian & Giltinan, 2003; Harring & Blozis, 2014). As a special case, Pinheiro and Bates (2000) note that the inclusion of moderator(s) can occasionally cause the variance of a random coefficient to drop so low that it can instead be treated as fixed; in these cases, all between-person variation is explained by the moderator(s).

As a reminder, in NLME growth models, variables may exist at level 1 or level 2. Level-1 variables change across timepoints or assessments, whereas level-2 variables are static and describe person-level characteristics. Level-1 variables are sometimes termed time-varying covariates (TVCs), and level-2 variables are sometimes termed time-invariant covariates (TICs).

Generally, when moderators are included in NLME models, they are level-2 variables (Blozis & Harring, 2021; Cudeck & Harring 2007, 2010; Davidian & Giltinan, 2003; Harring et al., 2012). In NLME models, the goal of including moderators is to explain across-person variability in the random coefficients, and this is best accomplished with predictors that change across (rather than within) persons. Therefore, the inclusion of level-2 moderators in NLME models has received much attention in the methodological literature. In terms of model specification, adding level-2 moderators to a NLME model closely resembles the process of adding moderators to a single-level nonlinear model, such that moderators are included as predictors of the moderated parameter.

As an example, consider a NLME Gompertz model that characterizes repeated measurements of math ability among elementary-aged children. Treating all four parameters as random, our model specification is:

$$y_{ti} = a_i + b_i * (\exp(-\exp(-c_i(t - d_i)))) + e_{ti}, \quad (4.10)$$

where

$$a_i = a_{00} + aResid_i,$$

$$b_i = b_{00} + bResid_i,$$

$$c_i = c_{00} + cResid_i,$$

$$d_i = d_{00} + dResid_i.$$

We can add moderators to Eq. 4.10 by including person-level variables as predictors of each person-specific coefficient. In this way, we explain interindividual variation in the coefficients.

Adding *Gender* and *SES* as covariates, we obtain:

$$y_{ti} = a_i + b_i * (\exp(-\exp(-c_i(t - d_i)))) + e_{ti}, \quad (4.11)$$

where

$$a_i = a_{00} + a_{01}Gender_i + a_{02}SES_i + aResid_i,$$

$$b_i = b_{00} + b_{01}Gender_i + b_{02}SES_i + bResid_i,$$

$$c_i = c_{00} + c_{01}Gender_i + c_{02}SES_i + cResid_i,$$

$$d_i = d_{00} + d_{01}Gender_i + d_{02}SES_i + dResid_i.$$

Here, each individual-specific coefficient is now predicted by that individual's gender and socioeconomic status. Coefficient  $a_{00}$  is now interpreted as the mean value of  $a$  among children with  $Gender = 0$  and  $SES = 0$ . Coefficient  $a_{01}$  is the effect of *Gender* on  $a$ , and coefficient  $a_{02}$  is the effect of *SES* on  $a$ . Finally, the random component  $aResid_i$  is interpreted as individual  $i$ 's conditional residual, or in other words, their remaining deviation from the mean value of  $a$  after accounting for the effects of *Gender* and *SES*. The coefficients for the other parameters are interpreted analogously. In summary, both mathematically and conceptually, moderation in NLME models is similar to moderation in single-level nonlinear models.

In addition to incorporating moderators, it is also common to incorporate covariates into NLME models. Here, level-1 variables (TVCs) become more relevant, as both TVCs and TICs are often useful to include. Adding TICs is straightforward because level-2 covariates are mathematically the same as level-2 moderators. TICs are simply included as additional predictors of the person-specific coefficients. Therefore, the distinction between a level-2 moderator and a TIC is purely conceptual.

TVCs are often mentioned on a conceptual level in discussions of NLME growth models. For example, Blozis and Harring (2021) note: “A response may be assumed to follow a function that relies only on time, or the function may additionally include covariates such as time-varying covariates in which a response is assumed to be due to time along with variables that also change with time” (p. 541). However, there is sparse information regarding how to specify a NLME model involving TVCs. The incorporation of TVCs into NLME models is a more complex issue than for linear mixed models, where TVCs are simply added as additional level-1 predictors of the outcome (Grimm et al., 2016); for reasons outlined earlier, this approach is nonsensical for NLME models.

Davidian and Giltinan (1995, 2003) and Pinheiro and Bates (2000) have briefly addressed TVC specification for NLME models. These authors suggest that TVCs should be incorporated into the model in the same way that TICs are incorporated: as additional predictors of the person-specific coefficient. If the coefficient is predicted by both a TIC and a TVC, then the coefficient is both person-specific and time-specific. For example, let us add a TVC, executive function, as a predictor of parameter  $c$  in Eq. 4.11. According to Pinheiro and Bates (2000) and Davidian and Giltinan (1995; 2003), our model specification would be:

$$y_{ti} = a_i + b_i * (\exp(-\exp(-c_{ti}(t - d_i)))) + e_{ti}, \quad (4.12)$$

where

$$a_i = a_{00} + a_{01}Gender_i + a_{02}SES_i + aResid_i,$$

$$b_i = b_{00} + b_{01}Gender_i + b_{02}SES_i + bResid_i,$$

$$c_{ti} = c_{00} + c_{01}Gender_i + c_{02}SES_i + c_{03}ExecFunc_{ti} + cResid_i,$$

$$d_i = d_{00} + d_{01}Gender_i + d_{02}SES_i + dResid_i.$$

Here, parameter  $c$  now has the subscript  $ti$  to denote that it is time-specific as well as person-specific. In summary, some methodologists have proposed that TVCs can be incorporated into a NLME model in the same way as TICs, but the inclusion of TVCs yields a random coefficient with a slightly different interpretation. However, examples of this type of model specification are scarce. It may be a useful avenue for future research to further investigate the interpretational complexities that arise from incorporating TVCs into NLME models.

### **Summary**

Social scientists working with nonlinear models face a variety of conceptual challenges. Unique considerations arise when choosing a model, identifying a useful parameterization, incorporating moderators, and incorporating covariates. Many approaches that are familiar in linear regression are no longer applicable for nonlinear models. Therefore, the goal of this chapter was to synthesize recommendations and provide guidelines for approaching each stage of the model selection and specification process. Ideally, these resources will be useful for researchers seeking to optimize the substantive utility of their nonlinear models and make choices that are well grounded in theory.

## CHAPTER V

### EXTENDING THE JOHNSON-NEYMAN TECHNIQUE FOR MODERATED PARAMETERS IN NONLINEAR MODELS

In the previous chapter, I addressed a variety of conceptual and theoretical challenges that arise when choosing and specifying nonlinear models in social science research, including how to approach the incorporation of moderators. After those moderators have been incorporated, the model has been fit, and certain parameters are found to be significantly moderated, it is often of key substantive interest to extract more detail about the nature of that moderation. However, at present, researchers are limited in their ability to follow up on moderation results when working with nonlinear models.

As noted in Chapter 1, the JN technique is considered the optimal method for plotting and probing statistically significant moderation. The JN technique provides rich information about how the moderated parameter and its standard error (SE) change as the moderator changes. Additionally, the JN technique enables the computation of significance boundaries, which are moderator values at which the parameter goes from being statistically significant to nonsignificant. However, the JN technique was developed for linear models. While some work has discussed its application to quadratic models (e.g., Kim et al., 2023; Miller et al., 2013), at present, use of the JN technique is restricted to intrinsically linear models. Therefore, the purpose of this chapter is to present novel extensions of the JN technique – both conceptual and mathematical – to facilitate its use for plotting and probing *any* linearly moderated parameter, particularly those in nonlinear models.

## Conceptual Extensions of the JN Technique

Before presenting mathematical extensions of the JN technique for use in moderated nonlinear models, it is important to address the conceptual extensions that are also necessary. To structure this discussion, I will describe how the JN technique has been used to date (i.e., in linear models), and then describe differences that arise for nonlinear models.

In linear models, when moderation is introduced, the moderated quantity is almost always the simple slope of the focal predictor. Therefore, when the JN technique is implemented, significance boundaries denote the value(s) of the moderator at which the simple slope passes from significance to nonsignificance. However, in moderated nonlinear models, any parameter other than a slope may be moderated. Therefore, the JN technique must be extended such that it can determine the value(s) of the moderator at which *any moderated parameter* passes from significance to nonsignificance. As noted in previous chapters, the parameters of nonlinear models map onto a diverse array of curve attributes, including rates of change, locations along the  $x$ -axis of inflection points or peaks, asymptotes, wave amplitudes, and more. For many of these parameters, it will be necessary to conceptualize “significance” in new ways.

Conceptualizations of significance are almost always the same in linear models. Generally, a slope is considered significant if it is statistically distinguishable from zero; significance tests for simple slopes treat zero as the null value, and the JN technique is designed to find moderator values at which the simple slope of  $x$  is detectably different from zero. However, for the parameters of nonlinear models, it may not make sense to treat zero as the null value. In other words, whether a parameter is statistically distinguishable from zero may not be useful substantive information.

The possibility of a nonzero null value is perhaps the most important conceptual extension that arises when applying the JN technique to moderated nonlinear models. As a running example, consider the study by Womack et al. (2022) in which Gompertz models characterized cognitive development among children from age 3 months to 15 years. This study utilized the popular parameterization of the Gompertz model:

$$y = a + b \left[ \exp \left( -\exp(-c(x - d)) \right) \right] + \varepsilon, \quad (5.1)$$

where  $a$  is the lower asymptote,  $b$  is the difference between the upper and lower asymptotes (i.e., total growth),  $c$  is the average rate of growth,  $d$  is the location along the  $x$ -axis (i.e., age) at which growth is the fastest, and  $\varepsilon$  is the residual. Multiple moderators were found to significantly affect the shape of the curve. First, gestational age moderated parameters  $a$ ,  $b$ ,  $c$ , and  $d$ , such that earlier gestational age was related to a smaller lower asymptote, greater total growth, slower average rate of growth, and an earlier inflection point. Second, household socioeconomic status (SES) moderated all four model parameters, such that higher SES was related to a smaller lower asymptote, greater total growth, a slower average rate of growth, and an earlier inflection point. Third, household chaos moderated parameters  $b$  and  $d$ , such that greater household chaos was related to less total growth and a later inflection point.

After identifying significant moderation, the next step is to probe these results to gain a more thorough understanding of how gestational age, household SES, and household chaos affect the development of cognitive ability. First, let us consider moderation of the inflection point (parameter  $d$ ). Greater household chaos and lower SES were related to a later inflection point. Womack et al. (2022) note that an earlier inflection point is desirable in this context; children with a delayed inflection point exhibit their most rapid gains in cognitive ability later in life, meaning that throughout much of childhood they are tasked with “catching up” to their peers



whose most rapid development occurred earlier. Therefore, the authors note that it may be worthwhile for interventions to target children with a later inflection point. It would be useful to probe moderation results to determine the levels of SES, household chaos, and/or gestational age at which the inflection point is significantly delayed. The JN technique is ideal for this purpose.

To find the moderator values at which the inflection point is significantly delayed, we must first define “significance” for this context. The default behavior of the JN technique is to find the moderator value(s) at which parameter  $d$  is significantly different from zero; however, a null value of zero is not sensible here. In this study, children were assessed from 3 months to 15 years of age; there is no “age zero” within the window of observation. Testing whether the inflection point is significantly different from zero will not yield substantively useful information, as the inflection point is expected to be – and indeed is – very far from zero years of age among all children in the study. Therefore, we must define a different null value, or in other words, a different benchmark with respect to which the “significance” of parameter  $d$  should be determined.

Choosing a useful null value for parameter  $d$  (or for any moderated parameter in a nonlinear model) will be inherently subjective; however, it is always possible to be transparent about how the null value was chosen. For example, we may use prior research and/or clinical cutoffs to determine a useful null value. Perhaps clinicians or other researchers have found that when most cognitive development occurs after four years of age, it becomes unlikely that the child will fully “catch up” to their peers by the time development is complete. In this case, four years of age may be a useful null value for parameter  $d$ . The JN technique would then answer: at what gestational age, or at what levels of household SES and chaos, does the inflection point become significantly different from four? Alternatively, we may use information from the

sample to inform our choice of null value. Among the Womack et al. (2022) sample, the mean age of inflection was 3.26 years, with a 95% confidence interval of [3.12, 3.41]. We may decide that the upper limit of the confidence interval (3.41), or one or two standard deviations above the mean of 3.26, should be treated as a benchmark for a “significantly” delayed inflection point.

Similarly, results indicated that parameter  $b$  was moderated by gestational age, SES, and household chaos. Because parameter  $b$  reflects total growth in cognitive ability over the course of ~15 years, a null value of zero is not appropriate for this parameter. Indeed, the average value of parameter  $b$  was 17.01 with a 95% CI of [15.55, 18.47]. Parameter  $b$  is notably different from zero among all children in the sample, and implementing the JN technique with zero as the null value is unlikely to yield substantively useful information. To choose a useful null value for parameter  $b$ , we may again turn to information from our sample, or to clinical and/or empirical findings regarding cognitive development. For example, perhaps children whose total growth is five or fewer points tend to end up with long-term cognitive deficits. Treating five as the null value may allow us to identify gestational ages, SES levels, and household chaos levels that do and do not correspond with deficits in asymptotic (i.e., long-term) cognitive ability. Regardless of the null value that we choose, the JN technique enables us to find the moderator values at which the parameter becomes statistically distinguishable from that null value.

It is also important to consider that it may not always be appropriate to apply the JN technique to moderated parameters in nonlinear models. First, it may not be possible to generate a useful null value. As an example, parameter  $c$  in Eq. 5.1 reflects rate of growth from the lower to upper asymptote. Parameter  $c$  was moderated such that earlier gestational age and higher household SES were related to a slower rate of growth. We *could* follow up on this result with the JN technique; however, it may not be sensible to do this, because there may not be a useful

null value for parameter  $c$ . Although all children's cognitive ability is expected to improve throughout childhood, there may not be a certain rate at which that improvement is expected to occur. Perhaps rate of improvement has not been found to be as clinically important as other aspects of the curve – like timing of the inflection point or total growth – such that there are no set benchmarks at which rate of growth is considered optimal or deficient. The absence of a useful null value reflects that there is no specific value against which the “significance” of the parameter can be evaluated. In these cases, rather than evaluating the significance of the parameter against a certain benchmark, it may be more substantively useful to rely on descriptive information about moderation. For example, it may be sufficient to use pick-a-point plots to visualize how the parameter changes as the moderator changes.

Second, there may not be useful substantive insight to be gained from applying the JN technique to a moderated parameter of a nonlinear model. Moderation of a parameter may be included simply to avoid model misspecification rather than to gain important substantive information. This is a common practice in linear models; higher intercepts often accompany lower slopes and lower intercepts often accompany higher slopes, such that if our goal is to meaningfully examine moderation of a slope, we must also moderate the intercept in order to obtain an accurate estimate of how the slope is moderated. As discussed in Chapter 4, this “omnibus” approach may also be useful for nonlinear models; for example, if working with a Gompertz model where we expect parameter  $b$  (total growth) to be moderated, it may be necessary to moderate parameter  $a$  (the lower asymptote) in order to accurately estimate how parameter  $b$  is moderated. In this case, the moderation of parameter  $a$  is simply included to allow for intraindividual variability in that parameter rather than to test specific hypotheses about moderation. Indeed, this may be the case for parameter  $a$  in the Womack et al. (2022) model,

which reflects the lower asymptote of cognitive ability. Parameter  $a$  was found to be moderated by gestational age and household SES; however, JN-derived information about the moderation of parameter  $a$  may not be useful. There may not be scientifically meaningful information to be gained, or hypotheses to be tested, by applying the JN technique to this result.

As a final note, the preceding discussion of null values for certain parameters, as well as the applicability of the JN technique for certain parameters, is not applicable to all research contexts. These hypothetical examples are only illustrations with which to demonstrate the conceptual considerations that arise when applying the JN technique to moderated nonlinear models, and the rationales provided here are not universal. For example, in the context of the Womack et al. (2022) data, it was clear that zero would not be a logical null value for parameter  $b$ , which reflected total cognitive growth over the course of ~15 years. However, in other contexts, it may be completely appropriate to compare total growth against a benchmark of zero. Similarly, in the Womack et al. (2022) example, I suggested there may not be a useful null value for parameter  $c$ , which reflected rate of growth in cognitive ability. However, there may be many contexts in which there is a well-established and useful benchmark against which to compare growth rates (for example, perhaps scores on a standardized assessment are expected to increase ten points per year). In summary, the rationales provided here should not be considered universal to all applications of sigmoidal curves. Whether the JN technique is appropriate for a given moderated parameter – and if so, the appropriate null value – will be a subjective conclusion that varies across models, measurement scales, and research contexts.

In summary, novel conceptual considerations arise when applying the JN technique to moderated parameters within nonlinear models. In many cases, the “significance” of a moderated parameter must be conceptualized in new ways, as comparing the parameter to a null value of

zero may not yield substantively useful information. Additionally, it will be important to consider whether implementing the JN technique is justified in the first place. In all cases, it will be essential to provide transparency and justification for JN-related decisions. Having addressed these conceptual extensions, in the following section I present a mathematical extension of the JN technique for use with nonzero null values.

### **Mathematical Extension of the JN Technique**

This section begins with a brief refresher of the key JN equations that were introduced in Chapter 1. Start with the simple linear regression equation for the expected value of  $y$ , conditional on values of  $x$  and  $z$ :

$$E[y|(x, z)] = \hat{\gamma}_0 + \hat{\gamma}_1x + \hat{\gamma}_2z + \hat{\gamma}_3xz, \quad (5.2)$$

where  $x$  is the focal predictor,  $z$  is the moderator, and the  $\hat{\gamma}$ s are the estimated regression coefficients. The simple slope of  $x$ , which is the effect of  $x$  on  $y$  at a particular value of the moderator, can be expressed as:

$$\hat{\omega} = \hat{\gamma}_1 + \hat{\gamma}_3z. \quad (5.3)$$

The standard error of  $\hat{\omega}$  is the square root of its variance, which is given by:

$$var(\hat{\omega}) = var(\hat{\gamma}_1) + 2zcov(\hat{\gamma}_1, \hat{\gamma}_3) + z^2var(\hat{\gamma}_3). \quad (5.4)$$

The first goal of this section is to establish that the JN technique can be applied to linearly moderated parameters in nonlinear models. To do so, we must obtain expressions for what I will refer to as the *simple parameter* (akin to a simple slope) and the standard error of that simple parameter.

To obtain an expression for a simple parameter, recall that in Chapter 1 we established that, generally, linear moderation occurs when a model parameter varies linearly as a function of

the moderator. Working from this definition, it is straightforward to incorporate linear moderation of any parameter into a nonlinear model specification. For example, we can extend the Gompertz model given in Eq. 5.1, such that parameter  $b$  is linearly moderated by  $z$ :

$$y = a + (b_0 + b_1z) \left[ \exp \left( -\exp(-c(x - d)) \right) \right] + \varepsilon, \quad (5.5)$$

where  $b$  has been replaced by  $b_0 + b_1z$ . Here,  $b_0$  is the value of parameter  $b$  when  $z$  is zero, and  $b_1$  is the change in parameter  $b$  when  $z$  increases by one unit. The expression for the estimate of the simple parameter  $b$  is given by

$$\hat{\omega}_b = \hat{b}_0 + \hat{b}_1z, \quad (5.6)$$

as this quantity reflects the estimated value of parameter  $b$  at a particular value of  $z$ . In summary, when any parameter is linearly moderated, the expression for the “simple parameter” is very similar to the expression for a simple slope given in Eq. 5.3.

Next, we must obtain an expression for the variance (and subsequently, SE) of a simple parameter estimate. To do so, we can apply the delta method, which is a very general method for deriving the variance of a function of one or more parameters – including a linear combination of parameters (Dorfman, 1938; Rao, 1965; Raykov & Marcoulides, 2004). Indeed, Aiken and West (1991) applied the delta method to derive the variance of a simple slope given in Eq. 5.4. To understand how Eq. 5.4 was derived, consider that a simple slope (Eq. 5.3) is a weighted linear combination. The elements are the estimated parameters which make up the simple slope,  $\hat{\boldsymbol{\gamma}}' = [\hat{\gamma}_1 \ \hat{\gamma}_3]$ , and the weight vector is  $\mathbf{w}' = [1 \ z]$ . More specifically, the weight vector contains the first partial derivatives of Eq. 5.3 with respect to each component parameter in turn (Raykov & Marcoulides, 2004). The variance of a linear combination in this form is a function of  $\Sigma_{\boldsymbol{\gamma}}$ , which is the asymptotic covariance matrix (ACOV) of the estimated coefficients, and the weight vector:

$$\sigma_{\boldsymbol{\gamma}}^2 = \mathbf{w}'\Sigma_{\boldsymbol{\gamma}}\mathbf{w}. \quad (5.7)$$

Aiken and West (1991) used this general fact to derive the variance of a simple slope. First, rewrite Eq. 5.3 as a weighted linear combination:

$$\hat{\omega} = (1)\hat{\gamma}_1 + (z)\hat{\gamma}_3. \quad (5.8)$$

To find the variance of  $\hat{\omega}$ , use the general formula for the variance of a linear combination given in Eq. 5.7. Here,  $\Sigma_\gamma$  is still the ACOV of the estimated coefficients, and the weight vector is:

$$\mathbf{w}' = [1 \ z]. \quad (5.9)$$

Therefore, we have:

$$\text{var}(\hat{\omega}) = [1 \ z] \begin{bmatrix} \text{var}(\hat{\gamma}_1) & \text{cov}(\hat{\gamma}_1, \hat{\gamma}_3) \\ \text{cov}(\hat{\gamma}_1, \hat{\gamma}_3) & \text{var}(\hat{\gamma}_3) \end{bmatrix} \begin{bmatrix} 1 \\ z \end{bmatrix}. \quad (5.10)$$

Simplifying this expression yields Eq. 5.4.

Aiken and West (1991) note that this method holds only for linear combinations.

Importantly, our scope here is restricted to *linear* moderation, and any simple parameter that is subject to linear moderation can be expressed as a linear combination, such as Eq. 5.6. Therefore, it is possible to derive the variance (and subsequently, SE) of any simple parameter estimate using the delta method. As long as the model is parameterized so that the moderated quantity is expressed as a linear combination, we will obtain an ACOV of parameter estimates that contains the necessary elements to derive the variance of the simple parameter. For example, in our moderated Gompertz model, the simple parameter  $b$  is given in Eq. 5.6. To obtain the variance of  $\hat{\omega}_b$ , express  $\hat{\omega}_b$  as a weighted linear combination,

$$\hat{\omega}_b = (1)\hat{b}_0 + (z)\hat{b}_1, \quad (5.11)$$

and apply Eq. 5.7,

$$\text{var}(\hat{\omega}_b) = [1 \ z] \begin{bmatrix} \text{var}(\hat{b}_0) & \text{cov}(\hat{b}_0, \hat{b}_1) \\ \text{cov}(\hat{b}_0, \hat{b}_1) & \text{var}(\hat{b}_1) \end{bmatrix} \begin{bmatrix} 1 \\ z \end{bmatrix}, \quad (5.12)$$

which simplifies to:

$$\text{var}(\hat{\omega}_b) = \text{var}(\hat{b}_0) + 2z \text{cov}(\hat{b}_0, \hat{b}_1) + z^2 \text{var}(\hat{b}_1). \quad (5.13)$$

The variance and covariance estimates in Eq. 5.13 will be contained within the ACOV of the nonlinear model's parameter estimates.

The expression for the variance of a simple parameter, given in Eq. 5.13, closely resembles the expression for the variance of a simple slope, given in Eq. 5.4. In both cases, the variance of the simple parameter depends on three estimates: the variance of the term which denotes the simple parameter when  $z$  is zero ( $\hat{\gamma}_1, \hat{b}_0$ ), the variance of the term which denotes the change in the simple parameter when  $z$  increases by one unit ( $\hat{\gamma}_3, \hat{b}_1$ ), and the covariance of those two terms. Eq. 5.13 shows that regardless of the complexity of the overall nonlinear model, the necessary elements of the ACOV pertain only to the parameter estimates within the linear combination.

In summary, for any linearly moderated parameter, we can obtain expressions for the simple parameter estimate and its variance. This result rests on the fact that, despite being couched within a nonlinear model, a linearly moderated parameter can be expressed as a linear combination. As a result, we can apply the JN technique to any linearly moderated quantity in a nonlinear model.

We are now in a position to conduct a significance test of any simple parameter at any value of the moderator. Therefore, we can proceed with the JN technique as we usually would. Let us briefly revisit the typical JN equation that was introduced in Chapter 1:

$$\pm t_{crit} = \frac{\hat{\omega}}{\sqrt{\text{var}(\hat{\omega})}}. \quad (5.14)$$

The JN technique reverses the process of the significance test. We first select a critical  $t$ -value ( $t_{crit}$ ), then we solve for the value(s) of the moderator that yield it. The numerator of the fraction in Eq. 5.14 is the simple slope of  $x$ , and is replaced with Eq. 5.3. Similarly,  $\text{var}(\hat{\omega})$  in the



denominator of the fraction is replaced with Eq. 5.4. Then, the equation can be solved for values of  $z$  using the quadratic formula.

No null value is explicitly represented in Eq. 5.14 because the JN technique assumes that the null value (i.e., the value against which “significance” is established) is zero. Next, I will present a more general version of the JN technique that allows the null value to be nonzero. We can develop this extension using the original JN formulae that were created in the context of linear regression, continuing with the notation in Eqs. 5.2 – 5.4. To allow for any null value of  $\hat{\omega}$ , which I will denote  $\omega_0$ , expand Eq. 5.14 to:

$$\pm t_{crit} = \frac{\hat{\omega} - \omega_0}{\sqrt{\text{var}(\hat{\omega})}}. \quad (5.15)$$

We must rearrange Eq. 5.15 such that the equation can be solved with the quadratic formula. In other words, we must obtain an equation of the form:

$$az^2 + bz + c = 0. \quad (5.16)$$

Begin by rearranging Eq. 5.15 so that it is set equal to zero:

$$\left(t_{crit}^2 \text{var}(\hat{\omega})\right) - (\hat{\omega} - \omega_0)^2 = 0$$

Next, substitute  $\text{var}(\hat{\omega})$  with Eq. 5.4, expand the squared term, and substitute  $\hat{\omega}$  with Eq. 5.3:

$$t_{crit}^2 \left( \text{var}(\hat{\gamma}_1) + 2z \text{cov}(\hat{\gamma}_1 \hat{\gamma}_3) + z^2 \text{var}(\hat{\gamma}_3) \right) - \left( \hat{\omega}^2 - 2\hat{\omega}\omega_0 - \omega_0^2 \right) = 0$$

$$t_{crit}^2 \left( \text{var}(\hat{\gamma}_1) + 2z \text{cov}(\hat{\gamma}_1 \hat{\gamma}_3) + z^2 \text{var}(\hat{\gamma}_3) \right) - \left( \hat{\gamma}_1^2 + 2\hat{\gamma}_1 \hat{\gamma}_3 z + \hat{\gamma}_3^2 z^2 \right) + 2(\hat{\gamma}_1 + \hat{\gamma}_3 z)\omega_0 - \omega_0^2 = 0.$$

Distribute, then rearrange to collect the terms with  $z^2$ ,  $z$ , and without either:

$$t_{crit}^2 \text{var}(\hat{\gamma}_1) + t_{crit}^2 2z \text{cov}(\hat{\gamma}_1 \hat{\gamma}_3) + t_{crit}^2 z^2 \text{var}(\hat{\gamma}_3) - \hat{\gamma}_1^2 - 2\hat{\gamma}_1 \hat{\gamma}_3 z - \hat{\gamma}_3^2 z^2 + 2\omega_0 \hat{\gamma}_1 + 2\omega_0 \hat{\gamma}_3 z - \omega_0^2 = 0$$

$$z^2 \left[ t_{crit}^2 \text{var}(\hat{\gamma}_3) - \hat{\gamma}_3^2 \right] + z \left[ 2 \left( t_{crit}^2 \text{cov}(\hat{\gamma}_1 \hat{\gamma}_3) - \hat{\gamma}_1 \hat{\gamma}_3 + \omega_0 \hat{\gamma}_3 \right) \right] + \left[ t_{crit}^2 \text{var}(\hat{\gamma}_1) - \hat{\gamma}_1^2 + 2\omega_0 \hat{\gamma}_1 - \omega_0^2 \right] = 0. \quad (5.17)$$

The bracketed terms in Eq. 5.17 are  $a$ ,  $b$ , and  $c$  in the quadratic formula:

$$a = t_{crit}^2 \text{var}(\hat{\gamma}_3) - \hat{\gamma}_3^2, \quad (5.18)$$

$$b = 2\left(t_{crit}^2 \text{cov}(\hat{\gamma}_1\hat{\gamma}_3) - \hat{\gamma}_1\hat{\gamma}_3 + \omega_0\hat{\gamma}_3\right), \quad (5.19)$$

$$c = t_{crit}^2 \text{var}(\hat{\gamma}_1) - \hat{\gamma}_1^2 + 2\omega_0\hat{\gamma}_1 - \omega_0^2. \quad (5.20)$$

Importantly, if  $\omega_0 = 0$ , then Eqs. 5.18-5.20 reduce to the  $a$ ,  $b$ , and  $c$  terms that were derived for the original JN technique (Bauer & Curran, 2005).

Using the  $a$ ,  $b$ , and  $c$  terms given in Eqs. 5.18-5.20, we can use the quadratic formula to solve for values of  $z$ , which are the significance boundaries:

$$z = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}. \quad (5.21)$$

Besides significance boundaries, another important component of the JN technique is to visualize the value of the simple parameter, as well as our confidence about that simple parameter, across all values of the moderator. We can use the expressions presented in this chapter for this purpose. For example, returning to the moderated Gompertz model given in Eq. 5.5, we can use the JN technique to plot the simple parameter  $b$  along with its confidence band at all values of  $z$ . The confidence band will be given by:

$$\hat{\omega}_b \pm t_{crit}\sqrt{\text{var}(\hat{\omega}_b)}, \quad (5.22)$$

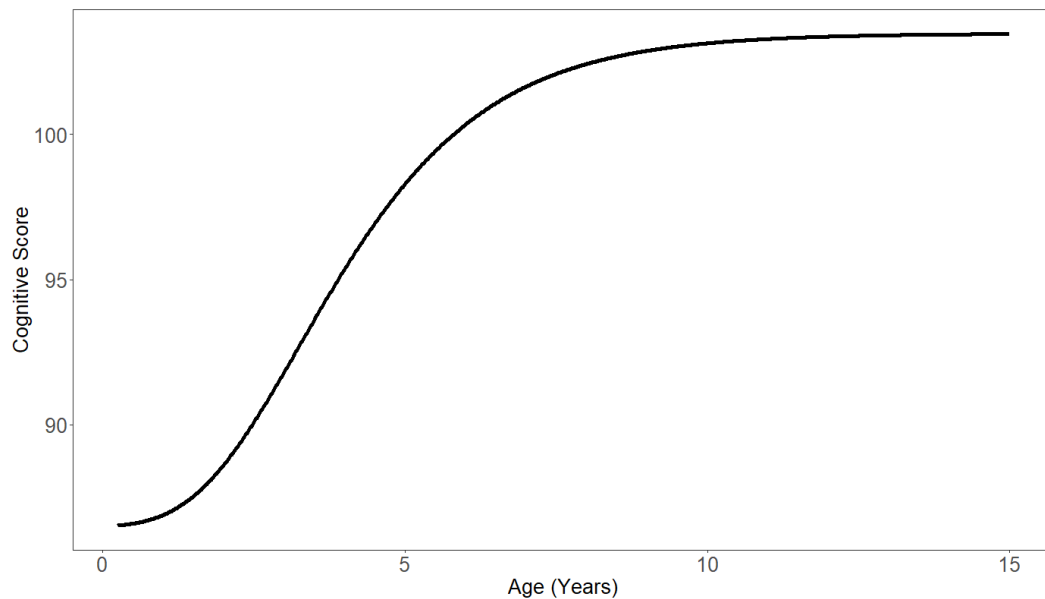
where both the simple parameter  $b$  and the width of the confidence band vary as a function of the moderator (Bauer & Curran, 2005).

In summary, I have shown that for any linearly moderated parameter in a nonlinear model, it is possible to obtain expressions for the simple parameter as well as its variance. Additionally, I presented a more general version of the JN technique that enables us to solve for significance boundaries using any null value of the moderated parameter, zero or nonzero.

## Demonstration

To illustrate the ideas and extensions presented above, let us revisit the Womack et al. (2022) example. In this section, I will present results and figures from simulated data that were designed to resemble those presented in the Womack et al. (2022) study. Figure 5.1 shows the mean function relating age to cognitive scores among the sample; using the parameterization of the Gompertz function given in Eq. 5.1, parameter estimates were  $a = 86.47$  (lower asymptote),  $b = 17.01$  (total growth),  $c = 0.58$  (rate of growth), and  $d = 3.26$  (location of the inflection point).

*Figure 5.1. Mean Function Relating Age to Cognitive Scores in Womack et al. (2022)*



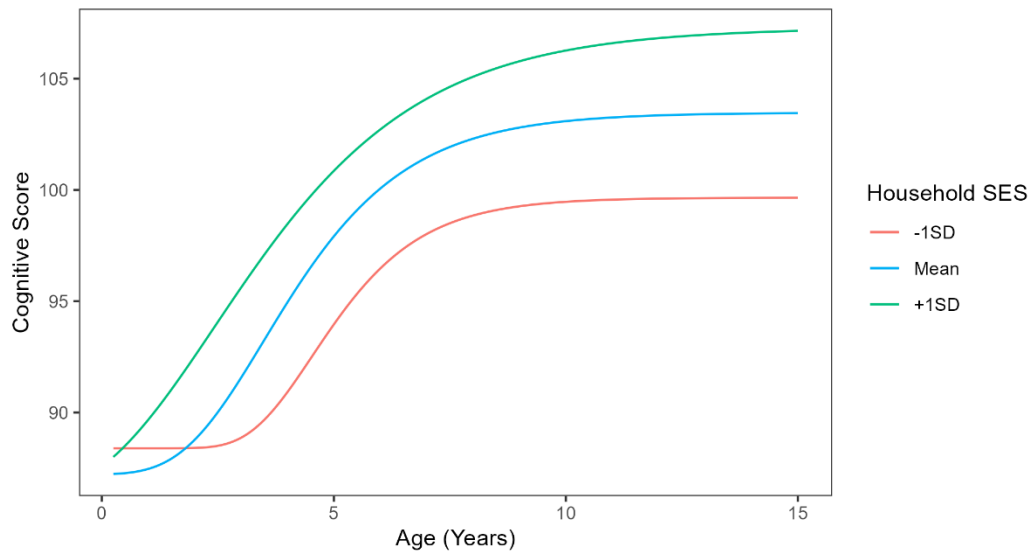
Our simulated data make use of the fact that household SES moderated all four model parameters, such that higher SES was related to a smaller lower asymptote, greater total growth, a slower average rate of growth, and an earlier inflection point. SES was standardized such that its  $M = 0$  and  $SD = 1$ . For simplicity (the real data were nested and modeled with a latent growth curve), data were simulated according to the following model specification:

$$\begin{aligned}
cogScore = & (a_0 + a_1SES) + \\
& (b_0 + b_1SES) \left[ \exp \left( -\exp \left( -(c_0 + c_1SES)(x - (d_0 + d_1SES)) \right) \right) \right] + \varepsilon.
\end{aligned} \tag{5.23}$$

Data were generated according to the parameter estimates reported in Womack et al. (2022), such that  $a_0 = 86.47$ ,  $a_1 = -1.31$ ,  $b_0 = 17.01$ ,  $b_1 = 5.57$ ,  $c_0 = 0.58$ ,  $c_1 = -0.17$ ,  $d_0 = 3.26$ , and  $d_1 = -1.00$ . Residual variance was set to 5.

For a preliminary visualization of this moderation, we can begin by inspecting a pick-a-point plot that displays the model-implied relation between age and cognitive score at three values of SES. The SES levels shown in Figure 5.2 are  $-1$ ,  $0$ ,  $1$ , which correspond to the mean  $\pm 1SD$ .

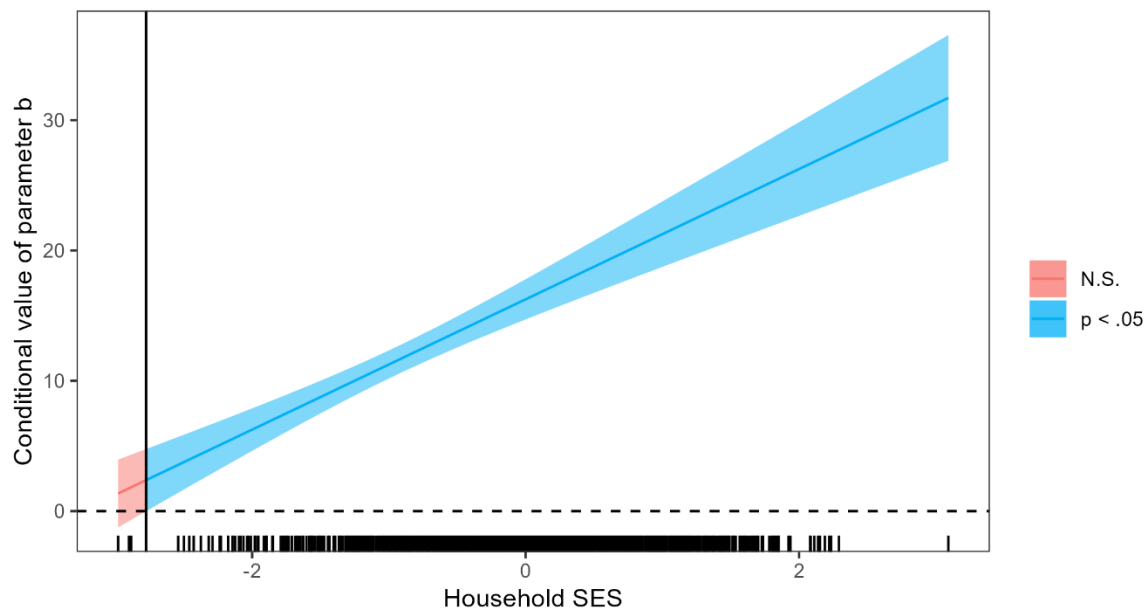
Figure 5.2. Pick-a-Point Plot of Cognitive Score vs. Age at Three SES Levels.



The pick-a-point plot indicates that household SES has quite a pronounced effect on total growth of the curve. To better understand how SES affects total growth in cognitive ability, let us create a JN plot depicting the relation between SES and parameter  $b$ . Using the formulae

given in the preceding equations, we can compute and plot (1) the conditional value of parameter  $b$  at each observed value of SES, (2) the corresponding confidence band surrounding the simple parameter, and (3) significance boundaries that denote SES values at which parameter  $b$  passes from statistical significance to nonsignificance. We can begin by implementing the default behavior of the JN technique, which finds significance boundaries using zero as the null value. Here, the significance boundaries are  $-3.991$  and  $-2.776$ , and we obtain the plot shown in Figure 5.3.

Figure 5.3. JN Plot for Parameter  $b$ , Using Zero as the Null Value.

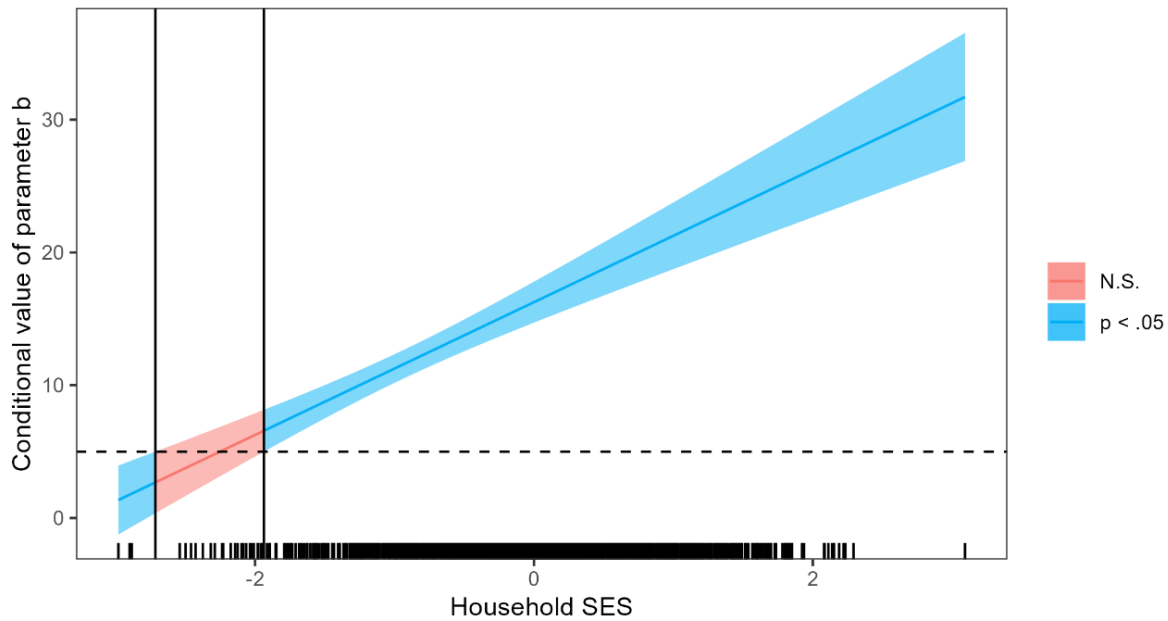


Only one significance boundary ( $-2.776$ ) is shown in Figure 5.3 because the other boundary ( $-3.991$ ) was outside of the observed range of SES. The boundary depicted in Fig. 5.3 indicates that when household SES is greater than  $-2.776$ , parameter  $b$  is significantly greater than zero. However, it does not seem sensible to treat zero as the null value here. First, it is not

substantively useful to assess whether total cognitive growth over ~15 years is different from zero. Second, the rug plot along the  $x$ -axis in Figure 5.3 – which shows the observed values of SES in our sample – indicates that only three individuals reported an SES level below the significance boundary. For basically all the children in our sample, the model implies that parameter  $b$  is significantly greater than zero. The lack of observed data around the significance boundaries, as well as the meaning of parameter  $b$  in this research context, suggest that this null value is not particularly useful or informative.

Let us recompute the significance boundaries using a more sensible null value. Again, suppose prior research indicates that total growth of five or fewer points is indicative of long-term deficiencies in cognitive ability. Treating five as the null value, we find that the significance boundaries are  $-2.715$  and  $-1.937$ , and we obtain the plot given in Figure 5.4.

Figure 5.4. JN Plot for Parameter  $b$ , Using Five as the Null Value.



Before unpacking these results, first observe the differences between Fig. 5.3 and Fig. 5.4. In both figures, the conditional value of  $b$  and its confidence band are the same across all observed values of SES, as these quantities are computed independently of the chosen null value. However, most other components of the plot have changed because they depend on the null value. First, the location of the horizontal dashed line has changed. This dashed line denotes the null value; in Fig 5.3 it intersects the  $y$ -axis at zero, whereas in Fig. 5.4 it intersects the  $y$ -axis at five. Second, the vertical lines that denote significance boundaries have moved. Third, the shading of the confidence band – which indicates regions of the moderator where parameter  $b$  is significant and nonsignificant – has also changed in accordance with the significance boundaries.

New results indicate that when household SES is less than  $-2.715$ , parameter  $b$  is significantly smaller than five, and when household SES is greater than  $-1.937$ , parameter  $b$  is significantly larger than five. At SES levels between the two boundaries, parameter  $b$  is statistically indistinguishable from five.

Our findings imply that, for children whose family SES is at or below about  $-1.937$  (i.e., about 2 SDs below the mean) on our standardized SES measure, additional intervention may be necessary to protect against long-term deficits in cognitive growth. When household SES is less than  $-1.937$ , model-implied total growth is either indistinguishable from five points, or is significantly smaller than five points. These children may show long-term cognitive deficits. On the other hand, when household SES is greater than  $-1.937$ , our model implies that total cognitive growth will be significantly greater than five points. These children are unlikely to show long-term cognitive deficits. In summary, we have pinpointed the SES levels at which total cognitive growth is and is not significantly reduced. Using the adapted version of the JN

technique with a nonzero null value, we have obtained more useful substantive information by finding the SES levels at which parameter  $b$  is detectably different from a meaningful value.

### **Summary**

To apply the JN technique for use in moderated nonlinear models, both conceptual and mathematical extensions are necessary. Conceptually, it becomes important to think critically about the “significance” of the moderated parameter, and whether zero is an appropriate value against which to compare the parameter. A nonzero null value may be more appropriate, and justification for the chosen value should be provided. Mathematically, after establishing that it is possible to obtain the necessary quantities for the JN technique for linearly moderated parameters in nonlinear models, I presented a more general version of the original JN formulae. The more general extension allows the moderated parameter to be tested for significance using a nonzero null value. In the following chapter, I present a software interface which incorporates these JN extensions.



## CHAPTER VI

### CURVEBUILDER: AN INTERACTIVE NONLINEAR MODELING TOOLKIT IN SHINY

For social scientists seeking to implement nonlinear models in their work, a major barrier is a lack of accessible software tools, as detailed in Chapter 3. Given the shortcomings of extant software, I created an open-source application, CurveBuilder, the aim of which is to unify and simplify each step of the nonlinear modeling process. CurveBuilder was created in R using the Shiny web application framework (Chang et al., 2022) and can be accessed at <https://haleyyaremych.shinyapps.io/CurveBuilder/>. The application provides a code-free environment for users to complete all steps of the analysis process, including uploading data, visually choosing start values, specifying models, plotting results, and probing significant moderation. This chapter begins by documenting the functionality of the application, followed by multiple examples of its use.

#### CurveBuilder Documentation

##### Visualize Curves

The *Visualize Curves* tab is intended to be a learning tool for researchers to familiarize themselves with popular nonlinear models and their parameters. There is no need to upload one's own data in order to use this tab. In this tab, the selected curve is plotted, and as users adjust parameter values, the plot updates. This display makes it easy to understand how each parameter governs the appearance of the curve. Ideally, this feature will help researchers understand which

model parameters are theoretically important and/or which parameters may be expected to be moderated.

There are a variety of pre-specified nonlinear functions available to view in this tab. Additionally, there is a “Write my own function” option, where the user can enter any equation with up to 5 parameters. This option is intended for nonlinear functions that are not included as pre-specified options, or for different parameterizations of the functions that are provided.

There are a few simple display options for the plot created in this tab. First is the “lock y-axis scale” checkbox, which, if checked, locks the y-axis range at -10 to 10. If unchecked, the y-axis will auto-scale to the curve. If viewing a custom curve, the user can also edit the minimum and maximum values of the  $x$ -axis.

An error message may appear if the user enters a custom function with incorrect syntax. See *Using the custom curve option*, below, for more detail about how to use the custom curve functionality.

## **Data Upload**

The Data Upload tab allows the user to begin working with their own data, which can later be used to fit models and create plots. Accepted file types are .csv, .sav, and .xlsx. Prior to uploading their data to CurveBuilder, users should conduct any necessary data cleaning and pre-processing, as this functionality is not available in-app. For example, if planning to fit a model containing a multicategorical predictor, the user should create coding variables prior to data upload (coding variables can be any type). Additionally, variable centering is not conducted in-app, so any desired centering and scaling should be conducted prior to data upload. Finally, if using a mixed-effects model for grouped data, data must be in long format.

Upon data upload, the app conducts basic checks to avoid downstream errors. First, any date variables (e.g., variables of the *POSIXct* class) are converted to character variables. Second, if a column name is duplicated, “.1” is appended to the second instance of the column name. For example, if two columns are named ID, then the second ID column will be renamed to ID.1.

### **Preview Start Values**

When fitting nonlinear models, start values for each parameter are required. These start values should yield a curve that corresponds relatively well with the data, or else convergence problems are likely. However, it can be difficult to generate adequate start values. The goal of the Preview Start Values tab is to ease this burden. In this tab, users can plot their observed data with a nonlinear curve overlaid. Parameter values can be adjusted until the curve appears to follow the data well. Those parameter values can then be imported as start values when the model is fit later, in the Create Model tab. The user simply selects a variable for the  $x$ -axis, a variable for the  $y$ -axis, a nonlinear function to display (pre-specified or custom), and can then begin adjusting parameter values until the curve corresponds well with the data.

There are a few plot options in this tab. First, rather than plotting all observations, the user may plot a random subsample of the data. This option is recommended for very large data sets (Cudeck & Harring, 2007); in addition to decluttering the plot, which can make it easier to visually identify trends, this option will also speed up the rendering of the plot. For very large data sets (i.e., tens of thousands of rows), plots may take a few minutes to render if plotting all observations. Second, the user may color-code the scatterplot according to a moderator. This functionality is intended to help the user get a sense of whether certain aspects of the curve (i.e., parameters) may be moderated, and if so, what reasonable start values for the effect(s) of the

moderator may be. If the moderator is categorical, the plot will be colored by each unique value of the moderator found in the data set. If the moderator is continuous, the moderator will be grouped into quintiles (five groups, which each contain 20% of the moderator values), and the plot will be color-coded according to moderator quintiles.

An error message may appear if one of the selected variables makes it impossible to create the plot (“*Plot couldn’t be created. Selected variable(s) may be of wrong type*”). This may occur if the user selects an  $x$ -variable that has all NA values, takes on just one unique value in the data set, or is read as a factor rather than a numeric variable. An error message may also appear if the user enters a custom function with syntax errors. See *Using the custom curve option*, below, for details about troubleshooting these errors.

## **Create Model**

The goal of the Create Model tab is to provide a code-free environment for users to specify and fit nonlinear models, which may include random effects and/or moderation. Required input from the user includes (1) a nonlinear function, (2) a predictor and outcome variable, and (3) start values for model parameters. All other input is optional. The outcome variable should be continuous, as the app cannot accommodate generalized nonlinear models.

Entered start values should yield a curve that corresponds with the data relatively well. The Preview Start Values tab may be helpful for identifying good start values; start values identified in the Preview tab can be easily imported by clicking the *Import start values from Preview tab* button. As a note, some readers may be aware that there are self-starter functions available in R, which automatically generate start values for a given nonlinear model (see Miguez, 2022; Onofri, 2020; Pinheiro et al., 2023; Ritz et al., 2015; Ritz & Streibig, 2008). Self-

starter functions are not implemented in CurveBuilder because they are highly specific to a given parameterization of a given nonlinear model; any changes or adjustments to that model necessitate a new self-starter function. For example, a Gompertz model with moderated parameter  $a$  and a Gompertz model with moderated parameter  $b$  require different self-starter functions. Therefore, the exclusion of self-starters enables maximal generality in terms of the nonlinear models, parameterizations, and moderation that the user may specify.

### ***Model Options***

If the user chooses to add moderation to the model, they will be required to indicate the parameter(s) that are moderated, moderator(s) for each of those parameters, and start values for each moderating effect. Any number of moderators can be added for any number of model parameters. Moderators can be continuous, binary, or multicategorical, in which case the user should enter the set of coding variables as moderators (any type of coding variable is allowed). Choosing start values for moderating effects is a required step. These start values can be thought of as the moderator's expected effect on the parameter; as the moderator increases by one unit, by how much is the moderated parameter expected to change? See Examples 1 and 2, below, for more detail.

The user may also choose to treat some parameters as random, creating a NLME model. If so, the user should simply indicate the name of the grouping variable and which model parameters should be treated as random, and should make sure data are in long format.

### ***Options for Troubleshooting Nonconvergence***

If attempting to fit a model that fails to converge, CurveBuilder offers a few options for users to try, each of which may help with convergence. First, the user may adjust the maximum iterations that will occur before the maximum likelihood algorithm stops. By default, this is set

to 50 (consistent with both *nls* and *nlme* defaults), but if experiencing convergence problems, it may help to increase this number.

Second, the user may adjust the tolerance for the convergence criterion. For models without random effects, tolerance is set to  $1 \times 10^{-5}$  (consistent with *nls* defaults), and for models with random effects, tolerance is set to  $1 \times 10^{-6}$  (consistent with *nlme* defaults). Making the criterion less strict (i.e., making it larger) may help achieve convergence. The maximum likelihood algorithm stops when likelihood values obtained from adjacent iterations change by an amount that is *less than* the convergence criterion; this signals that model estimates are not changing much from iteration to iteration, meaning the model has converged. Therefore, a less strict tolerance makes it easier for the convergence criterion to be reached.

Third, the user may toggle on the option to show the results from the final iteration. This option coincides with the *returnObject* argument in *nlme*, and the *warnOnly* argument in *nls*. By default, these are each set to FALSE, but turning on the toggle sets them to TRUE. If turned on, CurveBuilder will return results that were obtained on the final iteration of the estimation algorithm, even if convergence was not achieved at this point.

### ***R Code***

As the user specifies the model, the app builds the appropriate R code to fit the model. If there are no random effects, the app constructs a call to the *nls* function in base R. If there are random effects, the app constructs a call to the *nlme* function from the *nlme* package (Pinheiro et al., 2023). The first requirement of both *nls* and *nlme* is a nonlinear function representing the relation between  $x$  and  $y$ . The app starts with code for the nonlinear function given by the user (either prespecified or custom) and modifies that code to contain the correct variable names, as well as to reflect any moderation that is specified.

When the “Show R Code” option is switched on, the user can view the R code that is being generated as they specify the model. This may be helpful to ensure correct specification and for learning purposes. If the “Show R Code” switch is turned on and changes are made to the model, simply turn the switch off and back on to view these changes in the R code. Additionally, this R code may be copy-and-pasted into the user’s local R environment. From there, the model could be run locally (rather than in-app), which may be helpful for very large or complex models that are expected to take a long time to converge. Finally, the user may use this R code as a starting point for specifying a more advanced model, perhaps with additional features that are not enabled by the app (e.g., fitting a custom model with more than five base parameters, specifying an autocorrelation structure, modeling heteroscedastic variance, etc.). For a discussion and examples of incorporating the latter advanced features, see Davidian and Giltinan (1995) and Blozis and Harring (2021).

Next, we will review a variety of code examples to demonstrate correspondence between model specification and the R code that is created by CurveBuilder. In Example 1, we suppose the user selects the Gompertz model with no moderation and no random effects. For simplicity, let the predictor variable be  $x$  and the outcome be  $y$ . Code for the Gompertz model is:

$$y \sim a + b * (\exp(-\exp(-c * (x-d)))) , \quad (6.1)$$

and after the user has specified start values, the final *nls* call will look like this:

```
model = nls(y ~ a + b * (exp(-exp(-c*(x-d)))) ,
  data = data,
  start = c(a = 2, b = 2, c = 1, d = 5) ,
  control = nls.control(maxiter = 50,
    tol = 1e-05,
    warnOnly = FALSE) ,
  na.action = na.omit)
```

In Example 2, suppose the user selects a Gompertz model with no random effects, but indicates that a variable called *mod* should moderate parameter *b*. To incorporate this moderation, the code is updated as follows:

$$y \sim a + (b0 + b1*mod) * (\exp(-\exp(-c*(x-d)))) \quad (6.2)$$

Notice that parameter *b* has been replaced with  $(b0 + b1*mod)$ , such that *b0* is the value of parameter *b* when *mod* is zero, and *b1* is the change in parameter *b* when *mod* increases by one unit. After the user has specified start values and made any other desired adjustments, the final *nls* call will look like this:

```
model = nls(y ~ a + (b0 + b1*mod) * (exp(-exp(-c*(x-d)))) ,
  data = data,
  start = c(b1 = 3, b0 = 2, a = 2, c = 1, d = 5),
  control = nls.control(maxiter = 50,
    tol = 1e-05,
    warnOnly = FALSE) ,
  na.action = na.omit)
```

Notice that the *nls* call now contains start values for *b0* and for *b1*. In CurveBuilder, the start value entered for *b* will be treated as the start value for *b0*. Additionally, an input box will appear where the user can specify the start value for “*mod on b*,” which is *mod*’s effect on *b*, which is the parameter *b1*.

For Example 3, suppose the user has selected a Gompertz model with no moderation, but has specified that parameters *c* and *d* should be treated as random effects. Because random effects are involved, the app will construct a call to *nlme*. Code for the unmoderated Gompertz model remains the same as (6.1). Once the user has specified the grouping variable, start values, and any other adjustments, the final *nlme* call will look like this:



```

model = nlme(y ~ a + b*(exp(-exp(-c*(x-d)))) ,
  data = data,
  fixed = a + b + c + d ~ 1,
  random = c + d ~ 1,
  groups = ~grp,
  start = c(a = 2, b = 2, c = 1, d = 5),
  control = nlmeControl(maxIter = 50,
                        tolerance = 1e-06,
                        returnObject = FALSE),
  na.action = na.omit)

```

In Example 4, we will add complexity to the model in Example 3 by specifying that parameter  $b$  is moderated by the variable  $mod$ . Because parameter  $b$  is not random, the function code will be updated identically to (6.2). The final *nlme* call looks like this:

```

model = nlme(y ~ a + (b0 + b1*mod)*(exp(-exp(-c*(x-d)))) ,
  data = data,
  fixed = a + b0 + b1 + c + d ~ 1,
  random = c + d ~ 1,
  groups = ~grp,
  start = c(b1 = 3, b0 = 2, a = 2, c = 1, d = 5),
  control = nlmeControl(maxIter = 50,
                        tolerance = 1e-06,
                        returnObject = FALSE),
  na.action = na.omit)

```

Finally, for Example 5, we can add to the model by specifying that parameter  $b$  is moderated by  $mod$ , and that parameter  $b$  is a random effect. Code for this scenario is adapted from the code introduced by Grimm et al. (2016) for linear mixed growth models with time-invariant covariates. The function code will be updated as follows:

$$y \sim a + (b0 + b1*mod + bResid)*(exp(-exp(-c*(x-d))))). \quad (6.3)$$

Here, parameter  $b$  has been replaced with  $(b0 + b1*mod + bResid)$ . Parameter  $b$  now contains a moderated fixed component and a random component. The final *nlme* call will look like this:

```
model = nlme(y ~ a+(b0 + b1*mod + bResid)*(exp(-exp(-c*(x-d))))),
  data = data,
  fixed = a + c + d + b0 + b1 ~ 1,
  random = a + bResid + c ~ 1,
  groups = ~grp,
  start = c(b1 = 3, b0 = 2, a = 2, c = 1, d = 5),
  control = nlmeControl(maxIter = 50,
    tolerance = 1e-06,
    returnObject = FALSE)),
  na.action = na.omit)
```

### ***Troubleshooting***

If the model converges, then in the Create Model tab, “*Success message will appear here...*” is replaced with “*Model successfully converged!*” in green. Otherwise, R delivers an error, and a simplified error message will be shown in-app. Errors are caused by either user error or convergence failure. The app begins by checking for signs of user error. If *not* using the custom curve option, user errors are simple (e.g., a missing start value) and will be clearly communicated in the error message. If using the custom curve option, user error may arise from syntax errors in the custom equation. See the following section, *Using the custom curve option*, for details.

If user error is not detected, the app searches R’s error message for keywords that indicate convergence failure (e.g., “singular”, “singularity”, “convergence”). When these keywords are found, the app shows a simple message, “*The model failed to converge. Try entering different start values or simplifying model*” to remove the user burden of deciphering a cryptic error message. If the app cannot find a keyword, it will simply display the original error

message with “*The following error occurred:*”. However, even in these cases, the error message usually indicates convergence failure.

### **Using the Custom Curve Option**

The custom curve option – found in the Visualize Curves, Preview Start Values, and Create Model tabs – greatly enhances the generality of the app by allowing the user to visualize and fit any nonlinear (or linear) model. However, *the custom function entered by the user must be written with syntax that is readable in R*. Therefore, care must be taken by the user to ensure that the custom function is valid and has appropriate syntax. The purpose of this section is to provide guidelines for writing custom functions that are appropriate for R.

#### ***Parameter and Variable Names***

The custom function may contain up to five parameters. (However, in the Create Model tab, additional parameters can be added to the model by including any number of moderators, so the final model may have more than five parameters). Any parameters contained within the custom function must also be listed in the boxes below. Users should be sure to double check that the parameters listed in the custom function are also listed in the boxes, and check for typos – any discrepancies will result in an error message and a model that fails to converge. Parameters can have any name (e.g., “a”, “alpha”, “a0”), but parameter names *cannot* begin with a number or contain punctuation (e.g., “0a”, “a.”). Parameter names are *not* treated as case sensitive. Naming one parameter “a” and naming another parameter “A” will result in two parameters with the same name, leading to an error. The function *should* contain “x” and *should not* contain any variable names from the data set. The function *should not* contain “y =” or “y ~”. Following these guidelines will ensure that plots and models are created correctly by the app.

## ***Syntax Guide***

If the custom function contains R syntax errors, this will result in an error message and a model that fails to converge. Refer to Table 6.1 for a simple syntax guide for custom functions. Additionally, it is strongly recommended that users *do* write custom equations from scratch and *do not* copy and paste equations from LaTeX or any other equation display system. Copy-and-pasted equations likely contain R syntax errors; for example, there may be missing asterisks (\*) for multiplication, and symbols such as dashes and asterisks may be unreadable in R.

## ***Adding Moderation***

In the Create Model tab, any custom parameter may be moderated. Parameter names will auto populate in the appropriate input boxes, enabling the user to add moderation by point-and-click. Users *should* add moderators to the custom function with these point-and-click input boxes, and *should not* add moderation into the custom equation. If moderation is indicated in the custom equation but not with point-and-click input boxes, this will not be recognized by the app as moderation, and later functionality that is specific to moderated parameters (i.e., pick-a-point plots, Johnson-Neyman plots) will not be available.

## ***Troubleshooting***

If using the custom curve option in the Visualize Curves and Preview Start Values tabs, error messages are the result of user error. Check for syntax issues, as well as mismatches between the parameter names in the custom equation and the parameter names in the boxes below. *In the Create Model tab, the model may fail to converge due to user error, or because the model is too ill-fitting or complex.* Some straightforward user errors can be caught by the app (e.g., the custom equation does not contain “x”), and if these errors are detected, a simple error message will be displayed in-app. However, some syntax errors cannot be caught until the model

is fit and fails to converge. Therefore, if a custom model fails to converge, check carefully for syntax errors and/or parameter name mismatches. If all user errors have been corrected and the model still fails to converge, the model is likely too complex or ill-fitting, or the starting values need to be adjusted.

Table 6.1. Syntax Guide for Custom Functions.

Rule	Good Example(s)	Bad Example(s)
Multiplication must be indicated with an asterisk (*)	$a*x$	$a(x)$ $ax$ $a*x$ [center asterisk copied from a LaTeX equation]
Powers must be indicated with a carat (^)	$x^3$ $x^b$ $x^{-1}$ $x^{1/2}$	$x3$ $x**3$ $xb$
Euler's number ( $e$ ) must be indicated with $\text{exp}()$	$\text{exp}(b)$ $\text{exp}(7)$	$\text{exp}b$ $e(b)$ $e^b$ $e7$ $e(7)$ $e^7$
Subtraction must be indicated with a short dash (-)	$b - c$	$b - c$ [long dash copied from a LaTeX equation]
Open parentheses must be accompanied by closed parentheses	$a + b*(x^c)$	$a+b*(x^c$
Operators and/or symbols must be readable by R  <i>Note:</i> by default, the $\text{log}()$ function computes log base 10	$\text{pi}$ $\text{sqrt}(x)$ $\text{sin}(x)$ $\text{cos}(x)$ $\text{tan}(x)$ $\text{log}(x)$ [log base 10] $\text{log}(x, 20)$ [log base 20]	$\text{ln}(x)$ $\text{inv}(x)$ $\text{inverse}(x)$

## Results

If the model converges, the Results tab populates with model information and output tables. The model selection and performance indices are the log likelihood, AIC, BIC, and root mean squared error (RMSE), which have been widely recommended for the evaluation of nonlinear models (e.g., Archontoulis & Miguez, 2015; Cho et al., 2022; Wallach, 2006).

The Parameter Estimates table contains fixed effect estimates and their precisions. If moderation has been included in the model, the name of each moderated parameter (e.g.,  $b$ ) is replaced by multiple parameters (e.g.,  $b_0$  and  $b_1$ ). If parameter  $b$  is moderated, then  $b_0$  is the estimated value of  $b$  when the moderator is zero, and  $b_1$  is the estimated change in parameter  $b$  when the moderator increases by one unit. The parameter name will be accompanied by the moderator name to clarify these results. If parameter  $b$  is moderated by *Age* and *Gender*, then the table will contain rows showing  $b_0$ ,  $b_1$  (*Effect of Age on  $b$* ) and  $b_2$  (*Effect of Gender on  $b$* ). If the model includes random effects, then the Random Effect Variances table also appears. This table shows the level-2 variance and standard deviation (*SD*) of each random parameter, level-2 correlations among the random parameters, as well as level-1 residual variance and *SD*. Additionally, the user may choose to display the asymptotic covariance (ACOV) matrix of parameters, the asymptotic correlation matrix of parameters, and/or the raw R output for the model. All tables in the Results tab can be copy-and-pasted directly into a Word document; they will copy as tables and will maintain their formatting.

## Plots

The Plots tab has four parts, each of which yields plot(s) that enable the user to evaluate the model's fit to the data, visualize results, and test hypotheses about moderation if applicable.

## ***Model Evaluation***

This tab contains four plots. First, the residuals vs. fitted y-values plot is useful for evaluating residual homoscedasticity, and for identifying any remaining patterns in the data that are not accounted for by the model (Motulsky & Christopoulos, 2004; Seber & Wild, 1989). For models without random effects (i.e., those created with *nls*), the plot displays standardized residuals. For models with random effects (i.e., those created with *nlme*), the plot displays level-1 conditional standardized residuals, consistent with the recommendations given in Cho et al. (2022). Second, the residual autocorrelation plot is helpful for assessing the independence of residuals, particularly within longitudinal data. The x-axis of this plot is lag, where lag = 1 means the residual for observation  $t$  is correlated with the residual for observation  $t-1$ , and lag = 2 means the residual for observation  $t$  is correlated the residual for observation  $t-2$ , and so on. The x-axis ranges from lag = 0 to lag = 15. The y-axis of this plot is the average correlation of the given pair of residuals. Third and fourth, this tab displays a histogram of standardized residuals and a QQ-plot of standardized residuals, each of which are useful for evaluating whether the residuals are normally distributed (Cho et al., 2022).

## ***Observed Data and Fitted Values***

Here, the observed predictor and outcome variables are plotted with fitted values from the model. This plot is helpful for ensuring that model-implied values correspond well with the observed data. For models without random effects (*nls* objects), fitted values are obtained via the *fitted()* function in R. For models with random effects (*nlme* objects), fitted values are obtained from the fitted values attribute of the model (e.g., *model\$fitted*); from here, population fitted values are extracted, which correspond to the fixed effects only (see Pinheiro et al., 2023). The

plot is created with *geom\_smooth()* from the *ggplot2* package (Wickham et al., 2016). The axis labels and title can be easily edited to prepare the plot for inclusion in a publication.

The fitted values can also be viewed with a confidence band. The band shown in the plot is a 95% confidence band obtained through simulation. Here, we assume that the parameter estimates follow a multivariate normal distribution; the means are the parameter estimates given in the Results tab (for *nlme* models, the fixed effect estimates), and the (co)variances are the ACOV of the parameter estimates also shown in the Results tab. To obtain the confidence band, 1000 sets of parameter estimates are drawn from this multivariate normal distribution, and fitted *y*-values are obtained for each set of parameter estimates. Finally, the 2.5<sup>th</sup> and 97.5<sup>th</sup> percentiles of these *y*-values are extracted, and those percentiles are plotted to create the confidence band. For further detail about simulation-based confidence bands, see Bolker (2008).

### ***Pick-a-Point***

Pick-a-point plots display the relation between *x* and *y* at different values of the moderator. The focal predictor is on the *x*-axis, and the *y*-axis is the predicted value of *y* given *x* and given a certain value of the moderator. If the model contains multiple moderators, only one moderator can be plotted at a time.

Predicted values are obtained with the *predict()* function in R, which works for both *nls* and *nlme* objects. If there are other moderators in the model – besides the moderator that is the basis of the pick-a-point plot – they are held constant at their means when computing predicted values. If working with a *nlme* object (i.e., a NLME model), predictions are population level.

The pick-a-point plot created in CurveBuilder is highly customizable. First, along with predicted values, the plot also displays the observed data, and this feature can be switched on or off. Second, the user may choose to display the moderator with color-coding or with paneling. If



using color-coding, there is an option to convert to grayscale (e.g., if grayscale is needed for publication). Whether using color-coding or paneling, the moderator legend, axis labels, and title are always editable.

The app can create pick-a-point plots for a continuous, binary, or multicategorical moderator. If the moderator is binary, no further user input is needed. The user should ensure the binary variable takes on only two values in the data set (besides missing values). If the moderator is indicated to be binary but more than two values are detected, the plot will not render.

If the moderator is multicategorical (i.e., has three or more categories), the user must indicate how many categories there are (the app can accommodate up to 20 categories) and select the coding variables that represent the multicategorical variable. Any type of coding variable (e.g., dummy codes, (un)weighted effect codes, contrast codes) is allowed. If there are  $k$  categories, the user should ensure that  $k - 1$  coding variables are selected. Internally, the app iterates through the rows of the data set and stores each unique pattern that the coding variables take on (e.g., if there are three dummy codes, 1,0,0; 0,1,0; 0,0,1; 0,0,0). Based on these patterns, the app creates a single categorical variable that is used to color-code or panel the plot. The coding variable patterns that correspond with each category are displayed in-app, so the user can update the moderator labels appropriately. See Example 2 for more detail.

If the moderator is continuous, the user may plot three or five values of the moderator. The user must indicate these moderator values (the plot will begin rendering once the user begins entering them). To help choose moderator values, the app displays the moderator mean and  $SD$ . If plotting three values, the user may choose to plot the mean  $\pm 1SD$ . Similarly, if plotting five values, the user may wish to plot the mean  $\pm 1SD$  and  $\pm 2SD$ . However, any values may be entered here. Once the user enters moderator values, the data will be binned according to the

small multiples procedure described by McCabe et al. (2018). As an example of how this binning occurs, suppose the moderator's  $mean = 0$ ,  $SD = 1$ , and range is -3 to 3. Next, suppose the user has entered five moderator values to be plotted: -2, -1, 0, 1, and 2. The data will be binned as follows: bin 1 = [-3, -1.5], bin 2 = [-1.5, -0.5], bin 3 = [-0.5, 0.5], bin 4 = [0.5, 1.5], and bin 5 = [1.5, 3]. Bins are created by finding the halfway point between each entered moderator value. Then, the observed data are color-coded or paneled according to bin.

### ***Johnson-Neyman***

Johnson-Neyman (JN) plots offer a more detailed method for understanding and testing hypotheses about moderation. Here, the  $x$ -axis is the moderator, and the  $y$ -axis is the conditional value of the moderated parameter. This plot is available only for continuous moderators. If the model contains multiple continuous moderators, only one can be plotted at a time.

When JN plots are used for linear models, the moderated quantity on the  $y$ -axis is always a simple slope, i.e., the slope of the focal predictor conditional on the value of the moderator. In CurveBuilder, because any parameter of any nonlinear model may be moderated, the  $y$ -axis may contain any simple parameter, i.e., any parameter that is conditional on the value of the moderator, such as a simple asymptote or a simple rate of growth. The line in the JN plot depicts this simple parameter, and the surrounding confidence band depicts the standard error of the simple parameter. For details about how this simple parameter and its standard error are computed, see Chapter 5.

The app also computes significance boundaries for the JN plot. These significance boundaries depend on the null value for the moderated parameter, which is specified by the user. Significance boundaries are denoted by a solid vertical line, and the null value is denoted by a dashed horizontal line in the plot. By default, the null value is zero, but this can be changed

depending on the parameter and the research context (see Chapter 5 for a discussion of nonzero null values in moderated nonlinear models). If the null value is zero, then the significance boundaries indicate the moderator values at which the parameter goes from being significantly different from zero to non-significantly different from zero (using  $\alpha = .05$ ). In other words, significance boundaries indicate the moderator values at which the confidence band transitions from containing zero to not containing zero. The same logic applies to nonzero null values; for example, if the user indicates a null value of two, then the app implements the equations given in Chapter 5 to find the moderator values at which the parameter goes from being significantly different to non-significantly different from the new null value; the plot and significance boundaries are updated accordingly. Significance boundaries are displayed in the plot only if they fall within the observed range of the moderator. Thus, although up to two significance boundaries may exist, the plot may display one or zero.

Beneath the plot, a short sentence about the significance boundaries is displayed. Significance boundaries are presented here regardless of whether they are within the observed range of the moderator. Additionally, if there are two significance boundaries, the app indicates whether the parameter is significant between or outside the boundaries.

The JN plot has many customizable features. First, a rug plot is displayed along the  $x$ -axis, which depicts observed values of the moderator. This feature may be switched on or off, but keeping it on is recommended. If there are regions of the moderator where observed values are sparse, then conditional values of the moderated parameter in these regions may need to be interpreted with caution. (For example, if the moderator ranges from -3 to 3, but there are only two observations that are  $>2$ , then conditional values of the moderated parameter when the moderator is  $>2$  are likely unreliable.) Second, the confidence band is color-coded according to

statistical significance, and this color-coding may be converted to grayscale if needed for publication purposes. Finally, the axis labels and the plot title are editable.

## **CurveBuilder Examples**

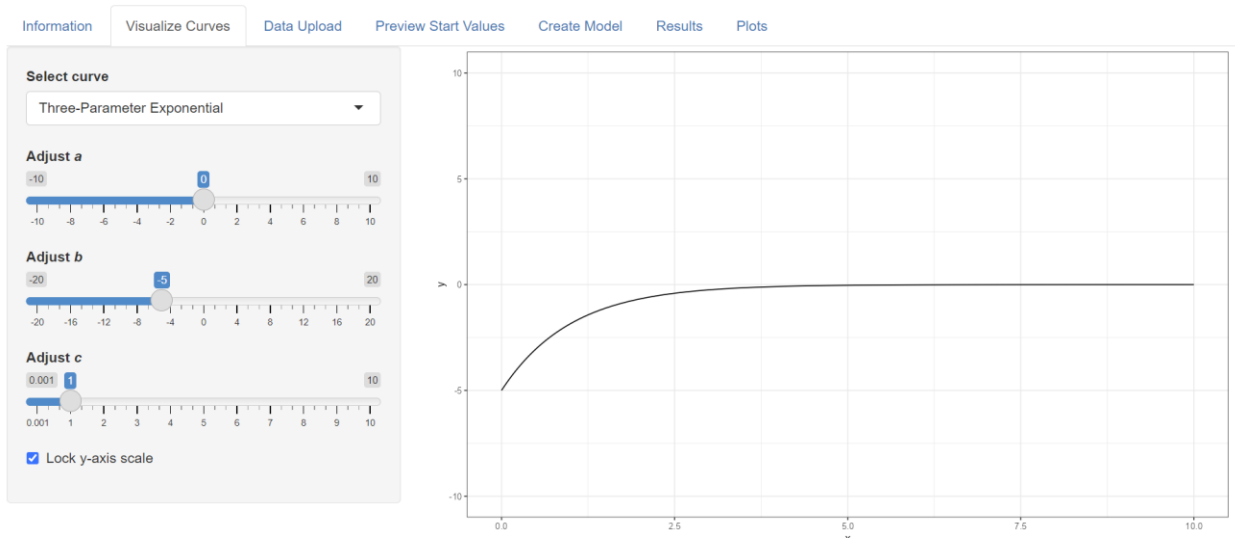
### **Example 1: Custom Functions and a Continuous Moderator**

In this example, we will explore the utilities available in CurveBuilder for creating custom functions, as well as visualizing results when the model involves a continuous moderator. We will work with a simulated data set inspired by Ren et al. (2022). The goal of this study was to characterize the relation between frequency of social interactions and psychological wellbeing. The authors sought to compare multiple competing hypotheses about this relation. First, the “More is Better” hypothesis assumes a linear relation between interaction quantity and wellbeing. Second, the “Inverted U” hypothesis can be roughly approximated by a quadratic relation, such that more interaction promotes greater wellbeing, but at the highest interaction frequencies, there is a detrimental effect. Third, the “Diminishing Returns” hypothesis posits that at the highest levels of interaction quantity, interaction quantity has little impact on wellbeing, meaning the effect of interaction quantity levels off. Ren et al. (2022) evaluated these hypotheses by comparing the fit of linear, quadratic, and piecewise linear models. In this example, we will compare these same models, but we will replace the piecewise linear model with a nonlinear curve indicative of “diminishing returns.” Finally, the authors explored whether extraversion moderated the relation between interaction quantity and wellbeing; these results were null, but for demonstrative purposes, our simulated data will yield significant moderation that is consistent with the authors’ hypotheses.

### *Step 0: Visualize Curves*

One goal of this analysis is to characterize the “Diminishing Returns” hypothesis with a nonlinear model rather than a piecewise linear model. (For a discussion of the advantages of nonlinear models for assessing hypotheses of “diminishing returns” or “plateauing associations,” see Chapter 2.) To explore our options, we can make use of the Visualize Curves tab. Within this tab, there is a group of functions listed under the exponential category, which yield curves that are consistent with the diminishing returns hypothesis. For each of these functions, we can read about the parameters that control the shape of the curve and use the available sliders to further understand each parameter. Upon exploring each option, we may note that the Jense-Bayley function and the Preece-Baines function each assume a two-phase relation between  $x$  and  $y$ ; there are parameters that govern the first “phase” of the curve and parameters that govern the second “phase” of the curve. Because our current hypothesis does not posit a two-stage relation, we may choose to eliminate these options. Therefore, we can further explore the Three-Parameter Exponential (3PE) function (Fig. 6.1) and the Michaelis-Menten (MM) function (Fig. 6.2).

Figure 6.1. Three-Parameter Exponential Function in the Visualize Curves Tab.



Exponential curve:

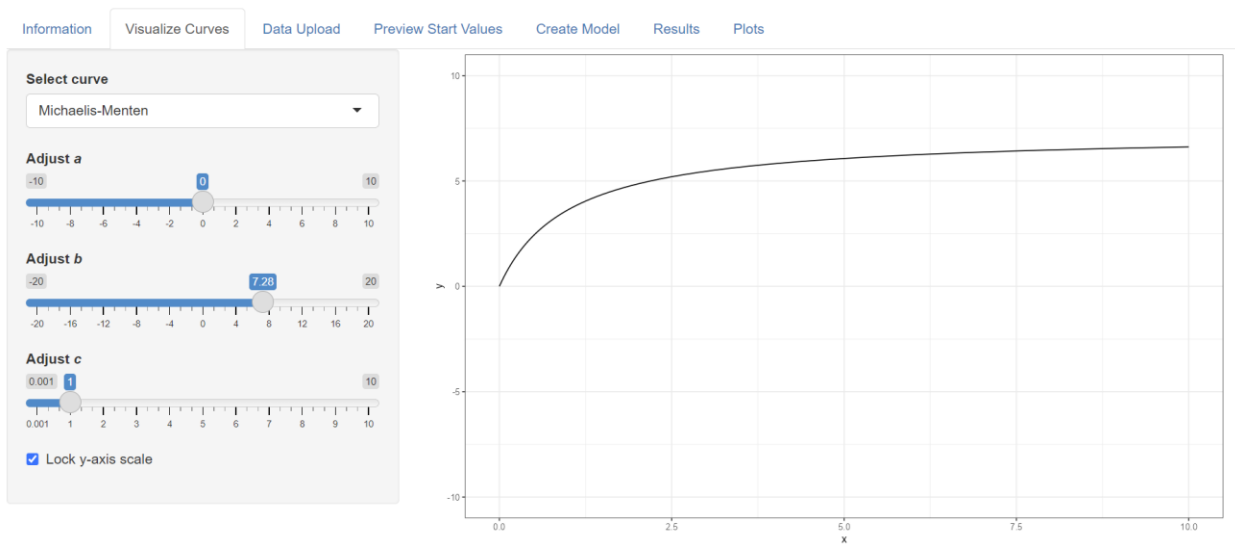
$$f(x) = a + b(\exp(-c * x))$$

**a** is the asymptote

**b** is the vertical distance between intercept and asymptote

**c** is the rate of change toward the asymptote

Figure 6.2. Michaelis-Menten Function in the Visualize Curves Tab.



Michaelis-Menten curve:

$$f(x) = a + \frac{bx}{c + x}$$

**a** is the intercept

**b** is the vertical distance between intercept and asymptote

**c** is the location at which half of the change between the intercept and asymptote has occurred

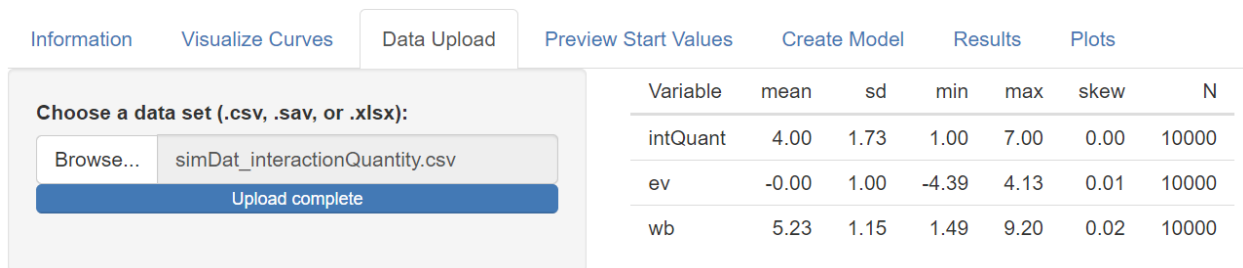
These functions yield curves that correspond well with our hypothesized trend.

Parameters  $a$  and  $b$  are interpreted similarly in the two functions, but the meaning of parameter  $c$  differs. In the 3PE function, parameter  $c$  is the rate of change, whereas in the MM function, parameter  $c$  is the location along the  $x$ -axis at which 50% of change has occurred. While either interpretation could be useful, parameter  $c$  of the MM function often yields more concrete insights (McNeish et al., 2023). Let us proceed with the MM model for further analyses.

### Step 1: Data Upload

Upon uploading our data, we see a summary of the variables available to us (Fig. 6.3): *intQuant* is interaction quantity, which ranges from 1 to 7. In Ren et al. (2022), this was the mean of three items that assessed how often participants spent an evening with family, someone from their neighborhood, or a friend. *ev* is the Extraversion factor from the Big Five, which has been standardized. *wb* is psychological wellbeing, which was an average of three measures which assessed happiness, life satisfaction, and social wellbeing on a scale ranging from 0-10.

Figure 6.3. Interaction Quantity Data Summary in Data Upload Tab.

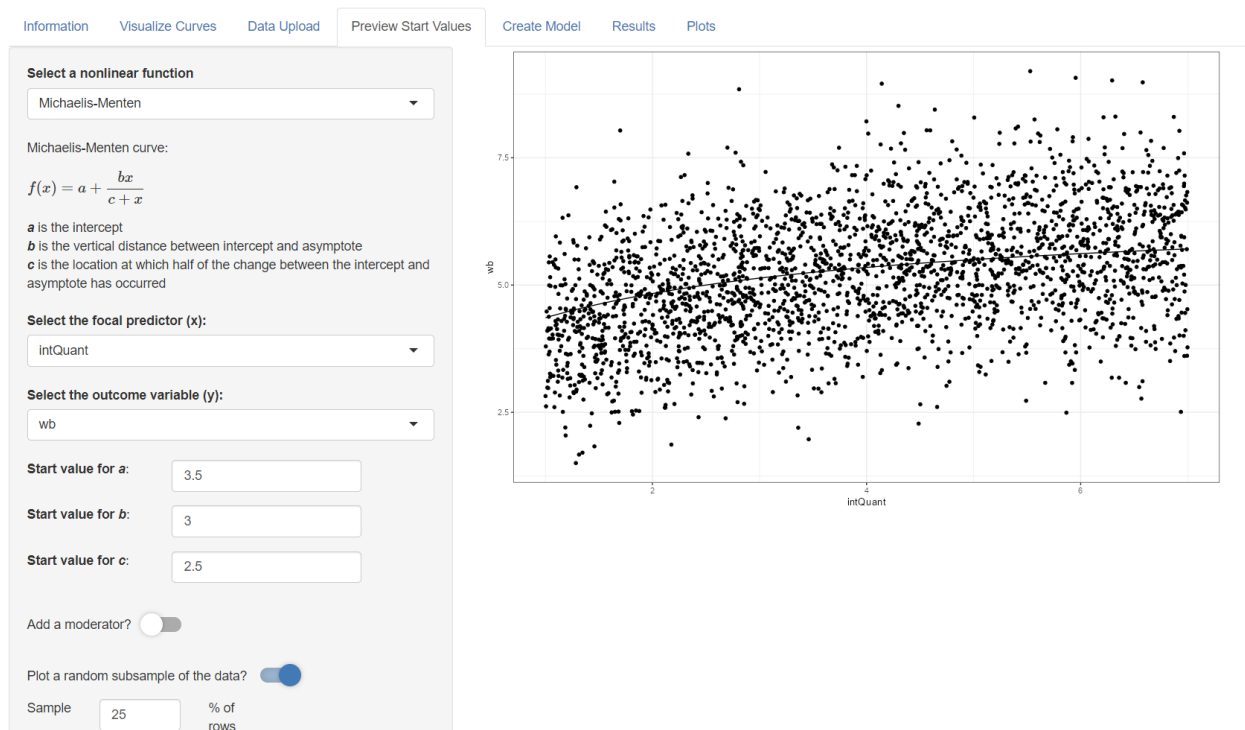


### Step 2: Preview Start Values

Next, we will use the Preview Start Values tab to identify parameter values for the MM model that correspond with our data relatively well. Because the data set is large (10,000 rows),

we will plot a subsample of the data for a less cluttered display. Any size subset of the data can be plotted here, but we will maintain the default value of a 25% random sample. After indicating our predictor and outcome variables, we see that parameter values of  $a = 3.5$ ,  $b = 3$ , and  $c = 2.5$  yield a relatively well-fitting curve (Fig. 6.4.).

Figure 6.4. Preview Start Values Tab with Michaelis-Menten Curve.



### Steps 3 and 4: Create Model and Results

In this section, we will alternate between the Create Model and Results tabs to demonstrate the process of fitting multiple models and carrying out model selection. Let us begin by fitting the MM model, which is consistent with the Diminishing Returns hypothesis. To fit this model in the Create Model tab, we simply select Michaelis-Menten as our desired function, indicate *intQuant* and *wb* as our predictor and outcome variable, and import the start values that



were just identified in the Preview tab. Additionally, we specify that all three parameters are moderated by  $ev$ . CurveBuilder then prompts us to enter start values for the effects of  $ev$  on parameters  $a$ ,  $b$ , and  $c$ . As  $ev$  increases by one unit, about how much do we expect parameters  $a$ ,  $b$ , and  $c$  to change? To increase the likelihood of convergence, we should consider any prior knowledge and hypotheses when choosing these start values. Ren et al. (2022) suggest “less extraverted individuals may be more likely to experience reduced wellbeing at high levels of interaction quantity” (p. 1069). For less extraverted people, wellbeing may be lower at the highest levels of  $intQuant$ , meaning that for more extraverted people, wellbeing may be higher at the highest levels of  $intQuant$ . To incorporate this expectation into our start values, note that parameter  $b$  governs the vertical distance between the intercept and the asymptote of the curve. For more extraverted people, the asymptote may be higher, as it corresponds with wellbeing at the highest levels of  $intQuant$ . Therefore, we can enter a positive start value (say, 1) for the effect of  $ev$  on parameter  $b$ . We have insufficient information to inform start values for the effect of  $ev$  on parameters  $a$  and  $c$ , so we can leave these at zero. After entering these specifications and clicking Fit Model, the text under the button changes from “*Success message will appear here...*” to “*Model successfully converged!*”, meaning the model converged (Fig. 6.5).

In the Results tab (Fig 6.6), we see a table of parameter estimates. Note that parameter  $a$  has been replaced with  $a0$  and  $a1$  (*Effect of  $ev$  on  $a$* ), such that  $a0$  is the estimated intercept when the moderator  $ev$  is zero, and  $a1$  is the estimated change in the intercept when  $ev$  increases by one unit. Similarly, parameter  $b$  has been replaced with  $b0$  and  $b1$  (*Effect of  $ev$  on  $b$* ), such that  $b0$  is the estimated total growth when  $ev$  is zero, and  $b1$  is the change in total growth when  $ev$  increases by one unit. We also see that  $AIC = 28426$  and  $BIC = 28477$  for the MM model.

Figure 6.5. Fitting the Moderated MM Model in the Create Model Tab.

Figure 6.6. Results Tab for the Moderated MM Model.

Parameter Estimates				
	Estimate	Std. Error	t value	Pr(> t )
a1 (Effect of ev on a)	-0.491	0.081	-6.100	0.000
a0	2.796	0.194	14.403	0.000
b1 (Effect of ev on b)	0.951	0.099	9.582	0.000
b0	4.147	0.100	41.350	0.000
c1 (Effect of ev on c)	-0.417	0.087	-4.778	0.000
c0	2.603	0.425	6.126	0.000

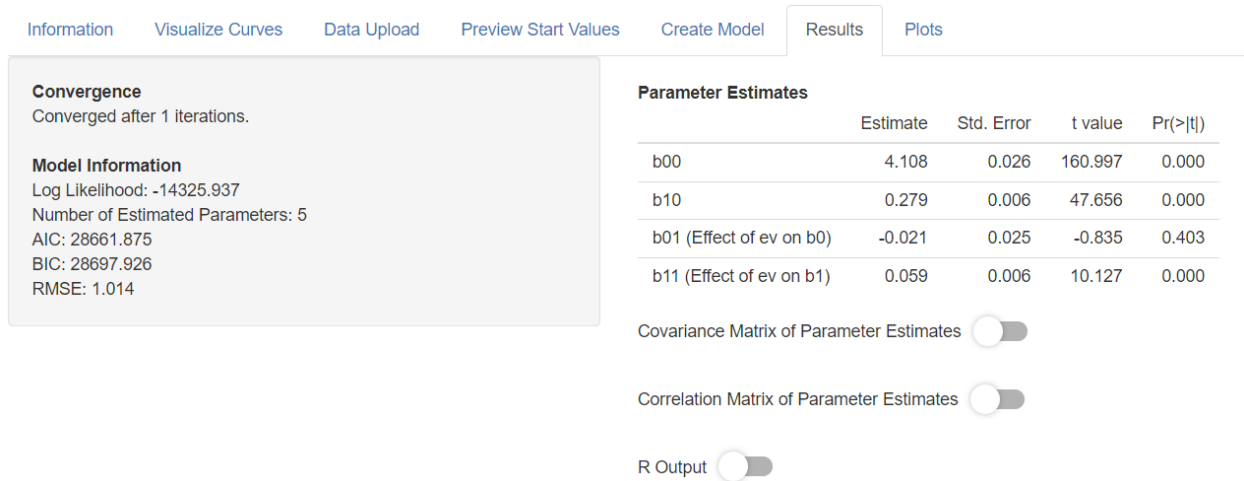
Next, we must compare the MM model to the linear and quadratic models, which correspond with the More is Better and Inverted U hypotheses, respectively. We can create these linear models as custom functions. (Although these models will be created via calls to *nls*, or to

*nlme* if random effects are included, both can accommodate linear models.) Let us begin by returning to the Create Model tab and specifying the moderated linear model. We simply enter the linear model,  $b_0 + b_1*x$ , into the custom function input box, and in the boxes below, indicate that  $b_0$  and  $b_1$  are the model parameters. Additionally, we specify  $ev$  as a moderator of both  $b_0$  and  $b_1$ . Because good start values are not essential for linear models, we can leave all start values at zero for simplicity. Upon fitting the model, the Create Model tab indicates that convergence was achieved (Fig. 6.7).

In the Results tab (Fig. 6.8), parameter names have been updated like they were in the MM model;  $b_0$  has been replaced with  $b_{00}$  and  $b_{01}$  (*Effect of  $ev$  on  $b_0$* ), and  $b_1$  has been replaced with  $b_{10}$  and  $b_{11}$  (*Effect of  $ev$  on  $b_1$* ). The model converged after 1 iteration because iterative estimation is not necessary for linear models. We also see that for this model,  $AIC = 28662$  and  $BIC = 28698$ .  $AIC$  and  $BIC$  for the linear model are both higher than those observed for the MM model. So far, we have garnered support for the Diminishing Returns hypothesis over the More is Better hypothesis.

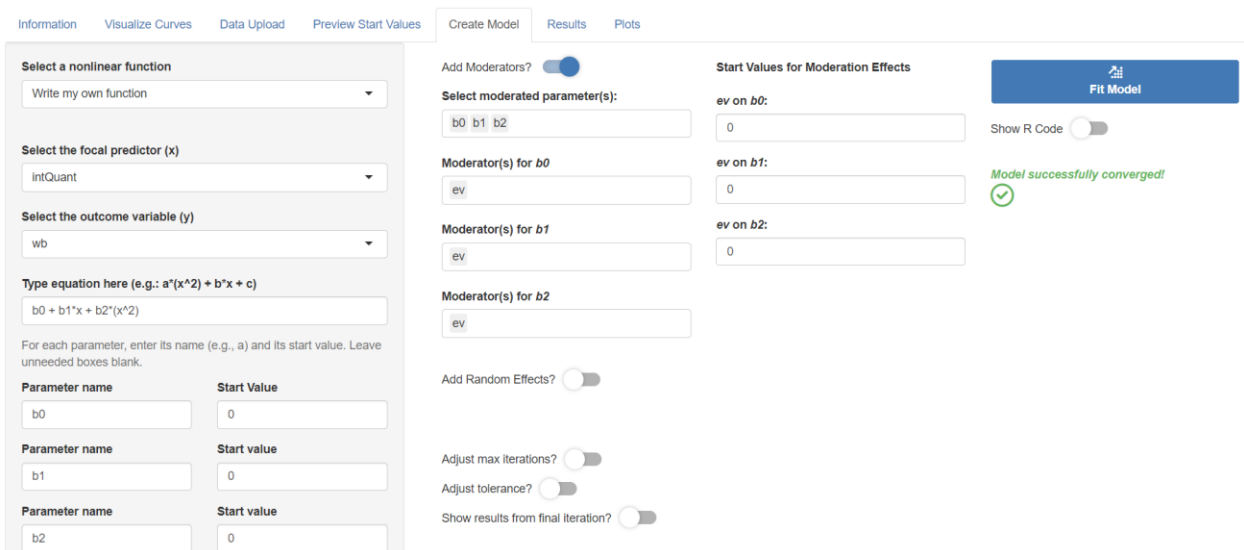
Figure 6.7. Fitting the Moderated Linear Model in the Create Model Tab.

Figure 6.8. Results Tab for the Moderated Linear Model.



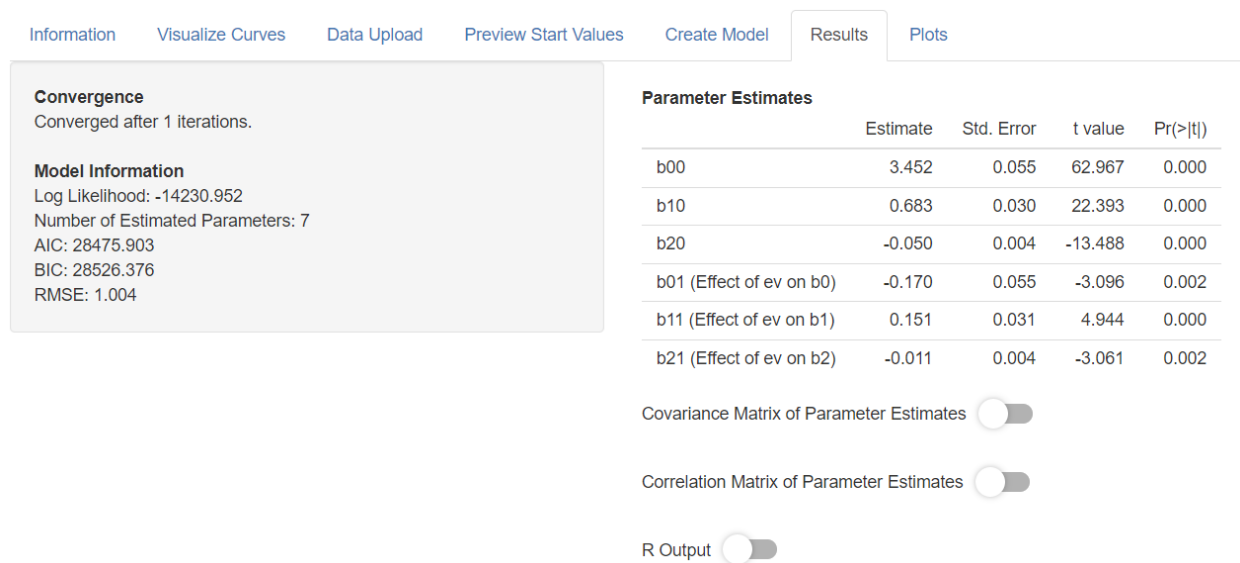
Next, let us return to the Create Model tab, and use the custom function feature to fit a quadratic model consistent with the Inverted U hypothesis. After entering the quadratic function, listing each parameter, and specifying *ev* as a moderator of each, CurveBuilder indicates that the model has converged (Fig. 6.9).

Figure 6.9. Fitting the Moderated Quadratic Model in the Create Model Tab.



In the Results tab (Fig. 6.10), we see parameter estimates for  $b00$  (the intercept when  $ev$  is zero),  $b10$  (the linear term when  $ev$  is zero),  $b20$  (the quadratic term when  $ev$  is zero),  $b01$  (change in intercept when  $ev$  increases by one unit),  $b11$  (change in the linear term when  $ev$  increases by one unit), and  $b21$  (change in the quadratic term when  $ev$  increases by one unit). For this model,  $AIC = 28476$  and  $BIC = 28526$ .  $AIC$  and  $BIC$  indicate that the quadratic model fits better than the linear model, but worse than the MM model. Overall, we have obtained support for the Diminishing Returns hypothesis over the More is Better and Inverted U hypotheses.

Figure 6.10. Results Tab for the Moderated Quadratic Model.



$AIC$  and  $BIC$  for the MM model are the lowest, suggesting that this model fits best to the data. Therefore, we will proceed with this model for further evaluation and interpretation. As shown in Figure 6.6, we have obtained estimates for  $a0$  (parameter  $a$  when  $ev$  is zero),  $a1$  (the change in parameter  $a$  when  $ev$  increases by one unit),  $b0$  (parameter  $b$  when  $ev$  is zero),  $b1$  (the change in parameter  $b$  when  $ev$  increases by one unit),  $c0$  (parameter  $c$  when  $ev$  is zero), and  $c1$

(the change in parameter  $c$  when  $ev$  increases by one unit). To interpret these estimates, note that  $ev$  has been centered such that its mean is zero. Therefore,  $ev = 0$  means that  $ev$  is at its mean.

Parameter  $a0 = 2.80$ , and parameter  $a$  is the  $y$ -intercept. Therefore, for individuals with mean levels of extraversion, we can expect a psychological wellbeing score of about 2.80 when social interaction frequency is zero. Parameter  $a1 = -0.49$ , indicating that as extraversion increases, the  $y$ -intercept decreases by about 0.49. In other words, more extraverted people are less happy and satisfied when interaction frequency is zero. Next, parameter  $b0 = 4.15$ , and parameter  $b$  is the vertical distance between the intercept and asymptote of the curve. For individuals with average extraversion, frequent social interaction results in a wellbeing score that is about 4.15 points higher than the  $y$ -intercept (i.e., wellbeing with zero interaction).

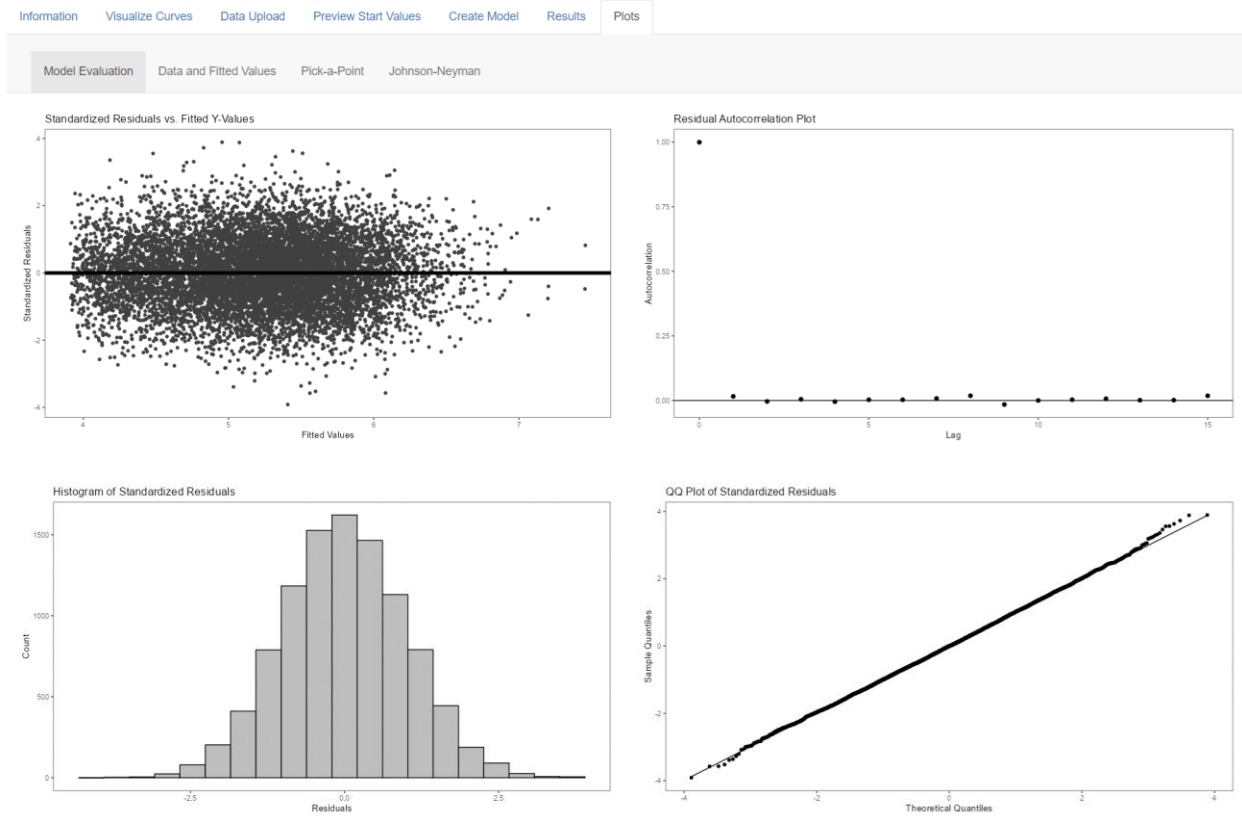
Additionally,  $b1 = 0.95$ , meaning that as extraversion increases, this vertical distance also increases; more extraverted people benefit more from frequent social interaction. Finally, parameter  $c0 = 2.60$ , and  $c$  is the location on the  $x$ -axis at which 50% of change has occurred. Here, “50% of change” can be interpreted as the halfway point of wellbeing relative to its maximum. For people with average extraversion, the halfway point of wellbeing occurs at an interaction frequency of about 2.6. Additionally,  $c1 = -0.42$ , meaning as extraversion increases, the halfway point of wellbeing occurs at a smaller  $x$ -value. In other words, more extraverted people require fewer social interactions to reach the halfway point of wellbeing.

### ***Step 5: Plots***

In the Plots tab, we can begin with Model Evaluation (Fig 6.11) to assess how well the moderated MM model characterizes our data. The Residuals vs. Fitted Y-Values plot shows no patterns in terms of residual mean or variance. The Residual Autocorrelation plot shows

correlations near zero for lag = 1 and beyond. The Histogram and QQ Plot of Residuals both indicate that residuals are normally distributed. All plots indicate good model-data fit.

*Figure 6.11. Model Evaluation Plots for the Moderated MM Model.*



Proceeding to the Data and Fitted Values tab, we can visualize how the model-implied y-values correspond with our observed data. Once again, this plot also indicates satisfactory model-data correspondence. To prepare this plot for publication, we can edit the x- and y-axis labels as desired (Fig. 6.12).

Figure 6.12. Data and Fitted Values Plot for the Moderated MM Model.

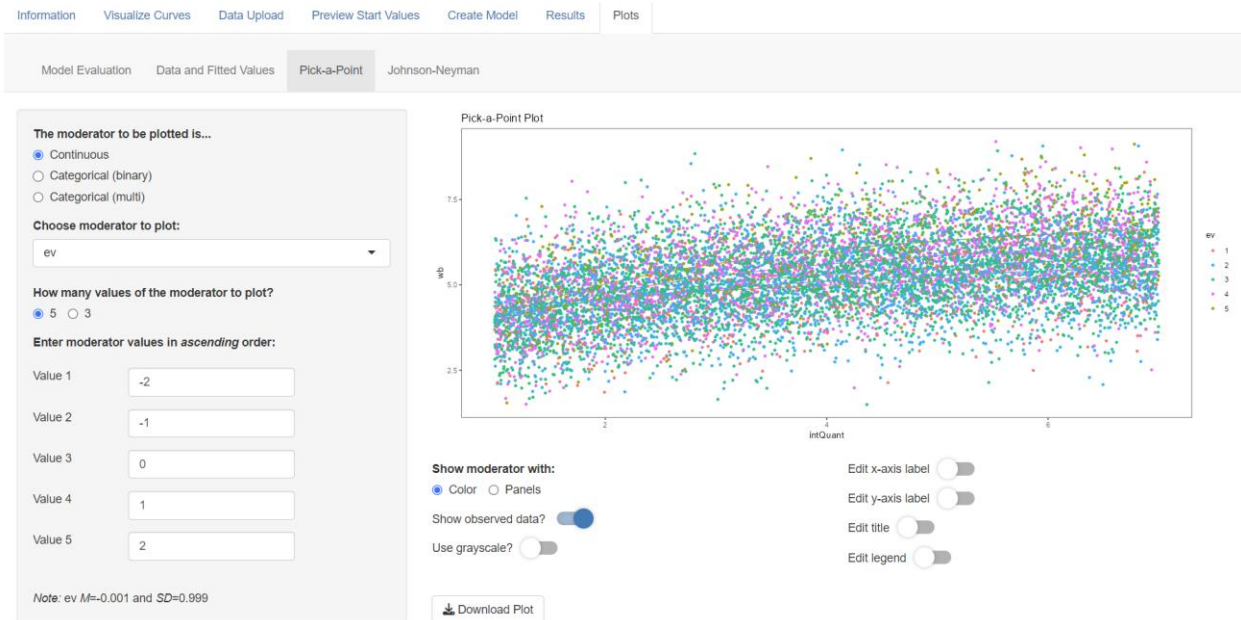


Next, we will use pick-a-point and JN plots to gain a better understanding of how extraversion moderates the relation between interaction quantity and wellbeing. The Pick-a-Point tab allows us to plot the curve linking *intQuant* to *wb* at various values of *ev*. Because *ev* is a continuous moderator, we can plot the curve at either three or five values of *ev*. Here, we will select five values. At the bottom of the left-hand panel, the mean and SD of *ev* are shown, which may help us choose values to plot. Because *ev* has been standardized, we see its mean is about zero and its *SD* is about one. Therefore, we may select -2, -1, 0, 1, and 2 as the *ev* values at which to plot the curve. The observed data will be split into five bins according to these values (see prior section for binning details).

We can choose to view the curves with or without the observed data, and we may display *ev* values either with color or with paneling. The default plot, with observed data and color, is shown in Figure 6.13.

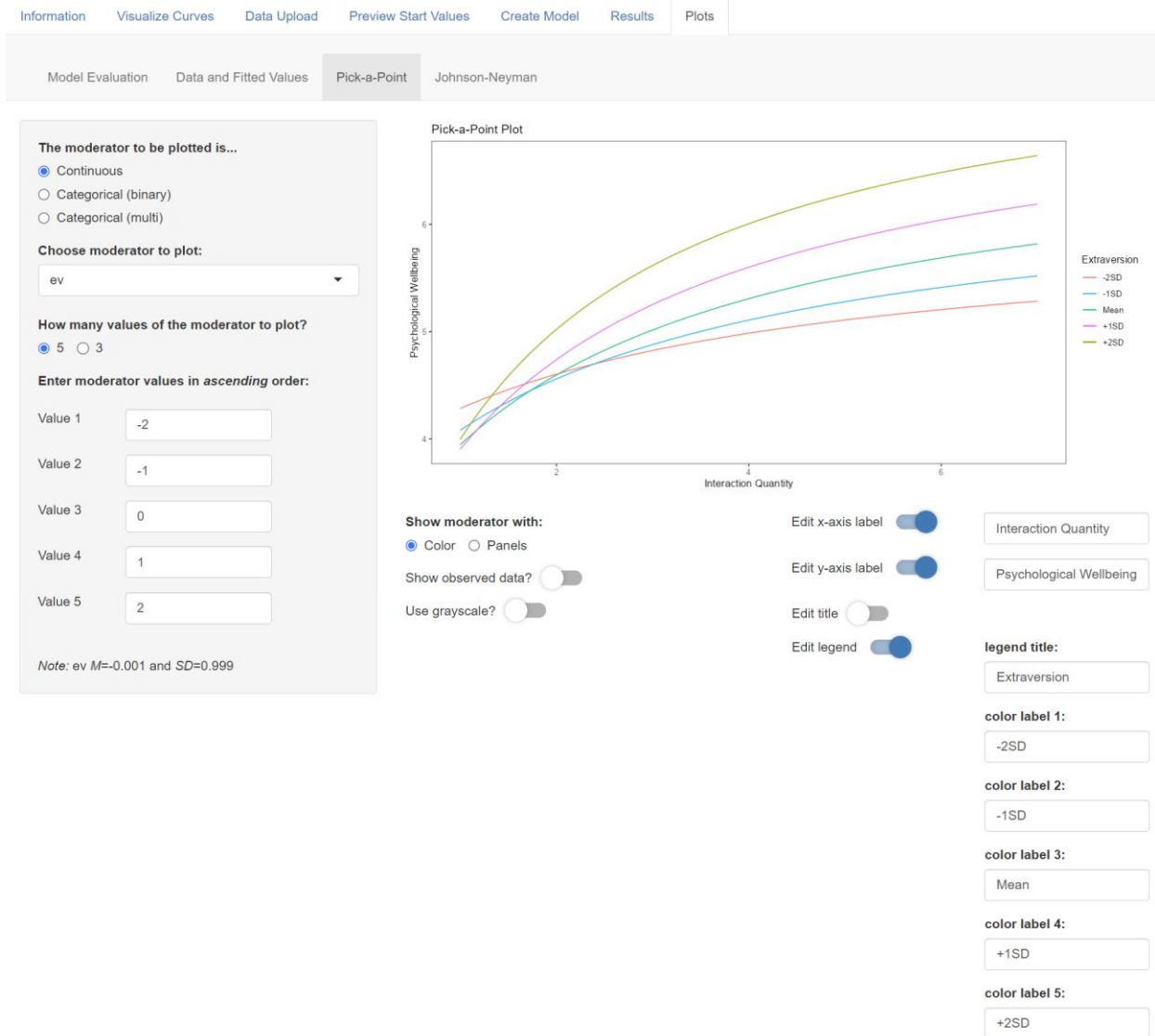


Figure 6.13. Pick-a-Point Plot with Default Settings for the Moderated MM Model.



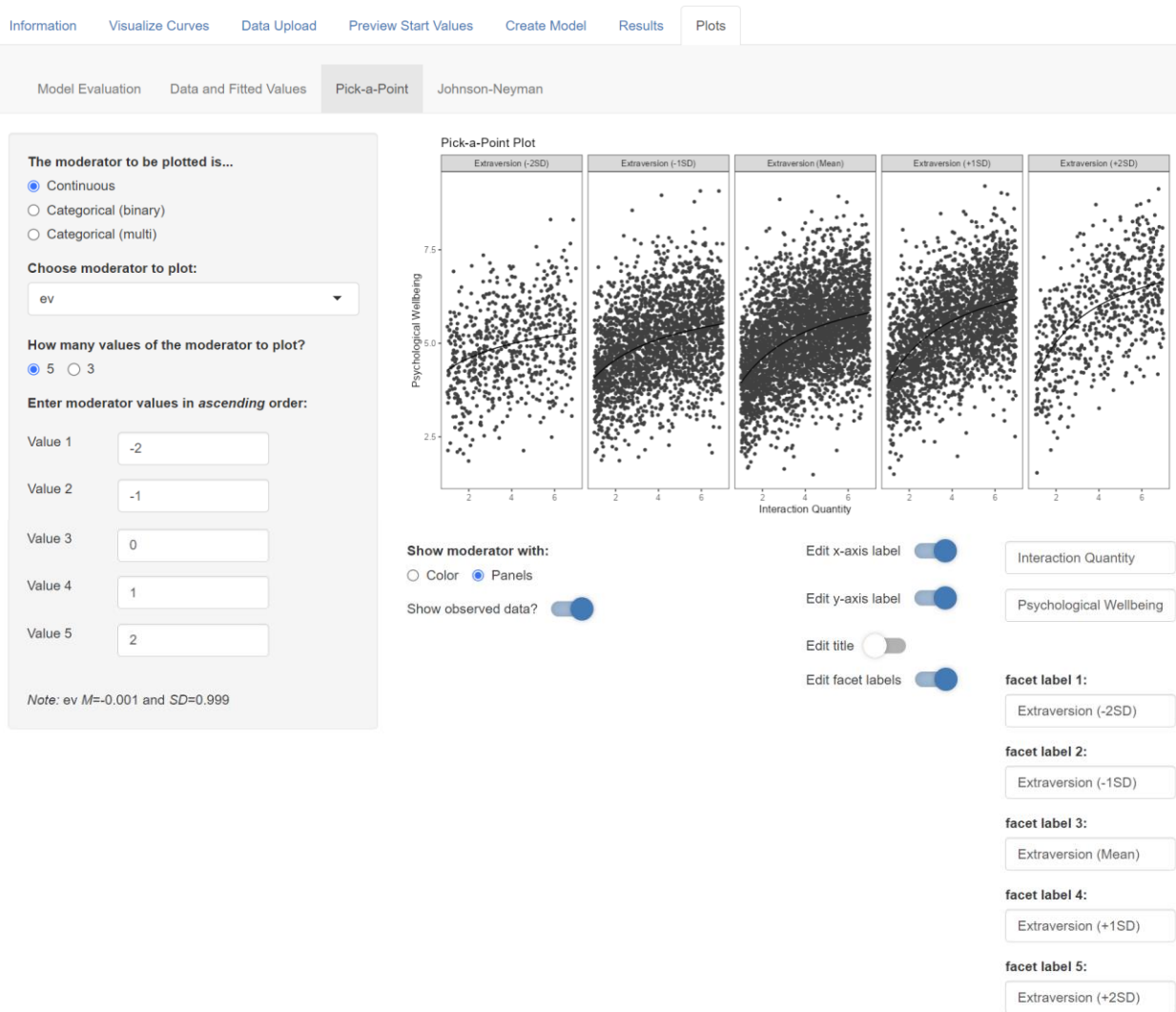
Because there are so many data points, the display in Figure 6.13 appears a bit cluttered. It would also be helpful to make the legend labels more descriptive. After making those edits, as well as editing the plot axes and title, and switching off the observed data layer, we obtain the plot shown in Figure 6.14.

Figure 6.14. Customized Pick-a-Point Plot for the Moderated MM Model.



Another way to declutter the plot – without sacrificing the observed data – is to use paneling rather than color coding. After selecting this option and editing the panel labels, we obtain the plot shown in Figure 6.15.

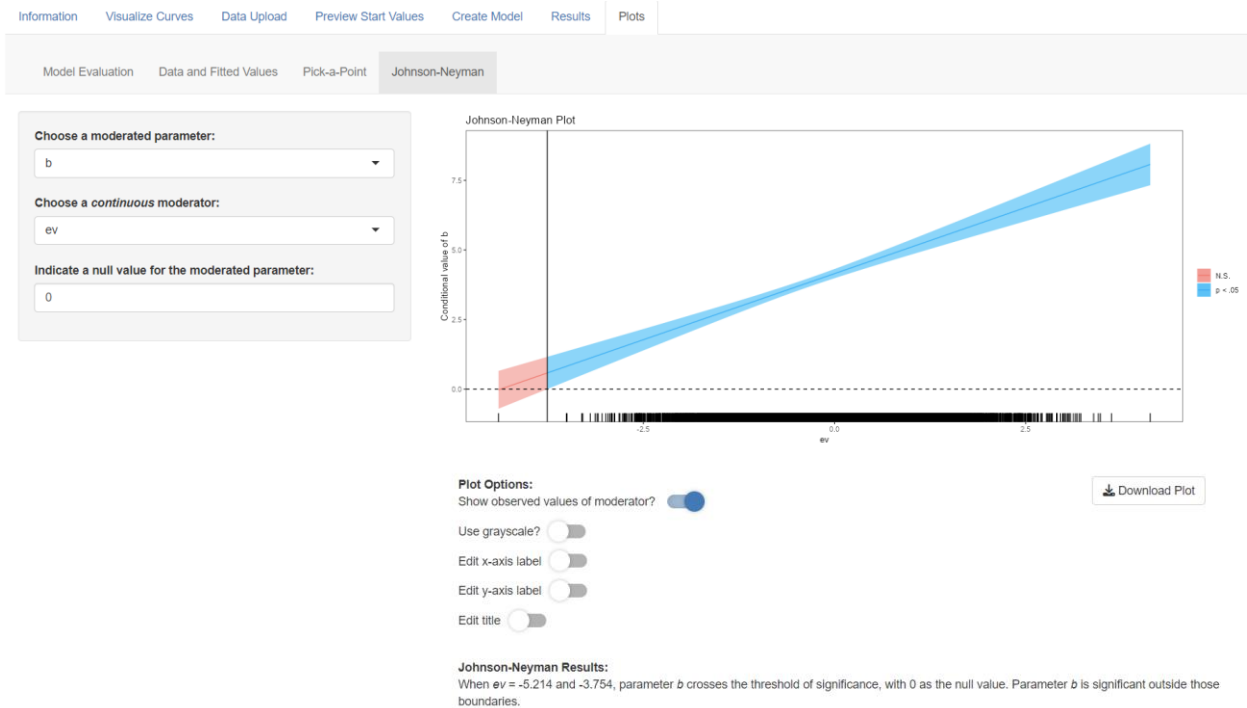
Figure 6.15. Pick-a-Point Plot with Paneling for the Moderated MM Model.



Next, we can gain even more detailed information about our moderation results by creating JN plots. The JN plot shows the moderator on the  $x$ -axis and the moderated parameter on the  $y$ -axis. Because parameters  $a$ ,  $b$ , and  $c$  are all moderated by  $ev$ , CurveBuilder allows us to choose which parameter to view on the  $y$ -axis. Ren et al. (2022) provided the most detailed hypothesis regarding  $ev$ 's moderation of parameter  $b$ , so here we will focus on parameter  $b$ . It was hypothesized that parameter  $b$ , interpreted as the difference in psychological wellbeing at very frequent social interaction compared to zero social interaction, would increase as

extraversion increased. Our findings supported this hypothesis. Placing  $ev$  on the  $x$ -axis and the conditional value of parameter  $b$  on the  $y$ -axis, we obtain the JN plot shown in Figure 6.16.

Figure 6.16. JN Plot with Default Settings for the Moderated MM Model.



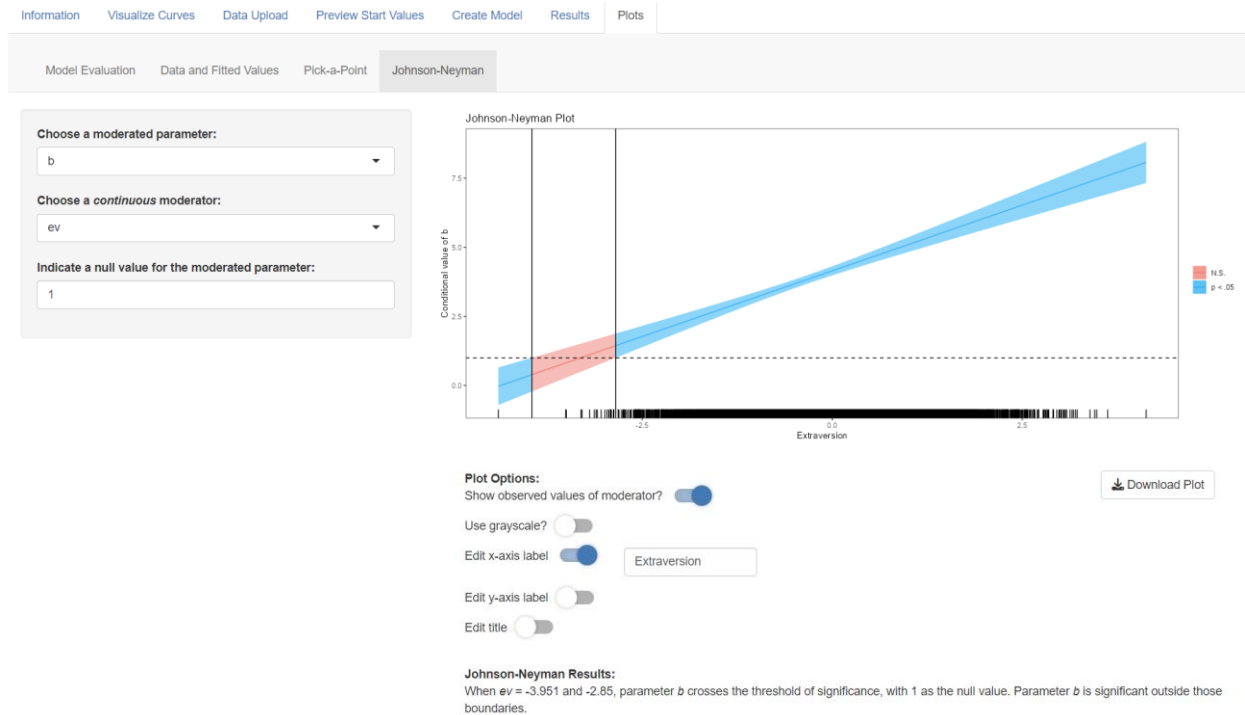
The increasing line indicates that as extraversion increases, parameter  $b$  increases. The surrounding confidence band is informed by the standard error of  $b$  across the observed range of extraversion. The rug plot along the  $x$ -axis shows observed values of  $ev$ .

Many components of the plot are informed by the null value that we have indicated in the left-hand panel. (By default, the null value is set to zero, but this can be changed.) The dashed horizontal line indicates the null value, and the confidence band is color-coded to denote whether the parameter is significant (blue) or not (red). The significance boundary – denoted by a vertical line – is the moderator value at which parameter  $b$  goes from being nonsignificant to significant.

Although two boundaries were calculated, only the boundary that falls within the observed range of the moderator is shown. The exact values of both significance boundaries are given in a sentence under the plot; the boundaries are -5.214 and -3.754, and when extraversion is outside of these boundaries (i.e., less than -5.214 or greater than -3.754), parameter  $b$  is significantly different from zero.

Suppose that for our purposes, a null value of zero is nonsensical for parameter  $b$ . We likely expect that more frequent social interaction will be related to greater wellbeing for all people in our study, so parameter  $b$  being greater than zero is not interesting. Indeed, the rug plot indicates that only one individual's realized value of  $ev$  falls outside the region of significance. Instead, we may want to know: at what levels of extraversion is parameter  $b$  significantly greater than one? In other words, at what levels of extraversion does frequent social interaction result in a greater than one-point boost to psychological wellbeing? Since our wellbeing scale ranges from 0-10, this would reflect a 10% change. Perhaps this is what we consider "significant," so let us instead enter 1 as the null value for parameter  $b$ . After making this change, and editing the  $x$ -axis label of the JN plot, we get the plot shown in Figure 6.17.

Figure 6.17. JN Plot with Custom Null Value for the Moderated MM Model.



The sentence below the plot reads: “When  $ev = -3.95$  and  $-2.849$ , parameter  $b$  crosses the threshold of significance, with 1 as the null value. Parameter  $b$  is significant outside those boundaries.” Before interpreting this output, note that the rug plot shows only one observation below the significance boundary of  $-3.95$ . This boundary should likely be interpreted with caution. Focusing on the second boundary, we find that when extraversion is greater than  $-2.849$ , parameter  $b$  is significantly greater than one. In other words, for individuals whose standardized extraversion score is greater than  $-2.849$ , frequent social interaction leads to a boost in psychological wellbeing that is significantly greater than one point. Only the individuals with extremely low extraversion experience a wellbeing boost that is not significant according to our definition.

In CurveBuilder, we could make more JN plots to visualize how parameters  $a$  and  $c$  change as extraversion changes, and for each plot, we could specify null values that are specific to the parameter and to our research context.

### ***Conclusions***

In this example, we compared the MM, linear, and quadratic models to characterize the relation between social interaction quantity and psychological wellbeing. We found that the MM model best characterized our data, providing support for the Diminishing Returns hypothesis described by Ren et al. (2022). Extraversion moderated all three parameters of the MM model. More extraverted people had a lower  $y$ -intercept (indicating lower wellbeing when interaction quantity was zero), greater growth from the  $y$ -intercept to the asymptote (indicating a greater boost to psychological wellbeing due to frequent social interaction), and a lower  $x$ -axis location of 50% growth (indicating that fewer social interactions were required to reach the halfway point of psychological wellbeing). Overall, it appears that more extraverted people are more negatively impacted by the absence of social interactions, and more positively impacted by a greater frequency of interaction. More extraverted people may also make the most of each social interaction, as they reach halfway levels of wellbeing with fewer interactions.

### **Example 2: Logistic Function and a Multicategorical Moderator**

Next, we will explore how to use CurveBuilder to fit a nonlinear model with a multicategorical moderator. For this example, we will work with a simulated data set based on findings from the field of hearing and auditory ability. In these applications, the  $x$ -axis reflects some aspect of difficulty of the auditory stimulus being listened to, such as the duration of sound exposure or the audibility of speech. The  $y$ -axis reflects some aspect of performance, such as the

proportion of trials where the tone with higher pitch is correctly identified or where a word is recognized correctly. These studies find that the relation between difficulty and performance is best characterized by a logistic function (McCrary & Cooper, 2004; Pogorzelski, 2022; Stelmachowicz et al., 2000). Additionally, one study (Stelmachowicz et al., 2000) found that the rate of approach toward the upper asymptote, as well as the location of the inflection point, differed across normal-hearing vs. hearing-impaired children. Given the consistency of past findings, in this example we will take a theory-driven approach to model selection, in which we choose our model *a priori* and do not empirically compare models.

In our simulated example, we suppose the children in our study listened to spoken words and the audibility of speech was varied. Our outcome of interest is the percentage of trials in which the word was correctly identified. Based on prior findings in this field, we select the logistic function to model the relation between audibility and correct word identification:

$$\text{percentCorrect} = a + b / (1 + \exp(-c * (\text{audibility} - d))).$$

Our key research question is whether parameters  $c$  and  $d$ , which correspond with the rate of approach toward the upper asymptote and the location of the inflection point, respectively, are moderated by hearing ability. The children in our study are grouped according to three hearing ability levels: (1) normal-hearing, (2) slightly hearing-impaired, and (3) severely hearing-impaired. The data set contains two dummy codes that reflect these groupings. Normal-hearing children are treated as the reference group and coded [0, 0]; slightly hearing-impaired children are coded [1, 0]; and severely hearing-impaired children are coded [0, 1].

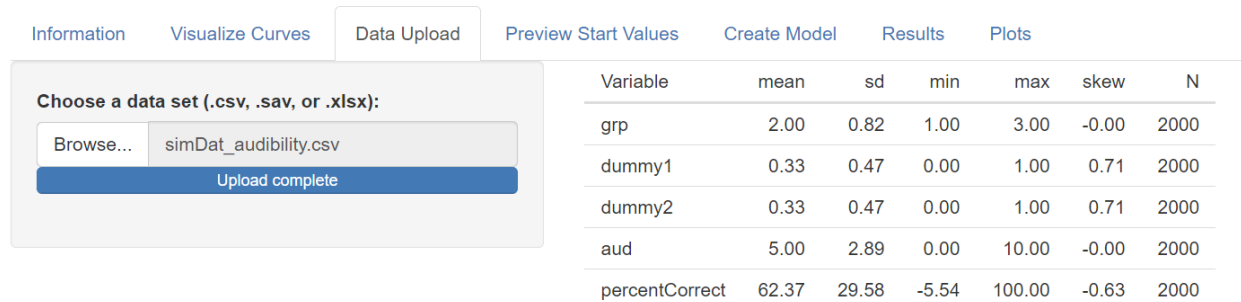
### ***Step 1: Data Upload***

Because we have chosen a nonlinear model *a priori*, we will bypass the Visualize Curves tab and begin with the Data Upload tab. Upon uploading our data, we see a summary of our



variables, including *grp* (a factor variable indicating hearing ability of the child), *dummy1*, *dummy2*, *aud* for audibility, and *percentCorrect*. See Figure 6.18.

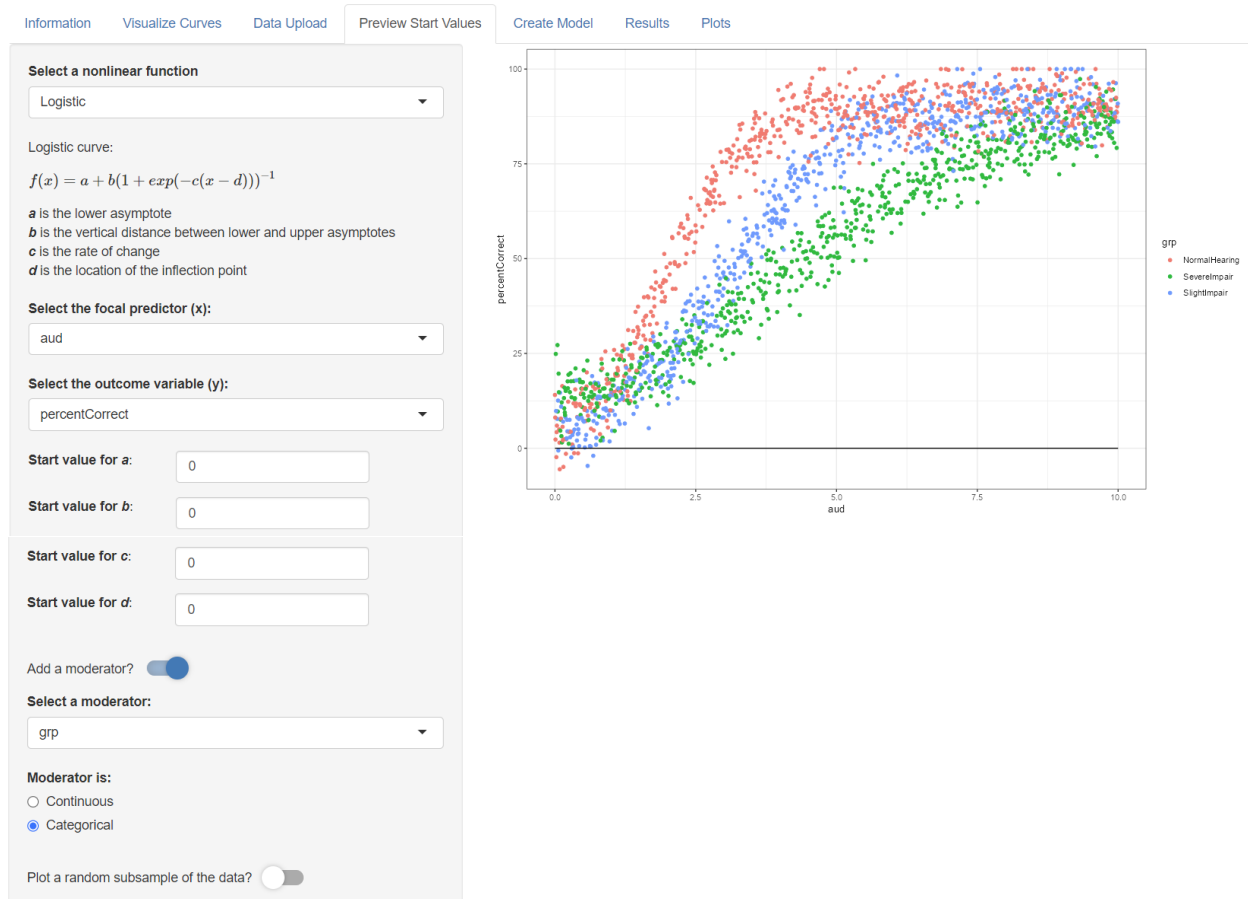
Figure 6.18. Audibility Data Summary in the Data Upload Tab.



### Step 2: Preview Start Values

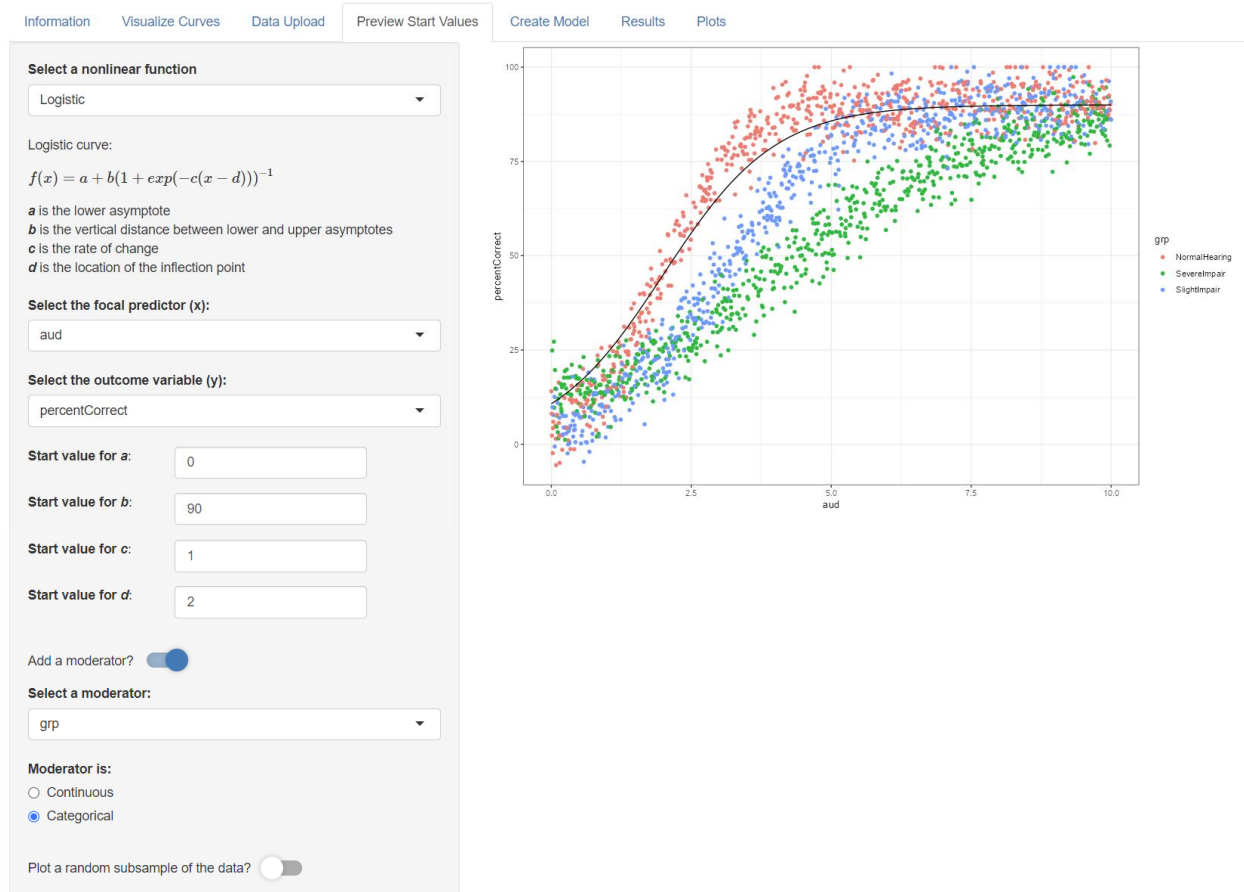
Before we fit the model, we must determine appropriate start values that yield a logistic curve that corresponds relatively well to our data. In the Preview Start Values tab, we begin by selecting the logistic function and indicating our predictor and outcome variables. We can also color-code the plot according to the moderator. Although we will use *dummy1* and *dummy2* in the model, we also have the *grp* available, which contains all grouping information in a single variable. Therefore, for visualization purposes we can indicate *grp* as the moderator. (We could also color-code by *dummy1* and *dummy2* separately.) Already, it is clear that the logistic curve is moderated by hearing ability. See Figure 6.19.

Figure 6.19. Preview Start Values Tab with Audibility Data.



From the plot, we see that different start values will correspond best with different groups of the moderator; understanding how these start values change across groups will help us when we specify the model in Step 3. To begin, let us identify the start values that match best with the reference group, normal-hearing children, which is shown in red. Start values of  $a = 0$ ,  $b = 90$ ,  $c = 1$ , and  $d = 2$  yield a curve that matches fairly well with the red points (Fig. 6.20).

Figure 6.20. Preview Start Values for Normal-Hearing Children.



Following this same process, we can visually choose start values for slightly hearing-impaired children (blue) and severely hearing-impaired children (green). Using the Preview Start Values functionality, we find that start values of  $a = 0$ ,  $b = 90$ ,  $c = 1$ , and  $d = 3$  seem to yield a well-matching curve to the blue dots, and start values of  $a = 0$ ,  $b = 90$ ,  $c = 0.5$ , and  $d = 4$  yield a well-matching curve to the green dots. These plots are not shown, but the reader is encouraged to use CurveBuilder to visualize these results.

By previewing start values, we gain a preliminary understanding of how parameters  $c$  and  $d$  change across groups. We find that parameter  $c \approx 1$  for normal-hearing children and slightly impaired children, and  $\approx 0.5$  for severely impaired children. We also observe that parameter  $d$  is

$\approx 2$  for normal-hearing children,  $\approx 3$  for slightly impaired children, and  $\approx 4$  for severely impaired children. For all groups, parameter  $a$  was held constant at 0, and parameter  $b$  was held constant at 90. We will use this information in the Create Model tab in Step 3.

### ***Step 3: Create Model***

To fit this model, we begin by selecting the logistic function, indicating  $aud$  as the predictor and  $percentCorrect$  as the outcome. We also indicate that parameters  $c$  and  $d$  are moderated by  $dummy1$  and  $dummy2$ . To select the best start values, it is ideal to incorporate what we know about how parameters  $c$  and  $d$  change across groups. It is not uncommon to simply indicate zero as the start values for any moderating effects (e.g., Grimm et al., 2016), and whereas this may yield convergence sometimes, the likelihood of convergence will be higher if we incorporate what we learned about parameters  $c$  and  $d$  in the Preview tab. We must indicate start values for  $c$ ,  $d$ , the effects of  $dummy1$  on  $c$  and  $d$ , and the effects of  $dummy2$  on  $c$  and  $d$ . The interpretation of the effect of a coding variable will change depending on the coding scheme. Because we are using dummy codes, we can interpret the effect of  $dummy1$  on  $c$  as follows: the difference in parameter  $c$  between slightly hearing-impaired children (coded 1 on  $dummy1$ ) and normal-hearing children (the reference group). Similarly, the effect of  $dummy2$  on  $c$  is the difference in parameter  $c$  between severely hearing-impaired children (coded 1 on  $dummy2$ ) and normal-hearing children (the reference group). Interpretations for parameter  $d$  are analogous. The start values we give for  $c$  and  $d$  will be treated as the start values for the reference group.

Beginning with a start value for  $c$ , we found that among normal-hearing children,  $c$  was  $\approx 1$ . Therefore, we can indicate 1 as our start value for  $c$ . Our Preview plots suggested that  $c$  was also  $\approx 1$  for slightly hearing-impaired children, suggesting that  $c$  may be the same for these groups; therefore, we can indicate 0 for  $dummy1$ 's effect on  $c$ . Among severely hearing-impaired

children we observed that  $c$  was  $\approx 0.5$ , suggesting that as we go from normal-hearing children to severely hearing-impaired children,  $c$  decreases by about 0.5. Therefore, we enter -0.5 as our start value for  $dummy2$ 's effect on  $c$ . We follow a similar process for parameter  $d$ . The start value for  $d$  is for normal-hearing children (the reference group). The start value for  $dummy1$ 's effect on  $d$  is difference in  $d$  between slightly impaired children and normal-hearing children. The start value for  $dummy2$ 's effect on  $d$  the difference in  $d$  between severely impaired children and normal-hearing children. Finally, we can indicate that start values for  $a$  and  $b$  should be 0 and 90, respectively. After entering all this information, the model converges (Fig. 6.21).

Figure 6.21. Fitting the Moderated Logistic Model in the Create Model Tab.

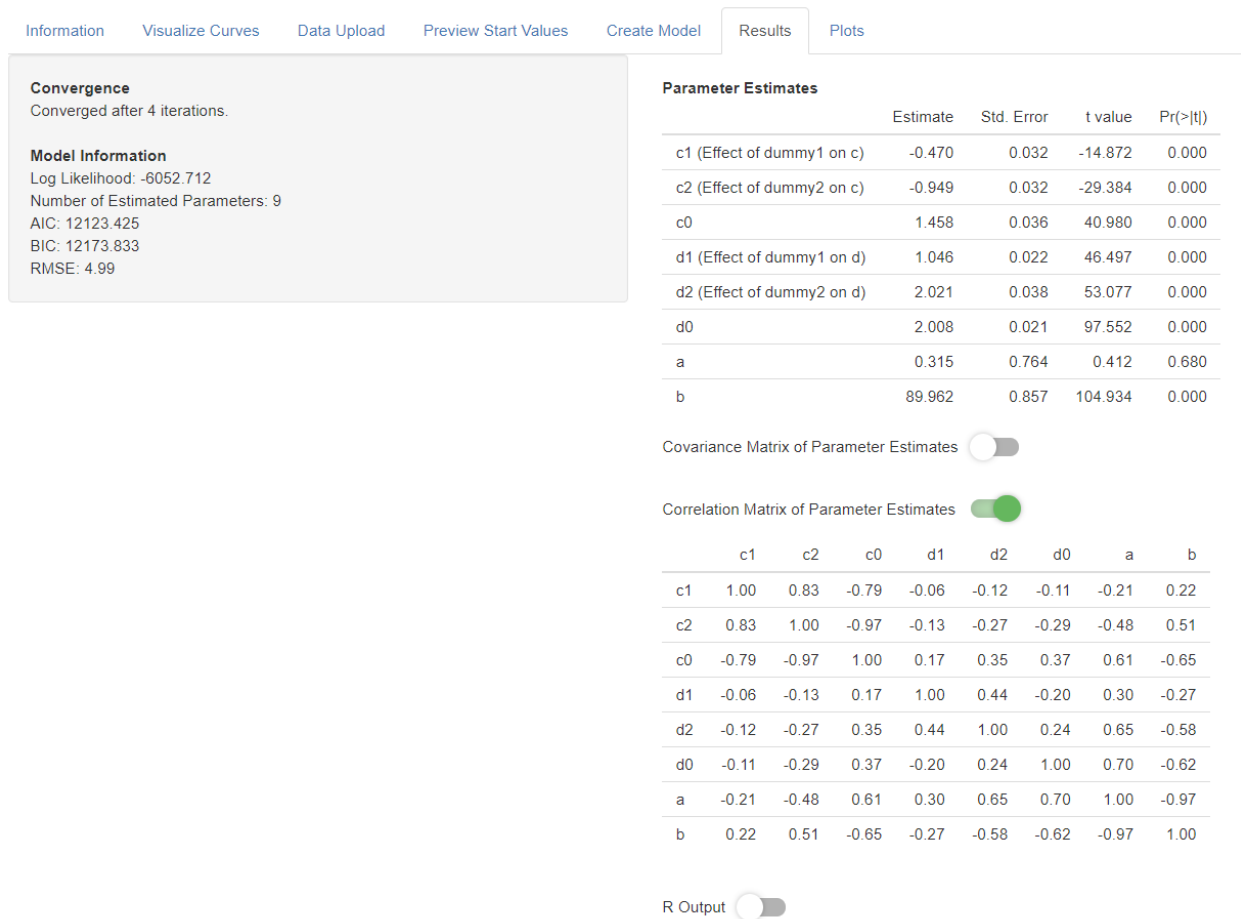
#### Step 4: Results

The Results tab (Fig. 6.22) shows the model converged after 4 iterations. In the estimates table,  $c$  has been replaced with  $c0$ ,  $c1$ , and  $c2$ . The value of  $c0$  indicates that  $c = 1.46$  among normal-hearing children. As we go from normal-hearing children to slightly impaired children,  $c$

decreases by 0.47. As we go from normal-hearing children to severely impaired children,  $c$  decreases by 0.95. Similarly,  $d$  has been replaced by  $d0$ ,  $d1$ , and  $d2$ . We find that  $d = 2.01$  among normal-hearing children, increases by 1.05 for slightly impaired children, and increases by 2.02 for severely impaired children. For all groups,  $a = 0.31$  and  $b = 89.96$ .

We can also choose to view the asymptotic correlation matrix of parameter estimates to assess whether the model is overparameterized. Highly correlated parameters sometimes suggest that the model can be simplified (Motulsky & Christopoulos, 2004). For this model, most correlations are low ( $<0.5$ ), suggesting this model is not too complex for our data.

Figure 6.22. Results Tab for the Moderated Logistic Model.



## Step 5: Plots

Because the Model Evaluation and Fitted Values plots are discussed in other examples, this example bypasses those tabs and begins with the Pick-a-Point tab. To create the pick-a-point plot, we indicate that the moderator is multicategorical and has 3 categories, and we select *dummy1* and *dummy2* as the indicator variables for the moderator. Given this input, CurveBuilder will create a pick-a-point plot with default settings, shown in Figure 6.23.

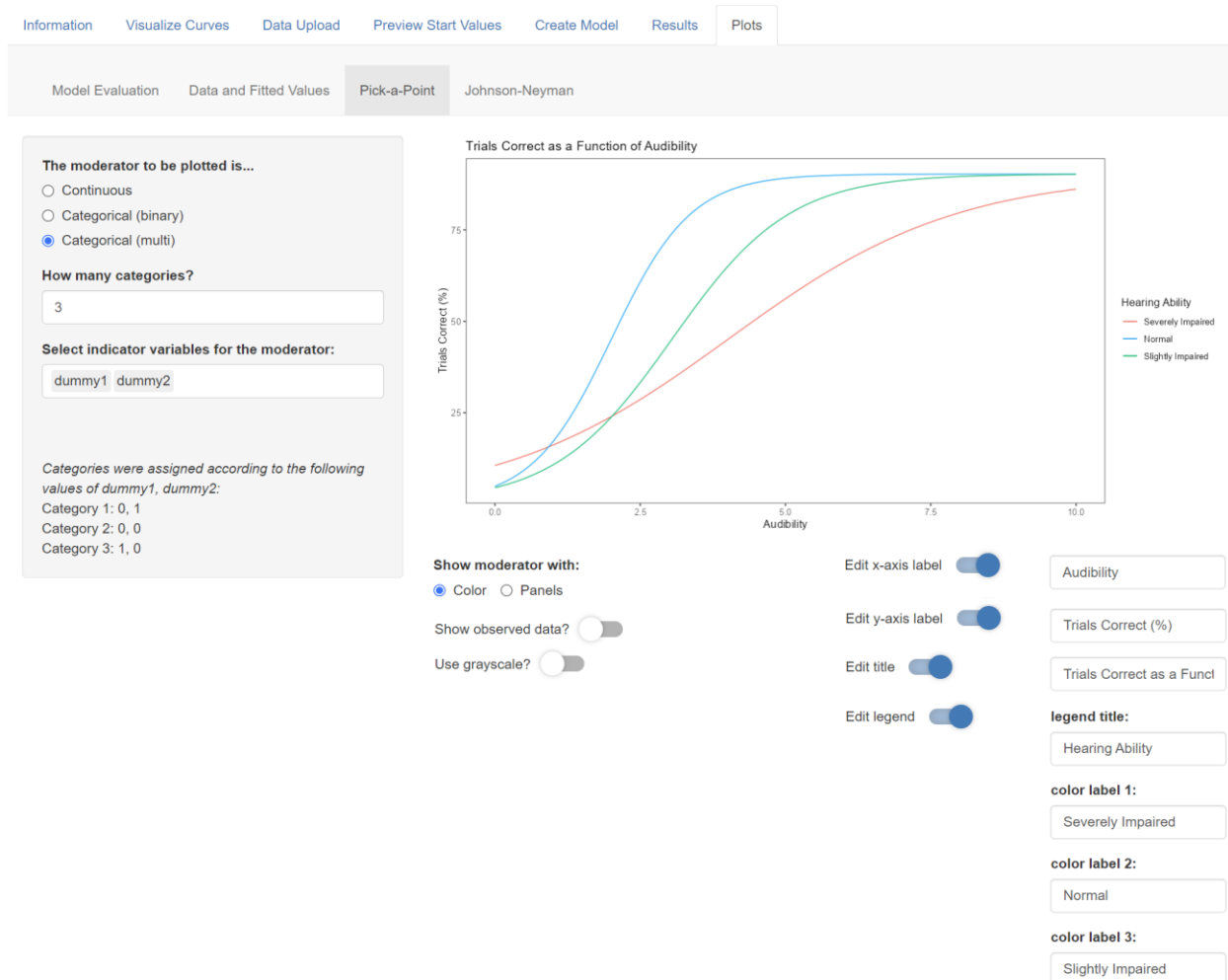
Figure 6.23. Pick-a-Point Plot with Default Settings for the Moderated Logistic Model.



In Figure 6.23, the plot is color-coded by hearing ability, but it would be ideal to add more descriptive labels to the legend. In the left-hand column, we are given information about how the labels in the plot correspond with the coding variables. The group labeled as “Category 1” in the plot is coded [0, 1] on *dummy1* and *dummy2*, which means that Category 1 is severely hearing-impaired children. Similarly, because “Category 2” is coded [0, 0], we know this group

is normal-hearing children. Finally, “Category 3” is coded [1,0], so this group is slightly hearing-impaired children. We can create a publication-ready plot by customizing the labels accordingly (see Fig. 6.24). Because the moderator is not continuous, the JN plot is not available.

Figure 6.24. Customized Pick-a-Point Plot for the Moderated Logistic Model.



## Conclusions

In this example, we fit a logistic model to characterize the relation between speech audibility and correct word identification, in which parameters  $c$  and  $d$  were moderated by hearing ability. We found that for all hearing ability groups, parameter  $a$  was close to zero,



suggesting that at low levels of speech audibility, children are unlikely to correctly identify any words. For all groups, parameter  $b$  was 89.96, suggesting that when speech was highly audible, children correctly identified the correct word about 90% of the time, regardless of hearing ability. Interestingly, we found that parameter  $c$  was greatest for normal-hearing children, and decreased as hearing impairment got worse. This implies that as speech becomes more audible, normal-hearing children more quickly transition to correct word identification. Hearing-impaired children have a slower rate of approach toward the upper asymptote, suggesting that as speech becomes more audible, their performance improves but does not improve as rapidly as normal-hearing children. Finally, we found that parameter  $d$  was lowest for normal-hearing children and increased as hearing impairment worsened. Parameter  $d$  is the location of the inflection point along the  $x$ -axis, or in this context, the speech audibility level at which children correctly identify words in 50% of trials. Therefore, among normal-hearing children, less audibility is required to successfully identify words half of the time. Hearing-impaired children require more audibility to reach 50% correct identification.

### **Example 3: Jenss-Bayley Function and Random Effects**

Finally, we will explore how to use CurveBuilder to fit a nonlinear model with random effects. NLME models are useful for modeling longitudinal data; when study subjects are each assessed on multiple occasions, mixed-effects models allow us to account for observations nested within individuals. In this example, we will work with height data collected as part of the Berkeley Growth Study (Jones & Bayley, 1941) and presented by Grimm et al. (2016). The Berkeley Growth Study tracked the height of 83 children over the course of 1 to 36 months of age – assessments were taken at 1, 3, 6, 9, 12, 15, 18, 24, and 36 months. The data set is freely

available for download at <https://www.guilford.com/companion-site/Growth-Modeling/9781462526062> (Grimm et al., 2016).

To characterize height trajectories, we will implement a Jenss-Bayley model. The Jenss-Bayley function was created to approximate changes in human height over time (Jenss & Bayley, 1937) and incorporates the fact that growth tends to occur in two distinct phases. During infancy, growth is rapid and can be characterized by an exponential model, whereas during the toddler years, rate of growth stabilizes, and can be characterized by a linear model. The Jenss-Bayley model is available in CurveBuilder with the following parameterization:

$$\text{height} = a + bt + \exp(c + dt),$$

where *height* is the outcome variable, *t* (*time*) is the predictor, *a* is the intercept of the linear asymptote, *b* is the slope of the linear asymptote,  $\exp(c)$  is the vertical distance between the *y*-intercept and the intercept of the linear asymptote, and  $\exp(d)$  is the ratio of acceleration of growth at time *t* to time *t* – 1.

### ***Step 1: Data Upload***

Because we have *a priori* knowledge about the nonlinear function that should be used for these data, we will bypass the Visualize Curves tab and proceed to Data Upload. Here we see a summary of the variables in the data set: subject ID, gender, age (the predictor), and height (the outcome). See Figure 6.25.

### ***Step 2: Preview Start Values***

Next, we will determine appropriate start values to use for the Jenss-Bayley model. Start values for *a* and *b* should reflect the intercept and slope of the linear portion of growth. Start values for *c* and *d* determine the shape of the early exponential portion of growth. It appears that  $a = 60$ ,  $b = 1$ ,  $c = 2$ , and  $d = -0.5$  fit the data relatively well; see Figure 6.26.

Figure 6.25. Summary of Height Data in the Data Upload Tab.

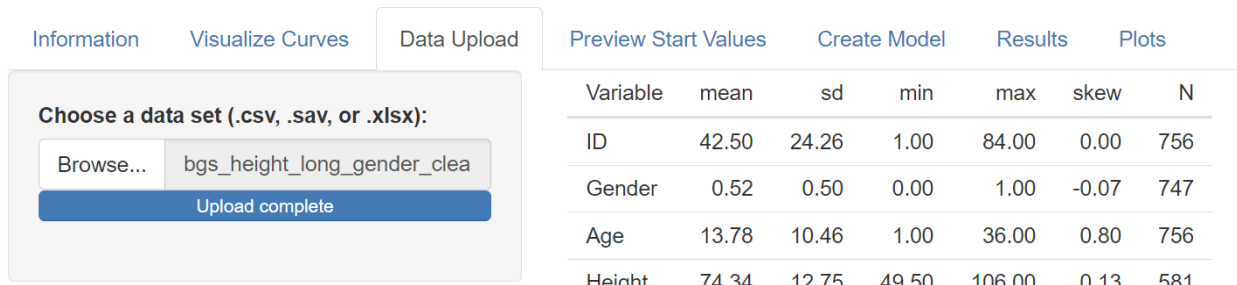
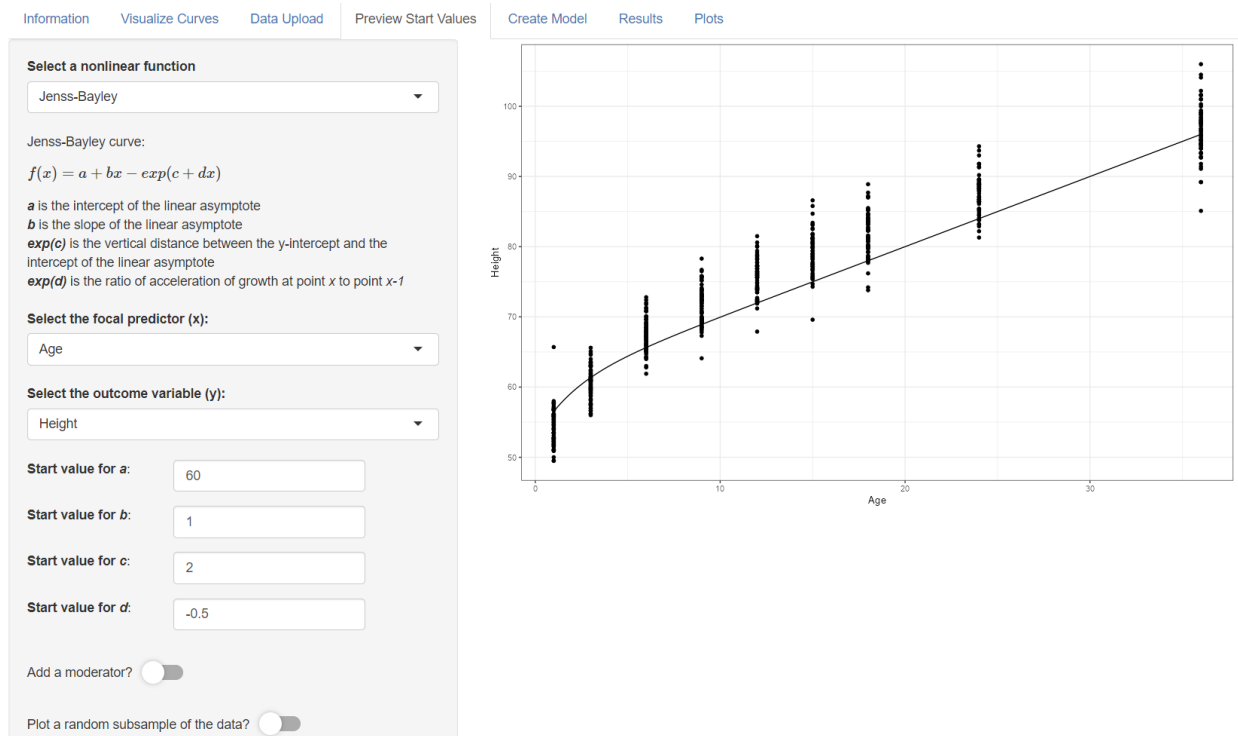


Figure 6.26. Preview Start Values Tab for the Jenss-Bayley Model.



### Steps 3 and 4: Create Model and Results

In this section, we will alternate between the Create Model and Results tabs (and briefly, the Plots tab) to demonstrate the process of fitting multiple models and carrying out model selection. In the Create Model tab, we select the Jenss-Bayley function and import the start

values that were found in Step 2. For demonstrative purposes, I will begin by specifying a model with no random effects. In other words, this model ignores the nested structure of the data. The model specification is shown in Figure 6.27.

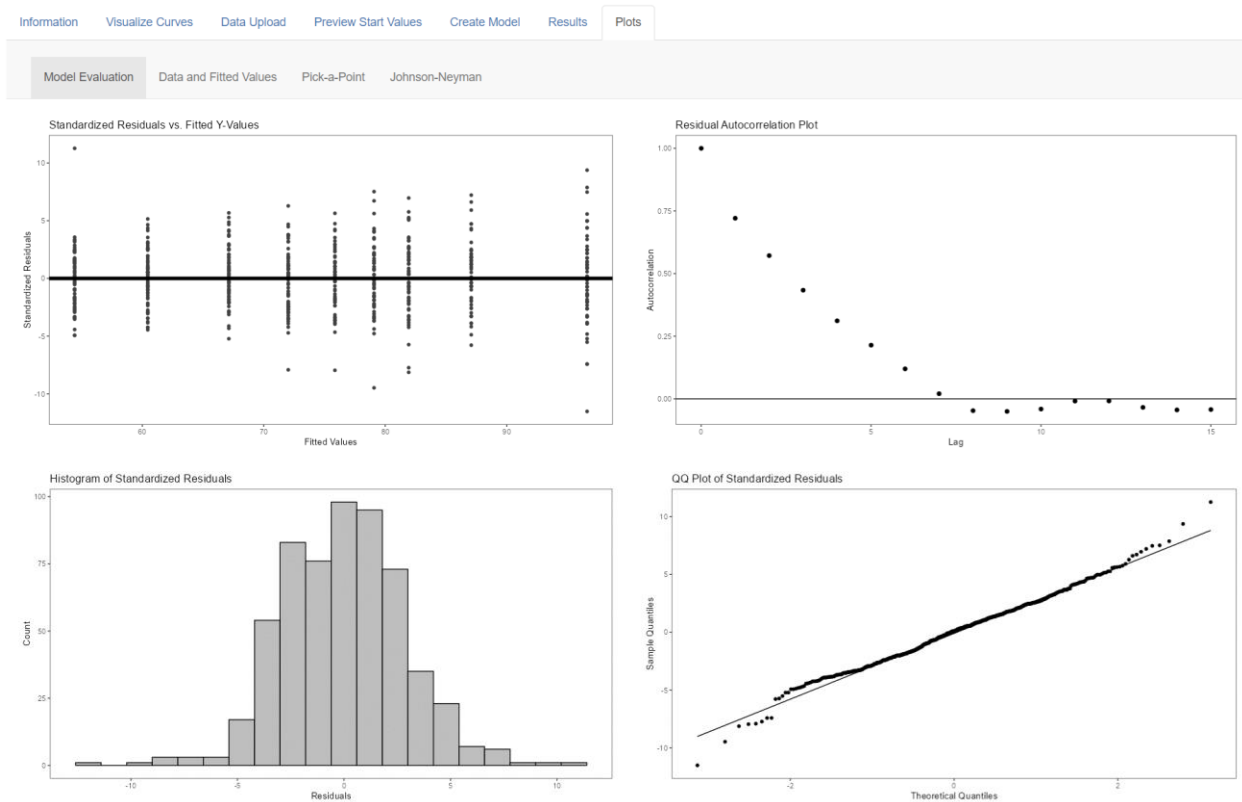
Skipping to the Model Evaluation tab under Plots, we immediately see that this is an insufficient model for the data (Fig. 6.28). The residual autocorrelation plot indicates that adjacent residuals are highly correlated, emphasizing the need for a mixed-effects model to account for dependencies within individuals.

Figure 6.27. Fitting the Jenss-Bayley Model without Random Effects.

The screenshot shows a software interface for fitting a Jenss-Bayley model. The interface is divided into several sections:

- Navigation Tabs:** Information, Visualize Curves, Data Upload, Preview Start Values, **Create Model**, Results, Plots.
- Select a nonlinear function:** A dropdown menu is set to "Jenss-Bayley".
- Jenss-Bayley curve:** The equation  $f(x) = a + bx - exp(c + dx)$  is displayed. Below it, definitions are provided: **a** is the intercept of the linear asymptote, **b** is the slope of the linear asymptote, **exp(c)** is the vertical distance between the y-intercept and the intercept of the linear asymptote, and **exp(d)** is the ratio of acceleration of growth at point x to point x-1.
- Select the focal predictor (x):** A dropdown menu is set to "Age".
- Select the outcome variable (y):** A dropdown menu is set to "Height".
- Start values for parameters:** Four input fields are provided: **a:** 60, **b:** 1, **c:** 2, **d:** -0.5. Below these is a button labeled "Import start values from Preview tab".
- Model Configuration:** Several toggle switches are present: "Add Moderators?" (off), "Add Random Effects?" (off), "Adjust max iterations?" (off), "Adjust tolerance?" (off), and "Show results from final iteration?" (off).
- Fit Model:** A blue button labeled "Fit Model" is located on the right side.
- Results:** A green checkmark icon and the text "Model successfully converged!" are displayed below the "Fit Model" button.
- Show R Code:** A toggle switch is currently off.

Figure 6.28. Model Evaluation Plots for the Jenss-Bayley Model without Random Effects.

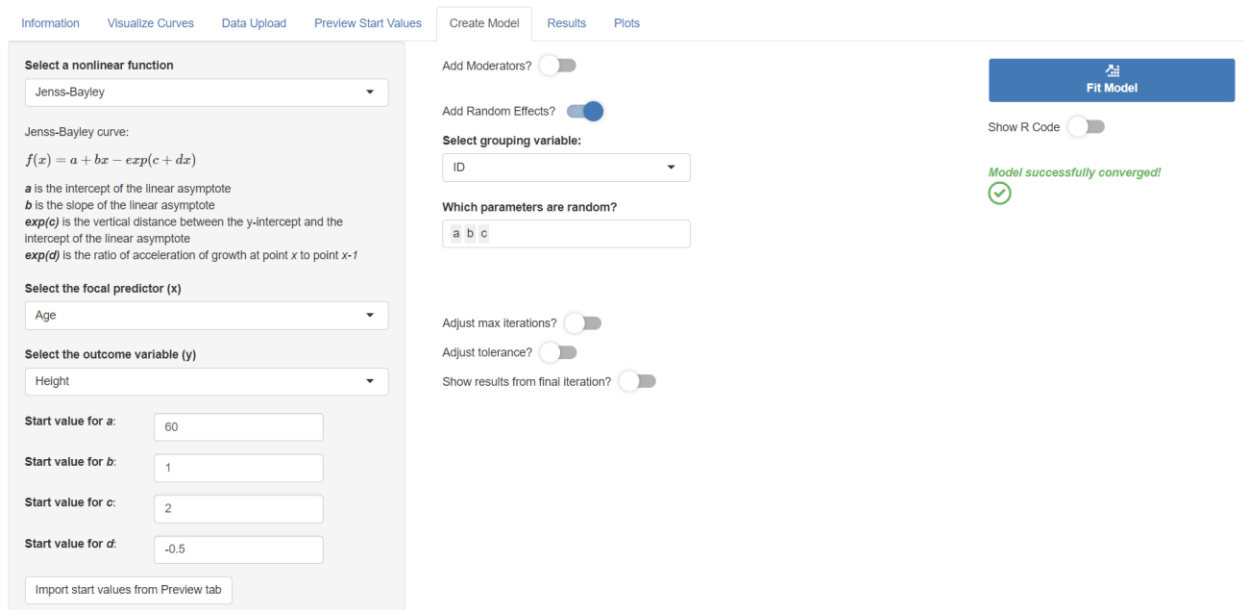


To add random effects to the model, we return to the Create Model tab. We select *ID* as the grouping variable, and we must select which parameters should be treated as randomly varying across individuals. A popular approach is to start with the maximal number of random effects, and if the model doesn't converge, to progressively remove random terms (e.g., McNeish et al., 2020; McNeish & Bauer, 2022). Therefore, we may begin by specifying that parameters *a*, *b*, *c*, and *d* are all random. However, this model fails to converge.

Deciding which parameter(s) to treat as fixed is often not a straightforward decision, as the parameters within nonlinear models typically are not organized into an intuitive hierarchy (McCormick et al., 2023). In this example, which parameter to treat as fixed is not obvious. As

one option, we may consider the fact that – as was seen in the Preview Start Values plot – most growth occurs within the linear portion of the Jenss-Bayley curve. Only the first two or three timepoints seem to correspond with the exponential portion of the curve. Therefore, it may be reasonable to expect that parameters  $a$  and  $b$ , which govern the linear portion of the curve, may be more variable across individuals. If we remove parameter  $c$  from the random effects, the model still fails to converge, but if we remove parameter  $d$  from the random effects, the model converges (Fig. 6.29).

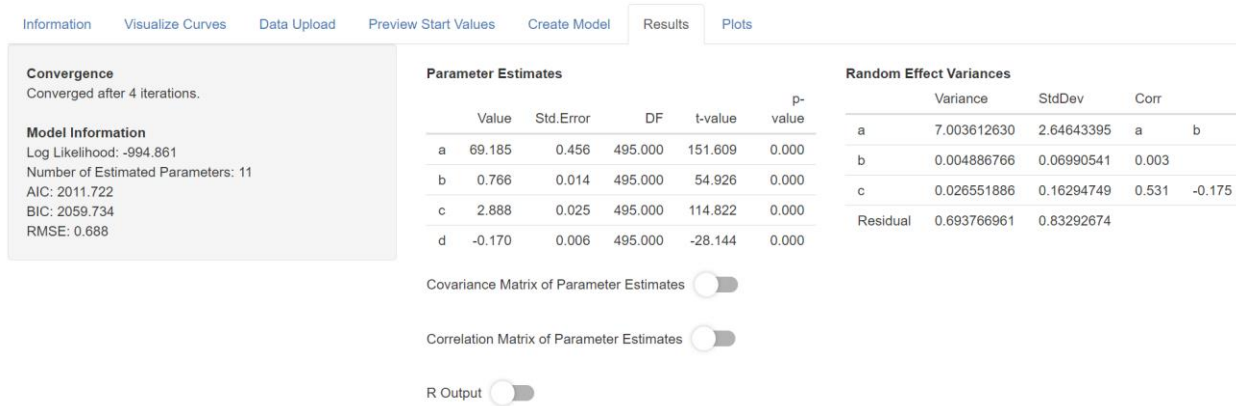
Figure 6.29. Fitting the NLME Jenss-Bayley Model in the Create Model Tab.



Results for this model (Fig. 6.30) indicate that, in our sample, the typical Jenss-Bayley curve is characterized by a linear intercept of 69.18 and a linear slope of 0.77. The distance between the linear intercept and the actual y-intercept is  $\exp(2.89) = 17.99$ , meaning the typical y-intercept is  $69.18 - 17.99 = 51.19$  cm. In the exponential portion of the curve, the ratio of growth acceleration is  $\exp(-0.17) = 0.84$ , meaning that as age increases, growth tends to slow by

a factor of about 0.84. Additionally, we found that the intercept of the linear portion of the growth curve ( $a$ ), the slope of the linear portion of the growth curve ( $b$ ), and the distance between the linear intercept and the actual  $y$ -intercept ( $c$ ) varied across individuals.

Figure 6.30. Results Tab for the NLME Jenss-Bayley Model.



### Step 5: Plots

Beginning with the Model Evaluation tab (Fig. 6.31), diagnostic plots indicate that this model fits well to the data. The Residuals vs. Fitted  $Y$ -Values plot shows that residuals have constant variance over the range of  $y$ . The Residual Autocorrelation Plot shows that at lag = 1 and beyond, adjacent residuals are correlated near zero. Incorporation of random parameters has accounted for all the dependency among the residuals. Finally, the Histogram of Residuals and QQ Plot of Residuals show that the residuals are relatively normally distributed.

Next, we examine the Data and Fitted Values plot (Fig. 6.32), which indicates that the model-implied  $y$ -values correspond well with the observed data.

Because this model does not contain moderators, the Pick-a-Point and Johnson-Neyman plots are not available.

Figure 6.31. Model Evaluation Plots for the NLME Jenss-Bayley Model.

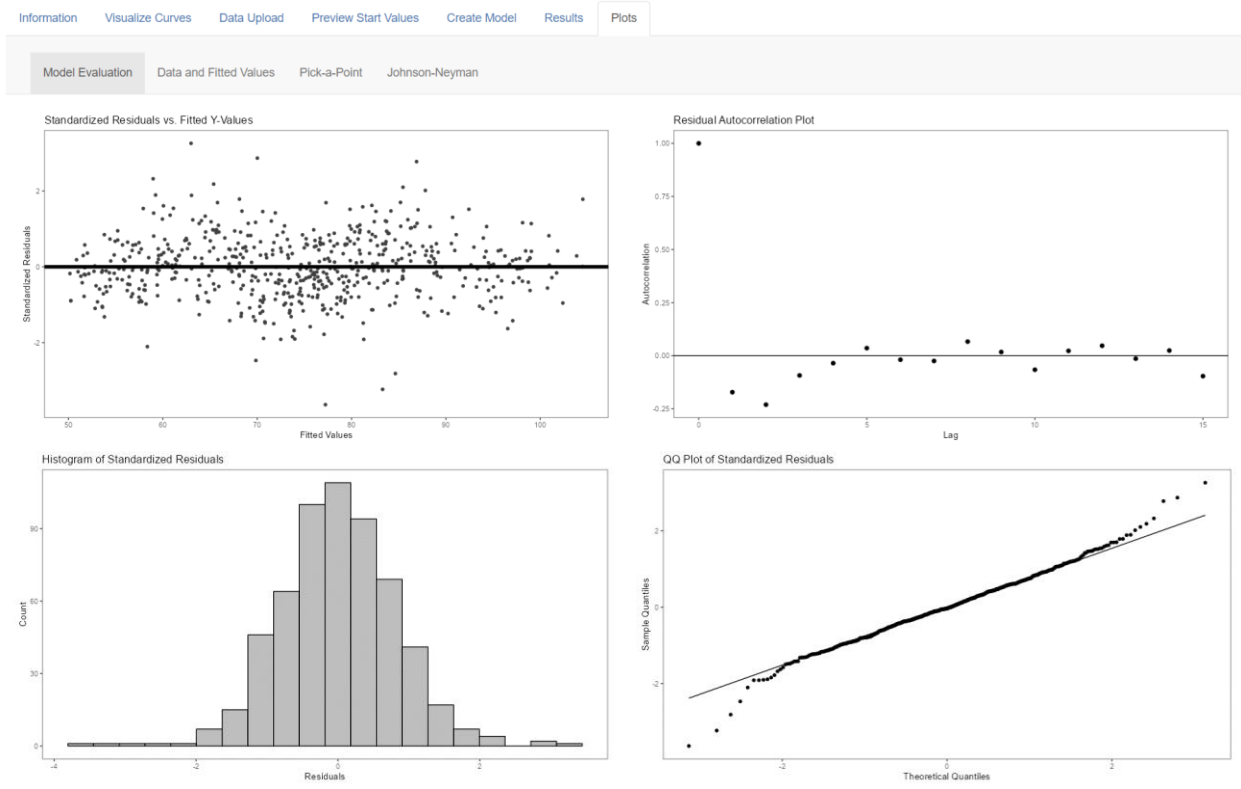
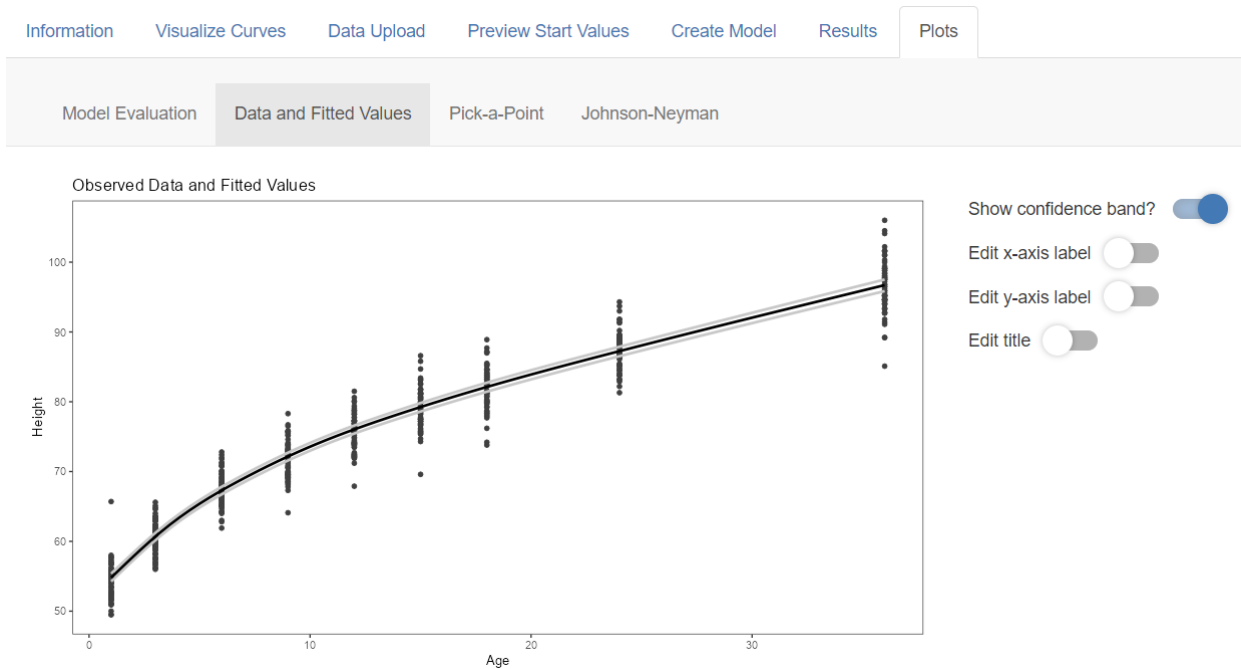


Figure 6.32. Data and Fitted Values Plot for the NLME Jenss-Bayley Model.





## *Conclusions*

In this example, we used CurveBuilder to fit a nonlinear mixed-effects model to characterize changes in height over the course of infancy and toddlerhood. We iteratively used the Create Model tab, Results tab, and Model Evaluation plots to arrive at the best-fitting model. We found that most aspects of the growth curve varied across individuals, including both parameters governing the linear portion of the curve, as well as the parameter related to the y-intercept of the curve; however, the growth rate during the exponential portion of the curve needed to be treated as constant to facilitate convergence. These results could be used to inform future analyses to find potential moderators of these variable aspects of the growth curve.

## CHAPTER VII

### DISCUSSION

Throughout the preceding chapters, I have presented methods and software that enable researchers to better integrate linear moderation and parametric nonlinear models. At the same time, there are abundant opportunities for extension of the models and techniques presented here, as well as myriad research questions regarding moderated nonlinear models that have yet to be answered. This chapter expands upon these unanswered questions, discusses extensions, and summarizes key considerations for successful implementation of moderated nonlinear models.

#### **Future Directions for CurveBuilder**

The primary goal of CurveBuilder is to simplify and unify each stage of the nonlinear modeling process, and there are many areas in which CurveBuilder may be expanded to further accomplish this goal. These include more avenues for dealing with convergence failures, broader utilities related to reparameterization, and advanced functionality for NLME models.

In its current state, CurveBuilder offers a few utilities for troubleshooting nonconvergence. The user may easily adjust the model specification by selecting a simpler functional form or by using graphical utilities to choose adjusted starting values, increase the iteration cap for the maximum likelihood estimator, adjust the convergence tolerance, or simply view the results that were obtained in the final iteration of the estimation algorithm. While these approaches have been suggested by various methodologists (e.g., Bates & Watts, 1988; Gallant, 1987; Ritz & Streibig, 2008), they may not always be effective. Because nonconvergence

remains a very common problem in nonlinear models, the practicality of CurveBuilder would notably increase if there were even more utilities available for addressing nonconvergence. Specifically, convergence problems are especially salient for NLME models, and specialized approaches to improve the likelihood of convergence have been developed for these models. Reparameterizing the random effects covariance matrix via a Cholesky decomposition has been shown to be effective for improving convergence rates (Lindstrom & Bates, 1988; McNeish & Bauer, 2022). More recently, McNeish and Bauer (2022) proposed decomposing the random effects covariance matrix via factor analysis; these authors note that it is possible to carry out this method in SAS and SPSS; however, extensions to the R environment have yet to be developed. In summary, there are a variety of approaches for dealing with nonconvergence, which range from basic to advanced. However, most of these approaches – especially those that are more complex – require fairly involved software procedures and have largely been restricted to more advanced applications. Any or all of these approaches will be useful to integrate into the easy-to-use interface provided by CurveBuilder.

Another important aspect of nonlinear model fitting is parameterization; however, CurveBuilder currently does not offer extensive utilities for reparameterizing a chosen model. If a user wishes to implement a model with a parameterization that differs from the prespecified offering, they must use the custom function option to manually create their desired reparameterization. There are many ways that CurveBuilder may be expanded in the future to enable easier reparameterization. First, a greater variety of parameterizations of each model could be offered as prespecified options. For example, the sigmoidal models provided in CurveBuilder contain parameters for (1) the lower asymptote, (2) the difference between the upper and lower asymptote (i.e., total change), (3) the rate of change, and (4) the  $x$ -location of

the inflection point. However, in some applications of sigmoidal models, it may be more useful to estimate the upper asymptote itself rather than total change. In other contexts, estimating jerk points (i.e., locations along the  $x$ -axis where the surge area begins and ends) may be more useful than estimating the location of the inflection point. Many of the models in CurveBuilder also exist in versions with fewer parameters, such as the three-parameter Gompertz and logistic, whose lower asymptote is constrained to zero (Sit & Poulin-Costello, 1994). Second, another area for expansion will be to provide easier functionality for constraining certain parameters to constants. Although the user may use the custom function option to create a model with constraints, it would be ideal for CurveBuilder to contain a code-free way of doing this. A simple interface for adding constraints would ease this aspect of parameterizing the chosen model, as well as aiding with nonconvergence problems as discussed in Chapter 4.

The utility of CurveBuilder for fitting NLME models could also be expanded by incorporating advanced functionality that is specific to these models. First, in order to obtain a well-fitting NLME model, it is often necessary to account for autocorrelation (i.e., when there is remaining correlation between adjacent observations, even after accounting for the nested structure of the data). Autocorrelation is commonly observed in longitudinal data, and there are a variety of ways to model it, such as by incorporating an autoregressive (AR) component and/or a moving average (ARMA) component (Cho et al., 2022; Davidian & Giltinan, 1995; Pinheiro & Bates, 2000). Additionally, heteroscedasticity is common to longitudinal data, wherein the variance of the residuals is not constant across the observed range of the predictor(s). It is often necessary to model heteroscedasticity explicitly, which may involve treating residual variance as a function of the predictor(s) (Blozis & Haring, 2021; Cho et al., 2022; Davidian & Giltinan, 1995; Pinheiro & Bates, 2000). Both autocorrelation and heteroscedasticity can be incorporated

into *nlme* objects (Pinheiro et al., 2023); however, in its current state, CurveBuilder does not provide functionality to do so. To incorporate these components, the user could use the R code generated by CurveBuilder as a starting point, and within their local R environment, add to that code such that it contains the desired autocorrelation and/or heteroscedasticity components. However, it would be ideal if these advanced features were incorporated within the simple interface provided by CurveBuilder. Incorporating these features into future versions of CurveBuilder will greatly enhance its practicality for fitting NLME models.

Many other advanced model specification options may be integrated into CurveBuilder in the future. In a maximally general app, users would be able to add complexity to the model in a variety of ways, such as by adding covariates and/or incorporating higher-order interactions. Additionally, enabling the user to select their choice of estimator (e.g., nonlinear least squares, weighted least squares, maximum likelihood, sandwich estimators) would likely be useful. At present, CurveBuilder implements the default estimator for *nls* (nonlinear least squares) and *nlme* (maximum likelihood) objects. However, depending on the model and data conditions, there are many scenarios in which it is useful or necessary to use a different estimator (see Appendix A). These are just a few ways that the model specification tools in CurveBuilder may be expanded in future versions to enable greater generality.

### **Moderated Nonlinear Model Extensions**

There are a variety of opportunities for extension of the moderated nonlinear models presented throughout this dissertation. While many of these extensions have been developed or proposed within the methodological literature, most have yet to enjoy regular use in empirical applications.

In all the examples presented throughout this dissertation, the functional form relating  $x$  to  $y$  is assumed to be the same across all values of the moderator (e.g., the curve is always characterized by a Michaelis-Menten or logistic function). However, there may be scenarios in which the fundamental shape of the curve is hypothesized to differ according to the moderator. Methodologists have proposed a few ways to test such a hypothesis. Codd and Cudeck (2014) and Kohli et al. (2016) presented a combination of the NLME model and the mixture model, which Kohli et al. (2016) termed the Nonlinear Random Coefficient Mixture Model (NRMM). Like other mixture models, the NRMM includes a group membership probability parameter, and various covariates and moderators may be included as predictors of group membership. Importantly, the NRMM allows the nonlinear trajectories of the latent classes to embody different functional forms. The authors note that such a model may be ideal for characterizing differential responses to treatment: “Suppose that some individuals improve more consistently throughout the observation period, while others improve initially but then relapse and decline after an unspecified amount of time. Assume the first group improves nonlinearly such that the Michaelis-Menten model is appropriate, and that the second group follows a quadratic function” (Codd & Cudeck, 2014, p. 65). The NRMM has many advantages; not only can the fundamental shape of the trajectory change across groups, but the use of a mixture model also reflects that those groups may be unobservable. Additionally, the researcher is required to specify the nonlinear functions for each group *a priori*, which encourages a theory-driven approach to model creation. In the above example, the Michaelis-Menten and quadratic models were chosen based on the *a priori* expectation that some individuals would respond continuously positively to treatment, whereas others would eventually relapse.

Implementing a different approach, Wood (2023) presented a combined model that contains both the logistic and exponential models as special cases, as well as a weight parameter that governs how closely the curve resembles either. The weight parameter may be allowed to vary across groups. As such, the model can accommodate different functional forms across values of the moderator, and allows the data to determine whether the curve more closely resembles the logistic or exponential model as the moderator changes. In addition, Wood (2023) proposes that this framework could be extended to create combined models involving other parametric curves; for example, the Jentsch-Bayley model could be combined with another model of physical growth. Extensions of the combined model framework are likely to be an interesting avenue for future research, as they enable straightforward examination of whether and how the functional form may vary according to an observed moderator.

Additionally, the scope of this dissertation was limited to *linear* moderation of the parameters within nonlinear models, as well as a single moderator acting in isolation. More complex patterns of moderation may be incorporated into nonlinear models in the future. First, the parameters of a nonlinear model could be governed by higher-order interactions, such as interactions among two or three moderators. Such higher-order terms are very commonly incorporated into moderated linear models (Aiken & West, 1991; Cohen et al., 2003); however, at present, their involvement in nonlinear models remains rare. A useful extension of CurveBuilder will be to incorporate easy specification of higher-order interactions, as well as more extensive graphical utilities that allow the user to visualize the nature of, for example, a two-way interaction. When higher-order interactions are probed within the linear framework, the pick-a-point plot is extended such that the line relating  $x$  to  $y$  is plotted at different values of the first moderator, and paneled according to values of the second moderator (e.g., Aiken et al.,

2012). Such an extension will be useful to add to CurveBuilder in the future. Second, it is also possible for nonlinear model parameters to be *nonlinearly* moderated. Here, the parameter does not change linearly according to the moderator; rather, any function relating the moderator to the parameter may be specified (Cudeck & Harring, 2007). Nonlinearly moderated parameters within nonlinear models will enable researchers to articulate and test more nuanced hypotheses.

### **Future Directions for the Johnson-Neyman Technique**

One goal of this dissertation was to extend the Johnson-Neyman (JN) technique to accommodate nonzero null values, which was accomplished in Chapter 5. At the same time, there are a variety of nuanced issues that arise when applying the JN technique to probe moderation within nonlinear models, raising interesting questions to be pursued in future work.

A unique feature of some nonlinear model parameters is that their ranges are bounded. The parameters of a linear model (e.g., intercept, slope, quadratic and cubic terms) are unbounded in that they may take on any value from positive to negative infinity. In contrast, some nonlinear model parameters must take on certain values in order for the model to be defined and/or for the model to make sense. For example, the symmetry parameter in the Richards function (Eq. 2.3) must be positive. Additionally, certain parameters may have logical bounds depending on the context of a study. If using a sigmoidal model to characterize learning, then the lower asymptote of the model cannot be smaller than the minimum observable  $y$ -value (e.g., the minimum score on a standardized test) and the upper asymptote cannot be larger than the maximum observable  $y$ -value (e.g., the maximum score on a standardized test).

The sampling distributions of bounded parameters may be nonnormal at sample sizes that are common in social science research (Feng et al., 2019). However, both nonlinear least squares



and maximum likelihood estimation assume that parameter estimates follow a normal sampling distribution (Motulsky & Christopoulos, 2004). This assumption underlies the computation of a simple parameter's standard error, and subsequently, the confidence bands of the JN plot. Thus, use of the JN technique rests on the assumption that parameter estimates follow a normal sampling distribution (Aiken & West, 1991; Bauer & Curran, 2005). Therefore, there are multiple questions that will be worthwhile to pursue in future work. First, under what conditions does the normality assumption tend to be violated for the bounded parameters of moderated nonlinear models? At what sample sizes do nonnormal sampling distributions begin to approach normality? Second, can the JN technique be adapted for use in conditions where the sampling distributions of parameters are known to be nonnormal? Such extensions will be important for ensuring that the JN technique yields accurate results when probing moderated nonlinear models.

Similar questions arise for parameters that are created via reparameterization of a given model. We can expect that sampling distributions for one parameterization of, say, the three-parameter exponential (3PE) model may differ in important ways from the sampling distributions for an alternative parameterization. The normality of parameters in one parameterization will not necessarily imply the normality of parameters in a reparameterization of the same model (Johnson & Hancock, 2019). In future work, it will be important to further examine the sampling distributions of parameters that result from reparameterization, given the cruciality of this assumption for the JN technique.

### **Considerations Regarding Sample Size, Temporal Design, and Measurement**

When working with nonlinear models, a variety of factors affect the likelihood of convergence, statistical power to identify effects and functional forms, and the accuracy of

parameter estimates. To enhance the probability that a theoretically well-motivated model will converge and will be estimated with reasonable accuracy, researchers must consider sample size, temporal design (in longitudinal contexts), and measurement reliability. Each of these factors has received varying amounts of attention in the methodological literature; extant findings and recommendations, as well as opportunities for future research, are summarized next.

First, sample size is a key consideration when working with nonlinear models. Generally, smaller sample size tends to be associated with a lower likelihood of model convergence, as well as reduced ability of model selection criteria to select the correct model. For example, in studies of longitudinal NLME models, the likelihood of convergence is found to be highly related to the number of measurement occasions (McNeish & Bauer, 2022). All extant studies of information criteria (ICs; e.g., AIC, BIC) for nonlinear model selection have found that sample size strongly impacts performance. Rohloff et al. (2022) observed that at smaller sample sizes, ICs were more likely to select an incorrect, overly complex model. Other studies (e.g., Christensen, 2019; Wood, 2023; Wood et al., 2015) have found that at smaller sample sizes, ICs are less likely to select the correct functional form, and less likely to select the correct predictor set for NLME models. However, researchers must balance the statistical advantages of larger sample size with the logistical costs of collecting more data (Moskowitz et al., 2017; Timmons & Preacher, 2015). Due to financial limitations, as well as concerns about participant attrition, fatigue, and/or practice effects, it is not always feasible to collect as much data as is ideal for convergence likelihood, accuracy, and precision of the nonlinear model to be estimated. Additionally, Timmons and Preacher (2015) note that in many cases, the relation between sample size and precision/accuracy embodies a pattern of diminishing returns, such that beyond a certain sample size, there is not much to be gained from collecting more data.

Given these findings, it appears that researchers would benefit greatly from the ability to easily conduct power analyses for a planned nonlinear model. However, at present, the tools to do so are limited. While power analysis approaches have been discussed in the context of (potentially nonlinear) growth curve models in the structural equation modeling framework (e.g., Diallo et al., 2014; Diallo & Morin, 2015; Zhang & Wang, 2009), there is less guidance for researchers going about sample size determination for nonlinear and/or NLME models. As an example of the tools that could be created, Lafit et al. (2021) recently developed a user-friendly Shiny app that conducts simulation-based power analysis for longitudinal multilevel models; however, this tool is restricted to linear models. A similarly user-friendly tool to conduct power analysis for nonlinear and/or NLME models would be a very useful avenue for future work.

The importance of sampling design is compounded when moderation is introduced. As discussed in Chapter 3, an inadequate number of observations across all regions of the design space is known to be a cause of nonconvergence for nonlinear models (Bates & Watts, 1988). Therefore, we can expect that when certain attributes of a nonlinear curve are hypothesized to be moderated, it will be important to obtain sufficient observations across a wide-enough range of the moderator, such that the effect of the moderation can be observed and estimated with reasonable accuracy and precision. However, methodological work has yet to address this topic. A useful direction for future work would be to provide more concrete recommendations and guidelines for researchers seeking to obtain adequate power to detect moderation within nonlinear models.

In addition to sample size considerations, researchers conducting longitudinal studies must also plan a *temporal design*, which is the timing and spacing of measurement occasions (Collins & Graham, 2002; Timmons & Preacher, 2015). Measurement occasions may be evenly

or unevenly spaced throughout a study period, and in unevenly spaced designs, occasions may be concentrated at the right, left, middle, or extremes of the range of the  $x$ -axis. Timmons and Preacher (2015) found that for intrinsically nonlinear models – including the power, exponential, and Gompertz models – concentrating measurement occasions where the curvature of the function was greatest tended to result in the best recovery of population parameters (i.e., the least bias). However, in order to strategically concentrate measurement occasions in this way, the researcher must have an *a priori* expectation of the timepoint(s) at which curvature is likely to be greatest. Therefore, the authors strongly encourage researchers to consider theory when planning a temporal design. Indeed, planning temporal design requires the researcher to consider similar questions as they would for a traditional power analysis (Timmons & Preacher, 2015), including anticipating the functional form, as well as reasonable parameter values for that form.

A unique aspect of nonlinear models is that many are asymptotic. Interestingly, models with asymptotes raise distinct issues with respect to sampling and temporal design. A common-sense argument is that in order to estimate an asymptote with reasonable accuracy, there must be a sufficient number of observations in the range of the  $x$ -axis where the asymptote occurs. If there are few or no observations in the asymptotic region, some methodologists have argued that it is nonsensical to estimate the asymptote and instead recommend constraining it to a constant (e.g., Motulsky & Christopoulos, 2004). However, in certain contexts, it may be difficult or impossible to obtain any observations within the  $x$ -axis range corresponding to the asymptote, especially within longitudinal studies of psychological change. Often, it is not feasible to observe individuals for so long that the asymptotic level of the outcome is reached, but at the same time, the asymptote may be of key substantive utility and important to estimate. McNeish and Dumas (2017) discussed this issue in their study of long-term growth in academic ability, wherein they

implemented Michaelis-Menten (MM) NLME models. Here, the upper asymptote of the MM model was a key substantive quantity referred to as the subject's *capacity*, or in other words, "the maximum amount of ability that an individual could develop given the individual's current and past ability levels" (p. 62). By design, there were no observations within the time period that corresponded with the asymptote, as the model was intended to predict *future* capacity. Indeed, the authors note that as observed timepoints become further away from the "future event" (i.e., the time at which asymptotic levels are reached), the estimate of those asymptotic levels becomes more uncertain. This raises the interesting question of "how close is close enough" in terms of the distance between the final measurement occasion and the time at which the final asymptote is reached. This question has yet to be addressed in methodological research (McNeish & Dumas, 2017), but is likely to be a viable avenue for future work.

Measurement reliability is another factor that strongly affects power, accuracy, and efficiency within the nonlinear modeling framework. In general, it is well-known that statistical power is affected by measurement reliability (i.e., the proportion of variability in observed scores that is attributable to true score variability rather than measurement error). However, measurement quality has received less attention in the nonlinear modeling literature (Jacobucci & Grimm, 2020); the few studies to have investigated reliability find that it strongly increases the probability that the researcher will arrive at the correct model specification. For example, Wood et al. (2015) generated data that followed a Gompertz curve, and found that BIC's ability to correctly select the Gompertz model (from among a candidate set of other parametric nonlinear models) was strongly impacted by the internal consistency of the outcome variable. Similarly, in his presentation of the combined exponential and logistic model, Wood (2023) found that in order for BIC to correctly select the combined model, an ICC of at least 0.7 and at least 10

measurement occasions were necessary. Finally, in their study of machine learning approaches for model selection, Jacobucci and Grimm (2020) found that when the data-generating function was nonlinear but measurement reliability was low, machine learning algorithms incorrectly selected a linear model in 97% of replications. In summary, extant findings suggest that measurement reliability is a key factor that impacts researchers' ability to correctly identify nonlinear functional forms; however, methodological work investigating this topic remains scarce. Future work may benefit from more in-depth explorations of the impact of measurement error within the nonlinear modeling framework.

### **Drawbacks of Nonlinear Models**

While a key goal of this dissertation has been to demonstrate the utility of nonlinear models for psychological research, it is also important to acknowledge that nonlinear models may not always be the optimal choice for every research context. Depending on the hypotheses to be tested and the goals of the analysis, there are situations where alternative approaches may provide more useful substantive insight. An example will be discussed next.

Recently, methodologists have pointed out potential drawbacks of nonlinear models when key hypotheses concern the demarcation between asymptotes and the growth area. McNeish et al. (2023) refer to these demarcation points as the  $x$ -axis location of “change onset” and “change offset.” Typically, a sigmoidal model would best characterize a trend that consists of an initial no-change period, a rapid-change period, and a final no-change period. However, sigmoidal curves never actually *reach* the asymptotes; rather, they infinitely *approach* the asymptotes. Therefore, change is always occurring to some degree, and defining the location at which change “begins” and “ends” will be arbitrary (Feng et al., 2019). As an example, working

with a logistic model, Choi et al. (2009) defined these locations as the two *jerk points* of the curve; jerk points were identified as the  $x$ -axis locations at which the function's third derivative was equal to zero. On the other hand, McNeish et al. (2023) argue that in order to define the point where a final asymptote is "reached," the researcher must set some threshold for declaring growth completed, such as finding the  $x$ -axis location at which 99% or 99.9% of growth toward the asymptote has occurred. Given these issues, piecewise models may be the better choice when key study hypotheses concern the timing of change onset and offset (Feng et al., 2019; McNeish et al., 2023), as piecewise models contain knot points that unambiguously define the transitions between change phases.

Importantly, the preceding arguments are motivated by the *theoretical* and *substantive* contribution that can be made by the model. Although practical factors (e.g., estimation difficulties, ease of software implementation) are not trivial and are often considered when researchers are deciding between linear and nonlinear models, the ultimate motivation for the chosen model should rest on its correspondence with theory and ability to test useful hypotheses.

### **Nonparametric Approaches**

The scope of this dissertation was intentionally restricted to parametric nonlinear models. However, it is useful to contrast these models with nonparametric approaches and discuss the pros and cons of each framework. The generalized additive mixed model (GAMM) is largely nonparametric and has been implemented in many social science research contexts. GAMMs enable the researcher to model complex nonlinearities that may not correspond with a known mathematical function. Rather than requiring the researcher to specify the functional form *a priori*, GAMMs estimate the functional form empirically by linking together a (potentially large)

number of curvilinear functions that are joined by knot points. The researcher may control the overall degree of curvilinearity by specifying the number of basis functions and/or the general “wiggleness” that is allowed (e.g., Cho et al., 2023), but overall, the functional form is informed by the data rather than by the researcher’s hypotheses about its shape.

A key advantage of GAMMs is that they are more flexible than parametric nonlinear models, as they can approximate any curvilinear functional form (Cho et al., 2022). Therefore, GAMMs may be best suited for research contexts wherein a highly complex curvilinear pattern is expected, “which cannot be described by a single, unified equation” (McCormick et al., 2023, p. 13), or wherein the researcher is uninterested in specifying the functional form *a priori*. For example, using illustrative data from a cluster randomized controlled trial (C-RCT) that aimed to reduce women’s depressive symptoms, Cho et al. (2023) specified a GAMM to evaluate the nonlinear interaction between the treatment effect and a level-1 predictor (pre-test depression). The functional form linking pre-test depression to post-test depression was curvilinear. To accurately estimate the interaction, it was necessary to account for the fact that the “wiggleness” of this curvilinearity differed across clusters – which was accommodated by the GAMM – but it was not substantively useful to obtain specifics about the nature or shape of that curvilinearity, as this was unrelated to key study hypotheses.

Despite the enhanced flexibility provided by nonparametric models like the GAMM, their essential drawback is that unlike the parametric nonlinear model, the parameters of a GAMM cannot be mapped directly onto specific attributes of a curve. Therefore, these parameters typically do not correspond to substantively meaningful quantities. McCormick et al. (2023) argue that GAMMs bear significant resemblance to machine learning models, and as such, may be better suited for explanation and/or prediction rather than hypothesis testing. Ultimately,



nonparametric and semiparametric methods embody a modeling framework that differs in important ways from the parametric framework emphasized in this dissertation. Nonparametric and semiparametric methods are better suited for exploratory endeavors, whereas parametric methods are better suited for confirmatory endeavors. The choice of which framework to implement will depend on the research context and study goals. Overall, it is important to understand that parametric nonlinear models are the optimal approach for linking model parameters to theory and for testing hypotheses developed on an *a priori* basis.

### **Dissertation Summary**

The overarching goal of this dissertation was to integrate the topics of parametric nonlinear models and linear moderation, which have largely been treated as disparate in extant literature. Key contributions include detailing the utility of nonlinear models for social science research, summarizing current barriers – both conceptual and logistical – to the uptake of nonlinear models, and providing guidelines for various stages of the model specification process, including choosing a nonlinear function, choosing a useful parameterization, incorporating moderators, and incorporating covariates. Additionally, conceptual and mathematical extensions of the JN technique were presented, such that the technique can now be applied to moderated nonlinear models. Finally, a new Shiny app was created that enables researchers to specify, fit, evaluate, and visualize moderated nonlinear models in a code-free environment. Ideally, the methods and software presented here will reduce most of the key barriers that social scientists currently face when implementing moderated nonlinear models, and the use of such models will increase across our field.

## APPENDIX A

### ESTIMATION METHODS FOR NONLINEAR MODELS

#### Nonlinear Least Squares

Nonlinear regression models can be estimated by a variety of iterative methods. Perhaps the most popularly discussed estimator is nonlinear least squares. Davidian and Giltinan (1995) refer to this as ordinary least squares (OLS) because the usual OLS criterion – minimizing the sum of squared residuals – is the same as it is for linear models. Most other sources refer to this estimator as “nonlinear least squares” to highlight the fact that estimates are now obtained via an iterative procedure. Many methodologists agree that when all assumptions of nonlinear regression are met, nonlinear least squares is the best estimator because it is the easiest to implement (Davidian & Giltinan, 1995; Motulsky & Christopolous, 2004).

However, if any assumptions are violated, nonlinear least squares becomes inefficient and standard errors become inconsistent, meaning they will *not* approach the true standard errors as sample size increases. The performance of nonlinear least squares estimation has never been investigated with respect to moderated nonlinear models specifically. However, given its sensitivity to assumption violations, it may not be robust enough to perform optimally in common moderation scenarios. For example, Franzese and Kam (2009) note that, in scenarios where the moderator is categorical, there is an implicit assumption that residual variance is equal across the groups defined by the moderator. However, this assumption is not often checked. It could be argued moderation introduces new assumptions and/or makes it more difficult for researchers to check whether assumptions have been violated; therefore, because of its strong

reliance upon all assumptions being met, nonlinear least squares may not be the best estimator for these models. This would be a useful topic for future research to examine.

### **Weighted Least Squares**

When assumption violations are present, specifically if error variance is found to be heteroscedastic, the weighted least squares estimator is a frequently suggested alternative for nonlinear regression (e.g., Davidian & Giltinan, 1995; Sit & Poulin-Costello, 1994). The weighted least squares estimator still seeks to minimize the sum of squared residuals. However, residuals are now given weights that are inversely proportional to the variance of  $y$  at that point. Through this procedure, residuals associated with  $y$ -values that are more variable (i.e., less certain) are given less weight in determining the parameter estimates. A drawback of this estimation method is that the user is required to supply a weighting scheme, which means they must choose from many schemes that exist. For example, Motulsky and Christopolous (2004) suggest “relative weighting” by the variance of  $y$ . In contrast, Davidian and Giltinan (1995) advocate for iteratively reweighted least squares (IRLS), where initial weights are derived from nonlinear least squares estimates, then the model is re-fit, the weights are updated, and this process is repeated until convergence is achieved. Still other options are available. The R function *nls* requires the user to compute and supply weights in vector form, whereas SAS PROC NLIN has the capacity to implement IRLS. Weighted least squares yields superior estimates in the presence of heteroscedastic residuals, which is sometimes cited as the most common assumption violation in nonlinear regression; however, regardless of the software chosen, incorporating weights is not straightforward for the user. The performance of the weighted least squares estimator with respect to moderated nonlinear models has never been assessed, but this

would be an important topic for future study. There may be additional considerations – which arise in moderated models specifically – that influence the performance of the weighted least squares estimator. For example, if a categorical moderator is present, and the residuals behave differently across groups defined by the moderator, the best weighting scheme may become unclear. Alternatively, the presence of a continuous moderator may further complicate matters. Future work should assess whether there are conditions under which weighted least squares is the optimal estimation method for moderated nonlinear regression models.

### **Sandwich Estimators**

Sandwich estimators are another option when errors are non-normal and/or residuals are heteroscedastic, and is recommended by Ritz and Streibig (2008). Here, parameters are estimated with nonlinear least squares, then the covariance matrix of parameter estimates is adjusted. The adjustment yields standard errors that are robust to residual heteroscedasticity and non-normal errors. Ritz and Streibig (2008) argue that this approach is more straightforward than explicitly modeling non-constant variance, and is easier than creating a weighting scheme for weighted least squares estimation. After fitting a nonlinear model, sandwich estimates can easily be obtained through the *sandwich()* function on *nls* objects in R, and significance tests of each parameter can be re-calculated from the adjusted standard errors. Indeed, in the presence of assumption violations, it seems that the simplicity of the sandwich estimator is its major strength relative to weighted least squares. The performance of this estimator has never been assessed with respect to nonlinear moderated models; however, it would be useful to examine whether the adjustment still functions as intended when parameters are moderated.

## Maximum Likelihood

When parameter estimates must be obtained iteratively, maximum likelihood (ML) is generally a popular estimation method. However, in the single-level nonlinear regression literature, ML has received less attention than least squares estimation methods. Davidian and Giltinan (1995) note that, asymptotically and when all assumptions are met, nonlinear least squares estimates are equivalent to ML estimates. However, these authors advocate for the use of least squares methods rather than ML. They note that ML estimation relies heavily on the normality-of-residuals assumption, and therefore is highly sensitive to outliers. Additionally, if the researcher chooses to explicitly model variance heteroscedasticity by incorporating a variance function, the ML estimator will be sensitive to misspecification. Likely for these reasons, ML estimation is not an option in popular software including SAS PROC NLIN and *nls* in R. However, it is the preferred and default method for NLME models.

Of the various R packages for fitting NLME models, each employs a slightly different estimation method that is based in ML. Stegmann et al. (2018) provide a useful review of these packages and their performance. The *nlme* package (Pinheiro et al., 2023) maximizes the log-likelihood by using an algorithm that alternates between two steps: a penalized nonlinear least squares step, and a linear mixed effects step. The algorithm alternates between updating the fixed effects estimates and the random effects estimates while holding the other constant. Stegmann et al. note that this estimation method is “state of the art for its speed and sensitivity.” The *lme4* package provides the *nlmer* function for nonlinear mixed-effects models. Here, the estimation algorithm alternates between three steps until convergence is achieved: penalized iteratively reweighted least squares, integrating out the random effects, and nonlinear optimization of the objective function. The *saemix* package uses a stochastic approximation of the likelihood by

using a modification of the E-M algorithm. Although *saemix* is slower to converge, simulation studies have shown that it yields substantially higher convergence rates than *nlme* and *lme4*, especially when models are more complex. This finding suggests that *saemix* may be especially well-suited for moderated nonlinear models. The performance of these packages for moderated NLME models has never been compared; however, such a comparison would be useful to explore in future research.

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