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ORIGINAL MANUSCRIPT

New methodological and software tools for probing moderation in intrinsically nonlinear models

Haley E. Yaremych[1,2] · **Kristopher J. Preacher**[1]

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Abstract
When modeling psychological processes and relationships, intrinsically nonlinear models often enhance researchers' ability to draw useful theoretical and substantive conclusions. In addition, psychological theories frequently suggest that such processes and relationships are moderated; therefore, it is often important to test for, probe, and plot moderation. However, extant methods for assessing and visualizing moderation are largely restricted to linear models. Therefore, the goal of this paper is to develop novel analytical and software tools that enable researchers to specify and examine moderated parameters within intrinsically nonlinear models. First, methods for testing, plotting, and probing moderation are expanded in novel ways for use in nonlinear models; specifically, we present conceptual and mathematical extensions of the Johnson-Neyman (JN) technique. The JN technique is currently used to probe moderation of simple slopes within the linear modeling framework; our extensions enable its application to any moderated parameter of an intrinsically nonlinear model. Additionally, we introduce a Shiny application called CurveBuilder, which unifies the process of choosing, specifying, fitting, and visualizing intrinsically nonlinear models that may include moderated parameters and/or random effects. 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 moderation with the extended JN technique. CurveBuilder examples are reviewed, and opportunities for future work in this area are discussed.

Keywords Intrinsically nonlinear models · Nonlinear models · Moderation · Interaction · Johnson-Neyman technique · Shiny

Intrinsically nonlinear models afford many advantages for modeling psychological phenomena. Additionally, psychological theories often involve moderation. However, due to both methodological and software limitations, researchers' options for testing, plotting, and probing moderation in nonlinear models are very limited. We present novel analytical extensions that enable the specification, testing, visualization, and probing of moderated parameters within intrinsically nonlinear models. Additionally, we introduce a Shiny app that unifies this process.

✉ Haley E. Yaremych
haley.yaremych@gmail.com

[1] Department of Psychology & Human Development, Vanderbilt University, Nashville, TN, USA

[2] JMP Statistical Discovery LLC, Cary, NC, USA

Intrinsically nonlinear models

First, it is important to define the *nonlinear models* that will be discussed throughout this paper, as *nonlinear* often takes on different meanings across contexts. In *intrinsically nonlinear regression models*, 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) is linear in its parameters whereas the three-parameter exponential (3PE) model (Eq. 2) is nonlinear in its parameters.

$$y = \hat{a} + \hat{b}x + \hat{c}x^2 + \varepsilon. \quad (1)$$

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$$y = \hat{a} + \hat{b} * \exp\left(-\hat{c} * x\right) + \varepsilon. \quad (2)$$

Throughout this paper, we use *nonlinear* to reference models that are nonlinear in at least one parameter in the regression equation, according to the above definition. More formally, these intrinsically nonlinear regression models can be defined in terms of 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). To demonstrate this point, consider the quadratic model, which characterizes a *curvilinear* relation between x and y, but is *linear* in its parameters. The first derivative with respect to parameter a, $\frac{dy}{da}$, is 1, whereas $\frac{dy}{db}$ is x and $\frac{dy}{dc}$ is x^2. Note that none of these first derivatives contain model parameters. In contrast, follow the same process for the 3PE model: $\frac{dy}{da} = 1$, $\frac{dy}{db} = \exp(-c * x)$, and $\frac{dy}{dc} = -bx * \exp(-c * x)$. Since derivatives with respect to b and c contain model parameters, this is an intrinsically nonlinear regression model.

Elsewhere, models may be described as *nonlinear* according to how parameters appear in the regression equation (as we have defined it here), according to the shape of the relation between x and y, or based on other features of the model. Sometimes, *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 nonlinear despite being linear in its parameters. For clarity, we will use *curvilinear* as a broader descriptor for relationships between x and y that do not follow a straight line. In still other contexts, *nonlinear* models refer to generalized linear models with link functions; these models are beyond the scope of this paper, as we limit our attention to models with continuous, normally distributed outcomes. Finally, nonparametric models such as the generalized additive mixed model (GAMM; Lin & Zhang, 1999; Wood, 2017) are termed *nonlinear* in other literature. These models take on a shape that is informed by the data rather than by prespecified functional form. The scope of this paper is limited to parametric intrinsically nonlinear models, which are defined prior to being fit to the data in terms of their shape and the parameters that govern that shape (Panik, 2014). These models do not involve transformations or link functions; x and y remain in their original units.

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 parameters reflecting 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 an intrinsically nonlinear model that can approximate that relationship. Each nonlinear model describes a specific functional form and often has been given a specific name. Though these models are distinct from one another, nonlinear models collectively offer greater flexibility than linear models (Archontoulis & Miguez, 2015).

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

For example, consider the 3PE model given in Eq. 2. Models in the exponential family (sometimes described as inverted J-shapes) are known to characterize processes 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). In cross-sectional contexts, they correspond to hypotheses involving "diminishing returns" or "plateauing associations." The relations between frequency of social contact and well-being (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 shown to follow such patterns.

The 3PE model is governed by three parameters, *a, b,* and *c*. Parameter a governs the vertical location of the asymptote, parameter b governs total growth/change (i.e., the vertical distance between the intercept and asymptote), and parameter c governs rate of change toward the asymptote. Figure 1 depicts how the shape of the 3PE curve changes as each parameter changes while the others are held constant.

Nonlinear models may contain even more parameters that each correspond with a unique attribute of the curve. As another example, consider the logistic model,[1] which belongs to the sigmoidal (S-shaped) family of nonlinear models. Models in this family characterize processes of learning, academic achievement trajectories, and skill acquisition in longitudinal contexts (e.g., Anthony & Ogg, 2020; Cameron et al., 2015; Ricker et al., 2018), as well as some

[1] The *logistic model* discussed in this paper is a type of intrinsically nonlinear regression model, where both the predictor and outcome variable are continuous. In other literature, the *logistic model* may refer to a linear regression model that includes a *logistic link function* because the outcome variable is binary.

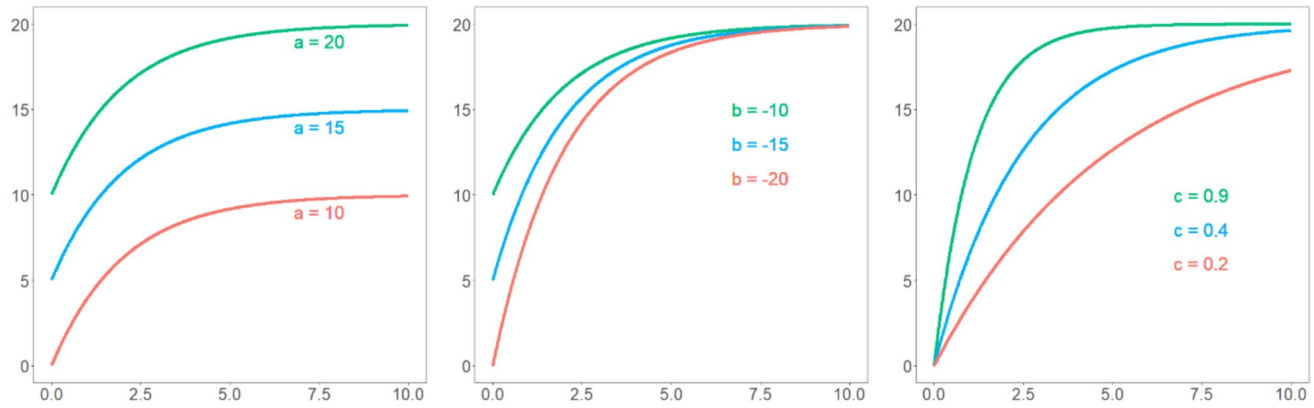

Fig. 1 Three-parameter exponential (3PE) curve examples

responses to experimental stimuli in cross-sectional contexts (e.g., D'Hondt et al., 2015; Zhao et al., 2022). One version of the four-parameter logistic model is

$$y = a + b * (1 + \exp(-c(x - d)))^{-1} + \varepsilon. \quad (3)$$

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 2 displays versions of the logistic curve where each parameter is varied and the others are held constant.

There are a wide variety of other intrinsically nonlinear models that characterize even more types of curves. For more examples, see Fig. 3. In all cases, when we fit intrinsically nonlinear models, our analysis goals are quite different

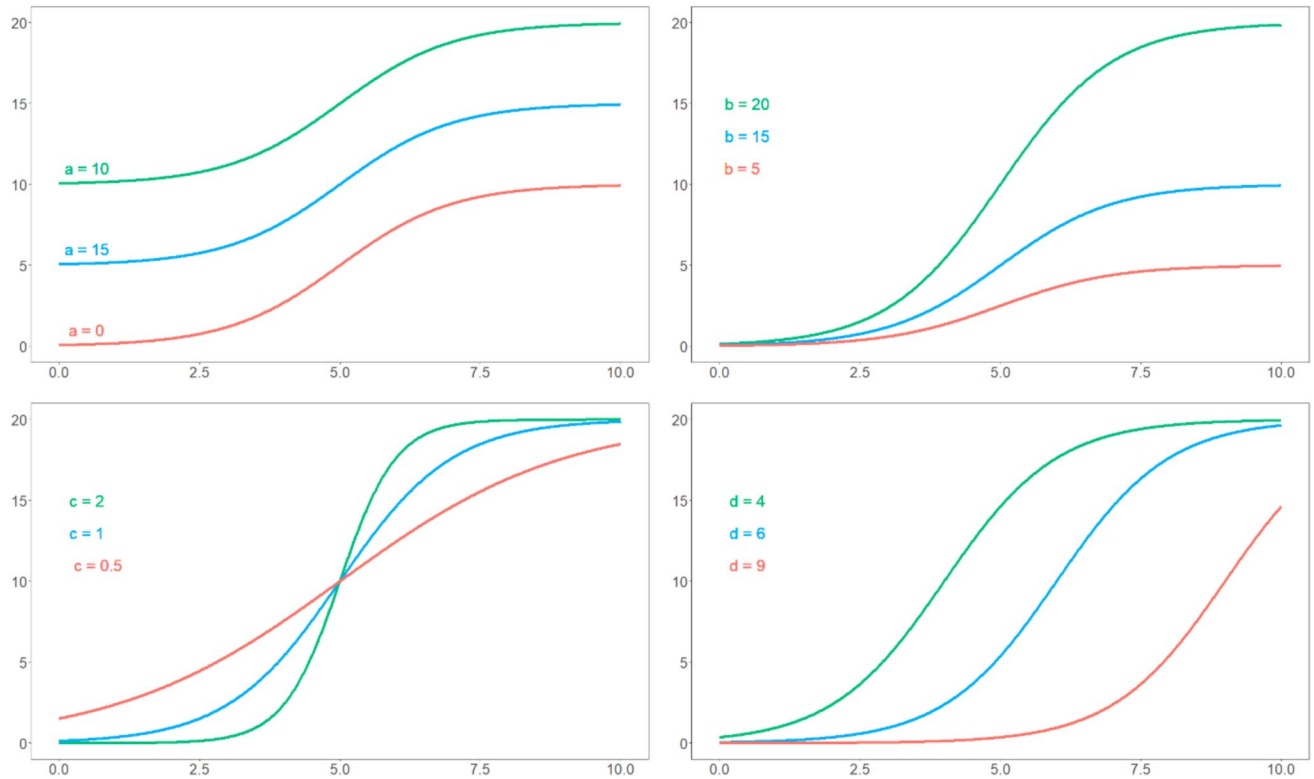

Fig. 2 Logistic curve examples

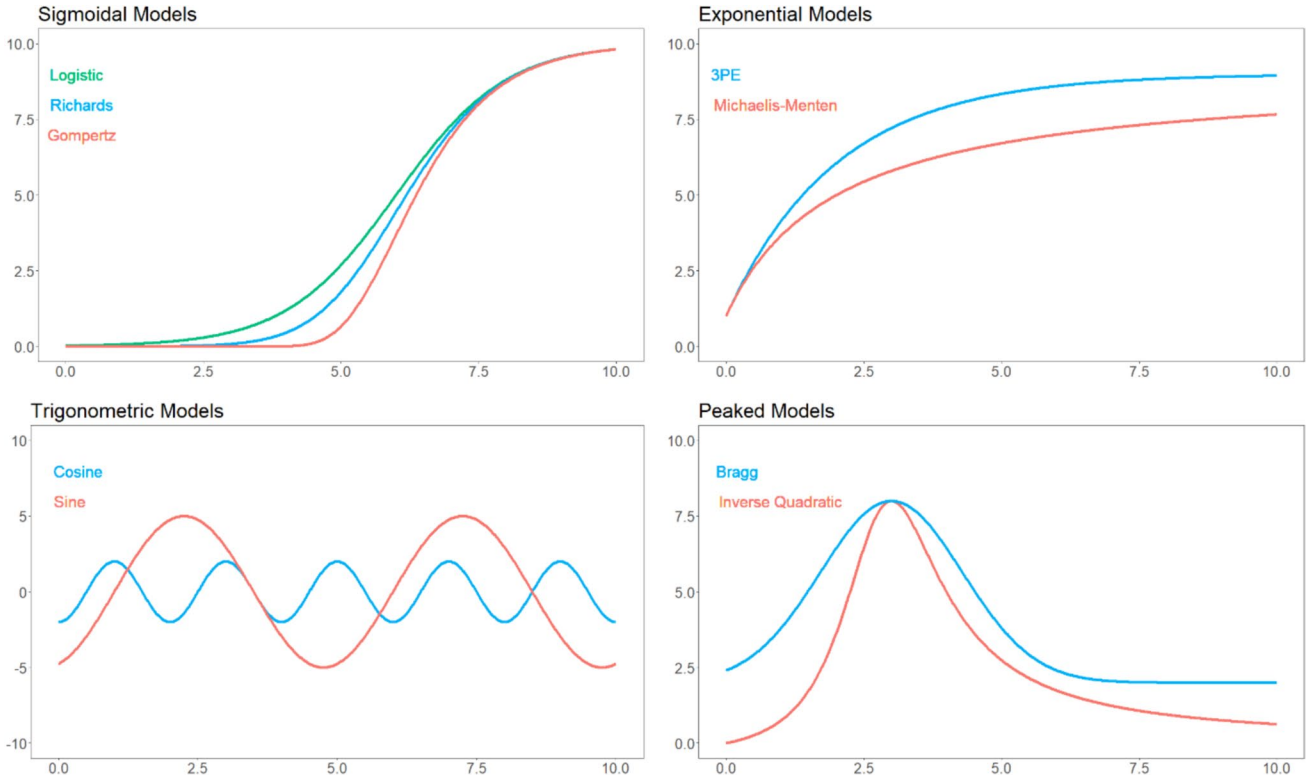

Fig. 3 Examples of intrinsically nonlinear models

relative to linear modeling. Rather than seeking to establish a "significant" association between x and y (as is often our goal in the linear framework), our goal in the intrinsically nonlinear framework is to choose a model that does a good job of characterizing the relationship between x and y, and that has interpretable parameters that correspond to something useful or interesting in our substantive context. Estimating and interpreting these parameters lends novel insight into this relationship that could not otherwise be obtained from a linear model.

Specifying and probing linear moderation

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 estimated regression equation:

$$y = \hat{\gamma}_0 + \hat{\gamma}_1 x + \hat{\gamma}_2 z + \hat{\gamma}_3 xz + \epsilon, \tag{4}$$

where the $\hat{\gamma}$ s are the estimated linear regression weights. Rearranging Eq. 4, 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 is the effect of x on y at a particular value of z:

$$\hat{\omega}_1 = \hat{\gamma}_1 + \hat{\gamma}_3 z. \tag{5}$$

When the slope of x is moderated, it is useful to analyze and visualize that result to understand the nature of the moderation. The most popular method for probing moderation is the pick-a-point plot (Aiken & West, 1991), also called spotlight analysis (Spiller et al., 2013). Here, the researcher chooses a few values of z (typically the mean $\pm$ 1 SD) and plots the relation between x and y at each of those values (Fig. 4). The pick-a-point approach is easy to implement and produces intuitive plots. However, the researcher evaluates the simple slope of x at only a few values of z; these values are inherently arbitrary and are often chosen automatically (Bodner, 2016). Additionally, the use of only a few z-values 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).

The Johnson-Neyman (JN) technique (Johnson & Fay, 1950; Johnson & Neyman, 1936) is a general method for evaluating the simple slope of x across all possible values of the moderator. The JN technique improves upon the major weaknesses of the pick-a-point approach (Bauer & Curran, 2005). First, results communicate whether the simple slope

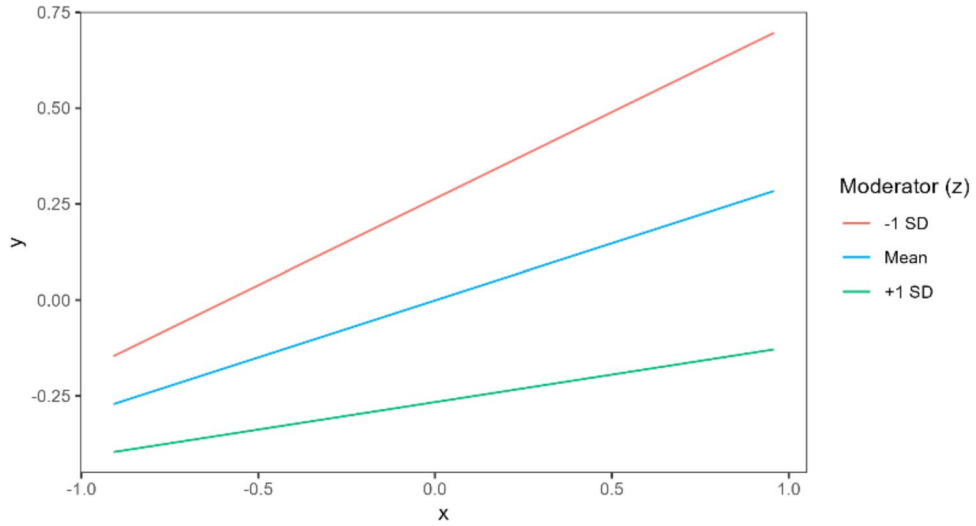

Fig. 4 Pick-a-point plot example

of x is significant at every possible value of the moderator. Second, confidence bands (i.e., confidence intervals for the simple slope plotted as a continuous function of a moderator) communicate how certain we are about the simple slope of x at all possible values of z, rather than at just a few. Additionally, by deriving significance boundaries, the JN technique allows us to answer the following question: given a continuous predictor x and a continuous moderator z, for which values of z is the simple slope of x significantly different from zero? Significance boundaries demarcate regions of significance, which contain the z-values at which the simple slope of x is significant.

Calculating significance boundaries is relatively straightforward with the JN technique. The simple slope of x is defined in Eq. 5, and the standard error of that simple slope is the square root of its variance, which is given by Aiken and West (1991) as

$$\text{var}\left(\hat{\omega}_1\right) = \text{var}\left(\hat{\gamma}_1\right) + 2z\text{cov}\left(\hat{\gamma}_1, \hat{\gamma}_3\right) + z^2\text{var}\left(\hat{\gamma}_3\right). \tag{6}$$

Under the pick-a-point approach, we choose a few values of z, compute $\hat{\omega}_1$ and $SE\left(\hat{\omega}_1\right)$ at each of those values, and assess the significance of $\hat{\omega}_1$ at each of those values with a t-test:

$$t = \frac{\hat{\omega}_1}{SE(\hat{\omega}_1)}, \tag{7}$$

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.

With the JN technique, rather than solving for t 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:

$$\pm t_{crit} = \frac{\hat{\omega}_1}{SE(\hat{\omega}_1)}. \tag{8}$$

Equation 8 is solved for values of z through use of the quadratic formula. The obtained values of z indicate the points at which the simple slope of x passes from non-significance to significance.

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 (Fig. 5). Here, we plot the moderator on the horizontal axis and the simple slope of x on the vertical axis. The confidence bands communicate our certainty about that simple slope at each value of z. In Fig. 5, the vertical line denotes a significance boundary, and the confidence band denotes z values at which the simple slope of x differs significantly 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 z. When there are two boundaries, the simple slope of x may be significant either between or outside of them.

In summary, when a parameter is 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, as it enables plotting the moderated parameter across every value of the moderator and pinpoints the value(s) of the moderator where that parameter is and is not statistically significant.

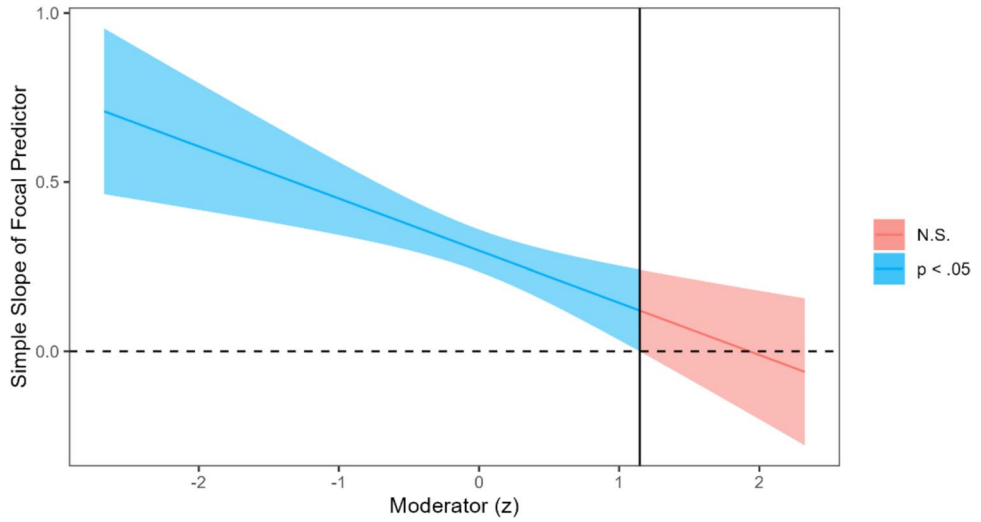

Fig. 5 Johnson-Neyman plot example

Barriers to fitting and probing moderated nonlinear models

For social science researchers seeking to test hypotheses of moderation within nonlinear rather than linear models, there is limited precedent for specifying and probing such models using the methods described in the previous section. Perhaps more problematically, many obstacles arise when attempting to carry out this process with software. Across software systems, the functions, formulas, and procedures for nonlinear models are often notably more complicated than those available for linear models (McCormick, 2023).

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 that moderation. Extant R packages for plotting and probing moderation cannot accommodate nonlinear models; functions developed for probing interactions, such as those in the *interactions* (Long, 2019) and *reghelper* (Hughes & Beiner, 2023) packages, accept only linear model objects. Additionally, most tools for fitting nonlinear models contain few or no plotting capabilities. Although SAS procedures like NLIN and NLMIXED permit moderated parameters, there is no straightforward way to plot or probe the output of such an analysis. In R, 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). The *marginaleffects* R package (Arel-Bundock et al., 2024) enables visualization of GAMs, which are nonlinear in the nonparametric sense, though JN functionality is missing. 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 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. 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.

Study goals

Given researchers' limited ability to probe moderation within intrinsically nonlinear models, the goals of this study are twofold. First, we present novel extensions of the JN technique to facilitate its application to moderated nonlinear models. Second, we introduce a new Shiny app called CurveBuilder, which provides a code-free environment wherein researchers can specify, fit, evaluate, probe, and visualize moderated nonlinear models.

Extending the Johnson-Neyman technique for moderated parameters in nonlinear models

The JN technique was developed for linear models. In rare instances, it has been applied to quadratic models (e.g., Kim et al., 2023; Miller et al., 2013), which allow for curvilinearity, but are intrinsically linear. Thus, the JN technique is currently restricted to intrinsically linear models. The purpose of this section is to present novel expansions of the JN technique to enable its use for plotting and probing *any* linearly moderated parameter, particularly those in nonlinear models. This section presents both conceptual and mathematical

extensions of the JN technique. For an in-depth example that further explicates these extensions, see the Online Appendix (available at https://osf.io/7gkny/).

Incorporating moderators into nonlinear models

We preface our discussion of the JN technique with details about how to specify linear moderation within nonlinear models. In general, linear moderation occurs when a parameter varies linearly according to the value of the moderator. To visualize this in the context of linear regression, we can rearrange Eq. 4 as $y = (\hat{\gamma}_0 + \hat{\gamma}_2 z) + (\hat{\gamma}_1 + \hat{\gamma}_3 z)x + \varepsilon$. The simple slope is $\hat{\gamma}_1 + \hat{\gamma}_3 z$, where $\hat{\gamma}_1$ is the slope when the moderator (z) is zero, and $\hat{\gamma}_3$ denotes the linear effect of z on the slope. When z increases by one unit, the slope changes by $\hat{\gamma}_3$. (Though often less substantively important, the terms that make up the simple intercept are analogous; $\hat{\gamma}_0$ is the intercept when z is zero, and when z increases by one unit, the intercept changes by $\hat{\gamma}_2$.)

We can follow the same procedure to specify linear moderation of parameters in nonlinear models. Recall the 3PE model given in Eq. 2: $y = \hat{a} + \hat{b} * \exp(-\hat{c} * x) + \varepsilon$. 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 specify the moderated model as follows: $y = (\hat{a}_0 + \hat{a}_1 z) + \hat{b} * \exp(-\hat{c} * x) + \varepsilon$. We replace parameter a with $\hat{a}_0 + \hat{a}_1 z$, such that a_0 denotes the value of parameter a when the moderator is zero, and a_1 denotes the linear effect of z on a. As the moderator increases by one unit, the vertical location of the asymptote changes by a_1. If a_1 is significantly different from zero, then z has a statistically significant moderating effect on the location of the asymptote.

Conceptual extensions of the JN technique

When moderation is introduced in linear models, the key moderated quantity is almost always the simple slope of the focal predictor. Therefore, significance boundaries from JN technique denote the value(s) of the moderator at which the simple slope passes from significance to non-significance. However, in moderated nonlinear models, any parameter may be moderated. The parameters of nonlinear models map onto a diverse array of curve attributes beyond linear rate of change, including peaks, asymptotes, wave amplitudes, locations along the x-axis corresponding to knots or inflection points, and more. Therefore, the JN technique must be extended such that it can identify the value(s) of the moderator at which *any moderated parameter* passes from significance to non-significance. For many of these parameters, it will be necessary to conceptualize "significance" in new ways.

Definitions of significance are almost always the same in linear models. Generally, a slope is "significant" if it is statistically distinguishable from zero. Therefore, 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; whether a parameter is statistically distinguishable from zero may not be useful substantive information.

The need for nonzero null values is perhaps the most important conceptual extension that arises when applying the JN technique to moderated nonlinear models. As a running example, we will reference a study by Womack et al. (2022) in which the Gompertz model (a popular model from the sigmoidal family) was used to characterize cognitive development among children from age 3 months to 15 years. The authors used a popular parameterization of the Gompertz model (hats and subscripts omitted for brevity):

$$y = a + b\left[\exp(-\exp(-c(x-d)))\right] + \varepsilon, \tag{9}$$

where a is the lower asymptote, b is total growth, c is rate of growth, and d is the inflection point, which is the location along the x-axis (i.e., age) at which growth is the fastest. Socioeconomic status (SES) moderated all parameters, such that higher SES was related to a smaller lower asymptote, greater total growth, a slower growth rate, and an earlier inflection point. The equation for the moderated Gompertz model looks like this:

$$y = (a_0 + a_1 SES) + (b_0 + b_1 SES)\left[\exp\left(-\exp\left(-(c_0 + c_1 SES)\left(x - (d_0 + d_1 SES)\right)\right)\right)\right] + \varepsilon. \tag{10}$$

Parameter estimates for a_1, b_1, c_1, and d_1 were all statistically significant, indicating that SES had a significant moderating effect on each parameter (i.e., each attribute of the curve). To visualize this result, see Fig. 6, which was created with simulated data to mimic the results reported in the study.

After identifying significant moderation, the next step is to probe these results to gain a more thorough understanding

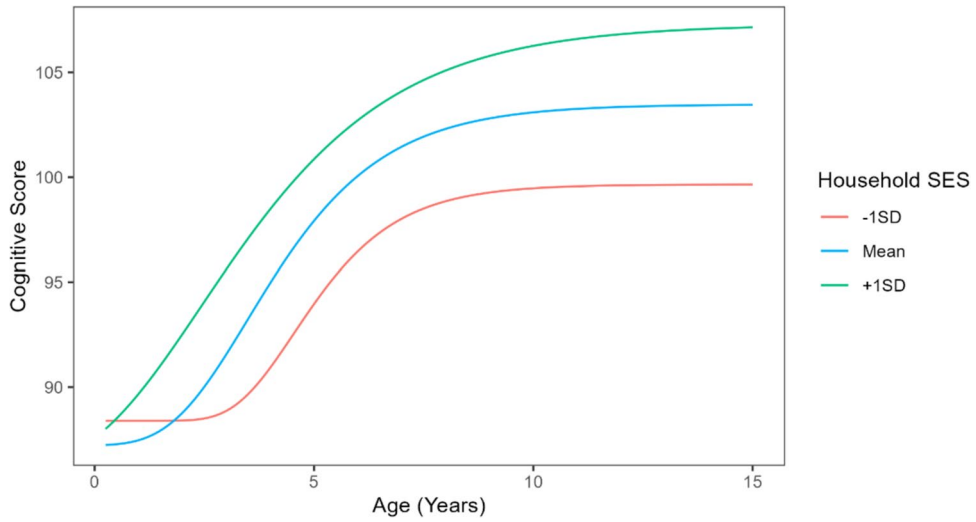

Fig. 6 Cognitive score versus age at three SES levels, adapted from Womack et al. (2022)

of how SES affects the development of cognitive ability. First, let us consider moderation of the inflection point (parameter *d*). The inflection point is the location along the *x*-axis (here, age) where growth is most rapid. 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. It would be useful to probe moderation results to determine the levels of SES at which the inflection point is significantly delayed. The JN technique is ideal for this purpose.

To find SES 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* differs significantly 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* can 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 is chosen. 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. Alternatively, 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 SES level(s) does the inflection point become significantly different from four? See Fig. 7 for a visualization.

Results also indicated that SES moderated parameter *b*. Parameter *b* reflects total growth in cognitive ability over the course of ~15 years. Its mean estimated value was 17.01; this can be observed in Figs. 6 and 7, where the blue curve (i.e., when SES is at its mean) begins at a *y*-value of about 86 and ends at a *y*-value around 103, showing about 17 points of growth. SES had a positive effect on parameter *b*; b_1 was estimated to be 5.57, indicating that as SES increases by one unit, total growth increases by about 5.57 points. This can also be observed in Figs. 6 and 7. Total growth is smaller when SES is 1 SD below the mean (red line) and total growth is greater when SES is 1 SD above the mean (the green line).

Indeed, a null value of zero is not appropriate for this parameter. 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

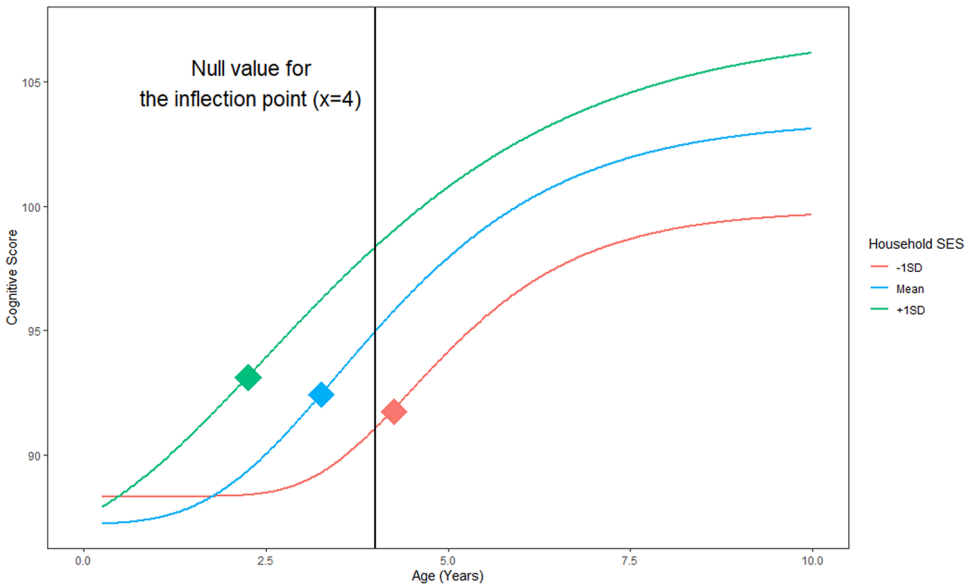

Fig. 7 Cognitive score versus age at three SES levels, including estimated inflection points at each SES level and a null value for the inflection point. *Note.* Diamonds are the estimated inflection points at each level of SES: mean −1 SD, mean, and mean +1 SD

regarding cognitive development. For example, perhaps children whose total growth is five or fewer points tend to suffer long-term cognitive deficits. Treating five as the null value may allow us to identify SES 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. 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, such as the visualization provided by the pick-a-point plot. Second, there may not be useful 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 test moderation of a slope, we must also allow the intercept to be moderated to obtain an accurate estimate of slope moderation.) 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) to accurately estimate how parameter b is moderated. Indeed, this may be the case for parameter a in the Womack et al. (2022) model; SES moderated parameter a, but there may not be useful information to be gained, or hypotheses to be tested, by applying the JN technique to this result.

Finally, 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 are hypothetical examples created for demonstration, and the rationales provided here should not be considered universal to all applications. 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 against a null value of zero may not yield substantively useful information. In all cases, transparency and justification will be essential for JN-related decisions. Having addressed these conceptual extensions, we next present a mathematical extension of the JN technique for use with nonzero null values.

Mathematical extension of the JN technique

To preface this section, we first note that our mathematical extension of the JN technique (which makes use of the delta method) relies on some key assumptions. The delta method is an asymptotic method that assumes the model's parameter estimates are normally distributed. This assumption is often tenable, but may not always hold for every parameter of a nonlinear model. Furthermore, in intrinsically nonlinear models, the sampling distributions of parameter estimates may not always be normal when sample size is small. See the Discussion section for more detail about these assumptions and limitations.

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 we refer to as the *simple parameter* (akin to a simple slope) and its standard error (SE).

To obtain an expression for a simple parameter, recall 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. 9, such that parameter b is linearly moderated by z:

$$y = \hat{a} + \left(\hat{b}_0 + \hat{b}_1 z\right)\left[\exp\left(-\exp\left(-\hat{c}\left(x - \hat{d}\right)\right)\right)\right] + \varepsilon, \quad (11)$$

where $\hat{b}$ has been replaced by $\hat{b}_0 + \hat{b}_1 z$. Here, $\hat{b}_0$ is the estimated value of parameter b when z is zero, and $\hat{b}_1$ is the estimated change in parameter b when z increases by one unit. The expression for the "simple parameter b" is given by

$$\hat{\omega}_b = \hat{b}_0 + \hat{b}_1 z, \quad (12)$$

as this quantity reflects the value of parameter b conditional on a particular value of z. 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.

Next, we must obtain an expression for the variance (and subsequently, SE) of a simple parameter. 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). Importantly, any simple parameter that is subject to linear moderation can be expressed as a linear combination, such as in Eq. 12; therefore, it is possible to use the delta method to derive its variance (and, subsequently, SE). As long as the model is parameterized so that the moderated quantity is expressed as a linear combination, the asymptotic covariance matrix (ACOV) of parameter estimates contains the necessary elements to derive the variance of the simple parameter. To obtain the variance of $\hat{\omega}_b$, first express $\hat{\omega}_b$ as a weighted linear combination:

$$\hat{\omega}_b = (1)\hat{b}_0 + (z)\hat{b}_1. \quad (13)$$

The elements of the combination are the estimated parameters, $\hat{\boldsymbol{b}} = [\hat{b}_0\ \hat{b}_1]$, and the weight vector is $\boldsymbol{w}' = [1\ z]$. More specifically, the weight vector contains the first partial derivatives of Eq. 13 with respect to each component parameter in turn (Raykov & Marcoulides, 2004). The variance of a linear combination in this form is a function of $\Sigma_{\hat{b}}$ (the ACOV of the estimated coefficients) and the weight vector:

$$\sigma^2_{\hat{b}} = w'\Sigma_{\hat{b}}w. \quad (14)$$

Applying Eq. 14, we obtain.

$$\mathrm{var}\left(\hat{\omega}_b\right) = \begin{bmatrix} 1 & z \end{bmatrix}\begin{bmatrix} \mathrm{var}\left(\hat{b}_0\right) & \mathrm{cov}\left(\hat{b}_0, \hat{b}_1\right) \\ \mathrm{cov}\left(\hat{b}_0, \hat{b}_1\right) & \mathrm{var}\left(\hat{b}_1\right) \end{bmatrix}\begin{bmatrix} 1 \\ z \end{bmatrix}, \quad (15)$$

which simplifies to

$$\mathrm{var}\left(\hat{\omega}_b\right) = \mathrm{var}\left(\hat{b}_0\right) + 2z\mathrm{cov}\left(\hat{b}_0, \hat{b}_1\right) + z^2\mathrm{var}\left(\hat{b}_1\right). \quad (16)$$

The variance and covariance estimates in Eq. 16 are contained within the ACOV of the nonlinear model's parameter estimates. Interestingly, Eq. 16 closely resembles the expression for the variance of a simple slope given by Aiken and West (1991) in Eq. 6. In both cases, the variance of the simple parameter depends on three quantities: the variance of the estimate denoting the simple parameter when z is zero ($\hat{\gamma}_1, \hat{b}_0$), the variance of the estimate 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 estimates. Regardless of the complexity of the overall nonlinear model, the necessary elements of the ACOV pertain only to the estimates within the linear combination.

In summary, for any linearly moderated parameter, we can obtain expressions for the simple parameter 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 can now 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. However, no null value is explicitly represented in the traditional JN equation (Eq. 8) because it is assumed that the null value is zero. Next, we present a more general version of the JN technique that allows the null value to be nonzero. We develop this extension from the original JN formulae that were

created in the context of linear regression, continuing with the notation in Eqs. 6–8. The simple parameter is denoted $\widehat{\omega}$. To allow for any null value, denoted ω_0, expand Eq. 8 to

$$\pm t_{crit} = \frac{\widehat{\omega} - \omega_0}{\sqrt{\text{var}(\widehat{\omega})}}. \tag{17}$$

Next, rearrange Eq. 17 such that the equation can be solved with the quadratic formula. In other words, we must obtain an equation of the form $az^2 + bz + c = 0$. After rearranging, expanding, and substituting terms (for details, see the Online Appendix), we get

$$a = t_{crit}^2 \text{var}(\widehat{\gamma}_3) - \widehat{\gamma}_3^2, \tag{18}$$

$$b = 2\left(t_{crit}^2 \text{cov}(\widehat{\gamma}_1\widehat{\gamma}_3) - \widehat{\gamma}_1\widehat{\gamma}_3 + \omega_0\widehat{\gamma}_3\right), \tag{19}$$

$$c = t_{crit}^2 \text{var}(\widehat{\gamma}_1) - \widehat{\gamma}_1^2 + 2\omega_0\widehat{\gamma}_1 - \omega_0^2. \tag{20}$$

Importantly, if $\omega_0 = 0$, then Eqs. 18–20 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. 18–20, we can use the quadratic formula to solve for values of z, which are the significance boundaries:

$$z = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}. \tag{21}$$

We can also visualize the value of the simple parameter and its surrounding confidence band across all values of the moderator. The confidence band will be given by

$$\widehat{\omega} \pm t_{crit}\sqrt{\text{var}(\widehat{\omega})}, \tag{22}$$

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

For an in-depth example that demonstrates the concepts and extensions presented in this section, readers are encouraged to visit the Online Appendix.

CurveBuilder

Given the shortcomings of extant software for integrating moderation and intrinsically nonlinear models, we created an open-source application called CurveBuilder. CurveBuilder was created in R using the Shiny web application framework (Chang et al., 2022) and is freely accessible at https://haleyyaremych.shinyapps.io/CurveBuilder/. The app provides a code-free environment for users to complete all steps of the nonlinear analysis process, including uploading data, visually choosing start values, specifying models, plotting results, and probing moderation. This section begins with a brief description of the app's functionality, then reviews two examples. Example 1 involves a continuous moderator, the Michaelis–Menten function, and custom functions; Example 2 involves a NLME model and the Jenss-Bayley function. Another in-depth example, involving a multi-categorical moderator and the logistic function, can be found at the app's OSF page: https://osf.io/7gkny/. The OSF page also houses extensive documentation and datasets for all the examples, as well as the Online Appendix for this paper. For researchers who are more comfortable with coding and/or wish to create reproducible code that exists outside the Shiny interface, all of the plotting and JN capabilities of CurveBuilder are also available as standalone R functions that accept a fitted model object (*nls* or *nlme*) as input. Two R files, one containing function definitions and one containing function descriptions and examples, are available on the project's OSF page.

CurveBuilder is divided into tabs that appear along the top of the interface. Users are encouraged to work from left to right across the tabs. This design feature was inspired by the *interActive* Shiny app (McCabe et al., 2018). The *Information* tab contains links to the app's documentation, vignettes and their datasets, and R files underlying the app. 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 to use this tab. Here, users select a nonlinear curve to plot, and as users adjust parameter values with sliders, the plot updates. This display makes it easy to understand how each parameter governs the appearance of the curve. The *Data Upload* tab allows the user to upload their own data, which can later be used to fit models and create plots. Accepted file types are .csv, .sav, .xlsx, and .xls. Also inspired by *interActive* (McCabe et al., 2018), data descriptives auto-populate upon upload.

In the *Preview Start Values* 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. The *Create Model* tab provides a code-free environment for users to specify and fit nonlinear models that may include random effects and/or moderation. When the model converges, the *Results* tab populates with convergence information; model selection indices; output tables including parameter estimates, random effect (co)variances (for NLME models), and the asymptotic covariance and correlation matrices of the parameter estimates; and raw R output, if desired.

The *Plots* tab is further divided into four sections, 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. The *Model Evaluation* section provides a plot of the residuals versus fitted y-values, an autocorrelation plot of the residuals, and a histogram and

QQ plot of the residuals. In *Observed Data and Fitted Values*, the observed predictor and outcome variables are plotted with fitted values from the model. The *Pick-a-Point* tab plots the model-implied relation between the predictor and the outcome at multiple values of the moderator, whether the moderator is binary, multi-categorical, or continuous. These plots utilize the "small multiples" principle recommended by McCabe et al. (2018). For continuous moderators, the *Johnson-Neyman* tab plots the moderator along with model-implied conditional values of the moderated parameter, and the user may enter a zero or nonzero null value. All sections provide a variety of customizable features that enable the creation and download of publication-quality plots.

In the *Visualize Curves*, *Preview Start Values*, and *Create Model* tabs, the user may select from a variety of prespecified nonlinear models or create a custom model. Available prespecified models are the Gompertz, logistic, Richards, 3PE, Michaelis–Menten, Jenss-Bayley, Preece-Baines, sine, cosine, inverse quadratic, and Bragg. For each, the model equation, parameters, and the attribute of the curve to which the parameter corresponds are all displayed in-app.

Example 1: Custom functions and a continuous moderator

In this example, we 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 simulated data inspired by Ren et al. (2022). The goal of this study was to characterize the relation between frequency of social interactions and psychological well-being. 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 well-being. Second, the "inverted U" hypothesis can be roughly approximated by a quadratic relation, such that more interaction promotes greater well-being, 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 well-being, 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. Here, we will compare these same models, but we replace the piecewise linear model with a nonlinear curve indicative of "diminishing returns." Finally, the authors tested whether extraversion moderated the relation between interaction quantity and well-being; results were null, but for demonstrative purposes, our simulated data 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. To explore our options, we begin with the *Visualize Curves* tab. Within this tab, there is a group of "exponential" functions that yield curves consistent with diminishing returns. For each of these functions, the user can read about the parameters that control the shape of the curve and use sliders to further understand each parameter. For example, compare the 3PE model (Eq. 2) to the Michaelis–Menten (MM) model:

$$y = \widehat{a} + \frac{\widehat{b}x}{\widehat{c} + x} + \varepsilon, \tag{23}$$

where $\widehat{a}$ is the estimated intercept, $\widehat{b}$ is estimated total growth, and $\widehat{c}$ is the estimated x-axis location at which 50% of growth has occurred. These models yield curves that correspond well with our hypothesized trend. Parameters a and b are interpreted similarly, but the meaning of parameter c differs. In the 3PE model, parameter c is the rate of change, whereas in the MM model, 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 model often yields more concrete insights (McNeish & Matta, 2018). We will proceed with the MM model for further analyses (Fig. 8).

Step 1: Data Upload

Upon uploading our data, we see a summary of the variables available to us (Fig. 9): *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 standardized Extraversion factor from the Big Five, and *wb* is psychological well-being, which was an average of three measures assessing happiness, life satisfaction, and social well-being on a scale ranging from 0 to 10.

Step 2: Preview Start Values

The *Preview Start Values* tab can be used to identify parameter values for the MM model that correspond with our data relatively well. Because the dataset is large (10,000 rows), we 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. Parameter values of $a = 3.5$, $b = 3$, and $c = 2.5$ yield a relatively well-fitting curve (Fig. 10).

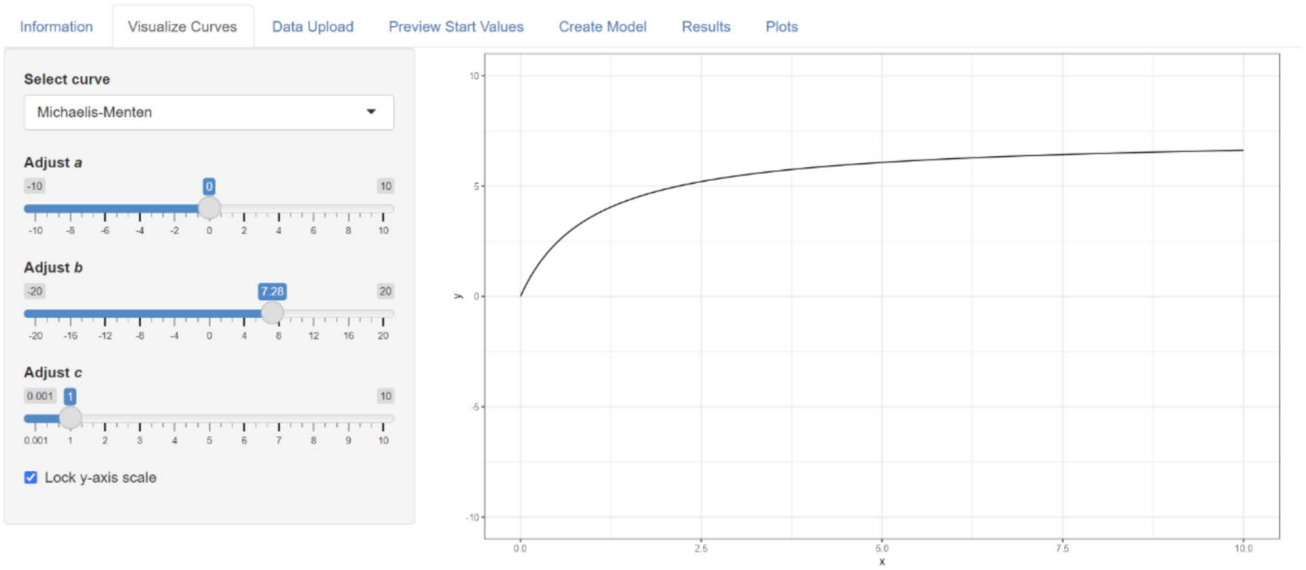

Fig. 8 Exploring the Michaelis–Menten function in the *Visualize Curves* tab

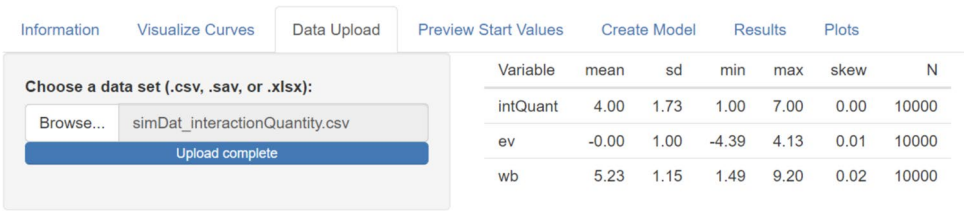

Fig. 9 Interaction quantity data summary in the *Data Upload* tab

Steps 3 and 4: Create Model and Results

In this section, we alternate between the *Create Model* and *Results* tabs to demonstrate fitting multiple models and carrying out model selection. We begin by fitting the MM model, which is consistent with the diminishing returns hypothesis. In *Create Model*, we simply select Michaelis–Menten as our desired function, indicate *intQuant* and *wb* as our predictor and outcome variables, and import the start values that were just identified in the *Preview* tab. Additionally, we specify that all 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, it is helpful to consider prior knowledge and hypotheses when choosing these start values. Ren et al. (2022) suggest that "less extraverted individuals may be more likely to experience reduced well-being at high levels of interaction quantity" (p. 1069), meaning that for more extraverted people, well-being may be higher at the highest levels of *intQuant*. To reflect this expectation in our start values, note that parameter *b* governs the vertical distance between the intercept and the asymptote. 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 *a* and *c*; we leave these at zero. After clicking Fit Model, the text under the button changes from "*Success message will appear here…*" to "*Model successfully converged!*" (Fig. 11).

Next, *Results* (Fig. 12) displays 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. Similar replacements have occurred for parameters *b* and *c*. Additionally, AIC = 28,426 and BIC = 28,477 for the moderated MM model.

Next, we will 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 *Create Model* and specifying

Fig. 10 *Preview Start Values* tab with Michaelis–Menten curve

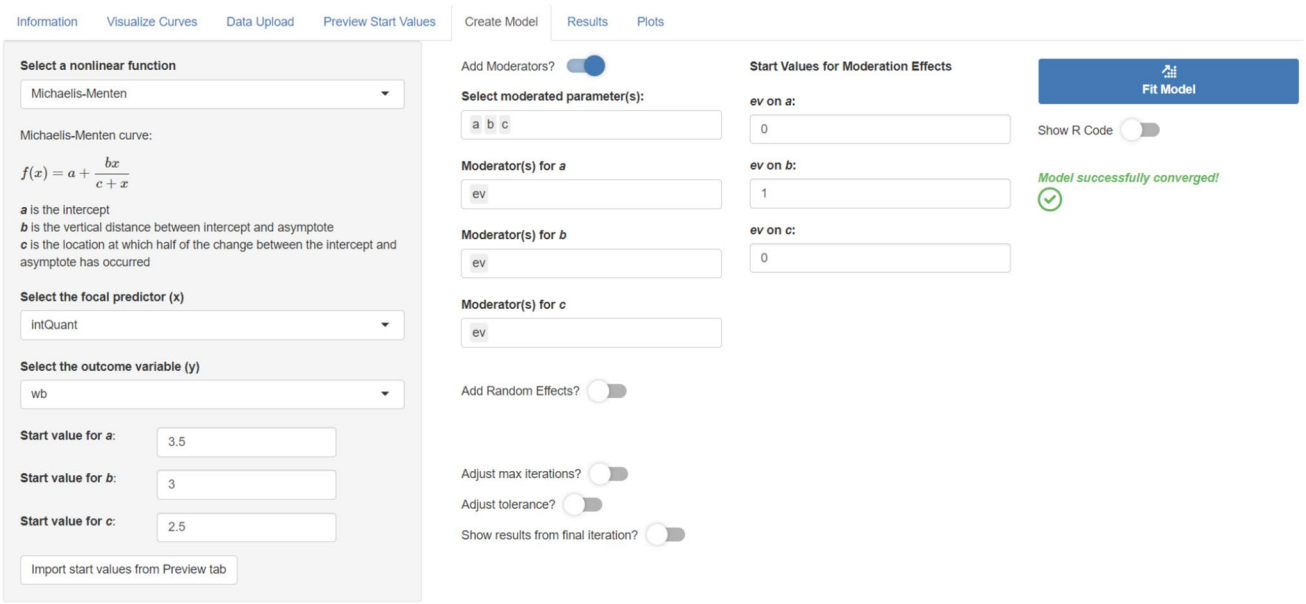

Fig. 11 Fitting the moderated MM model in the *Create Model* tab

the moderated linear model. We simply enter the linear model, *b0* + *b1***x*, into the custom function input box, and in the boxes below, indicate that *b0* and *b1* are the model parameters. Additionally, we specify *ev* as a moderator of both *b0* and *b1*. Because good start values are not essential for linear models, we can leave all start values at zero for simplicity. Upon fitting the model, convergence is achieved (Fig. 13).

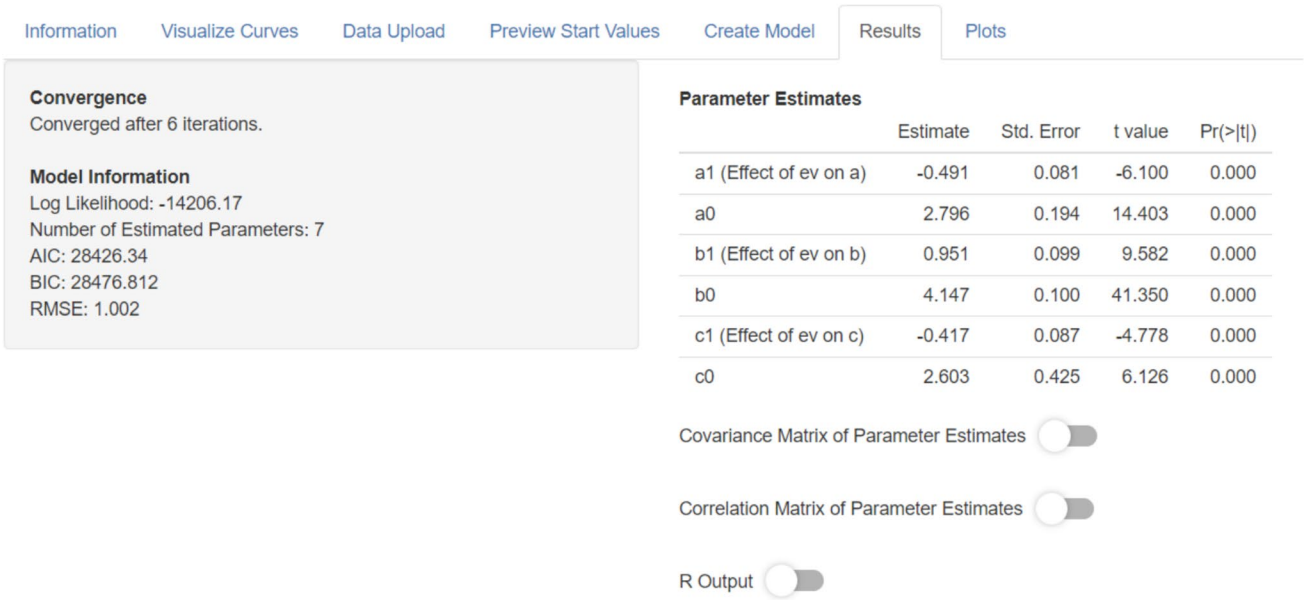

Fig. 12 *Results* tab for the moderated MM model

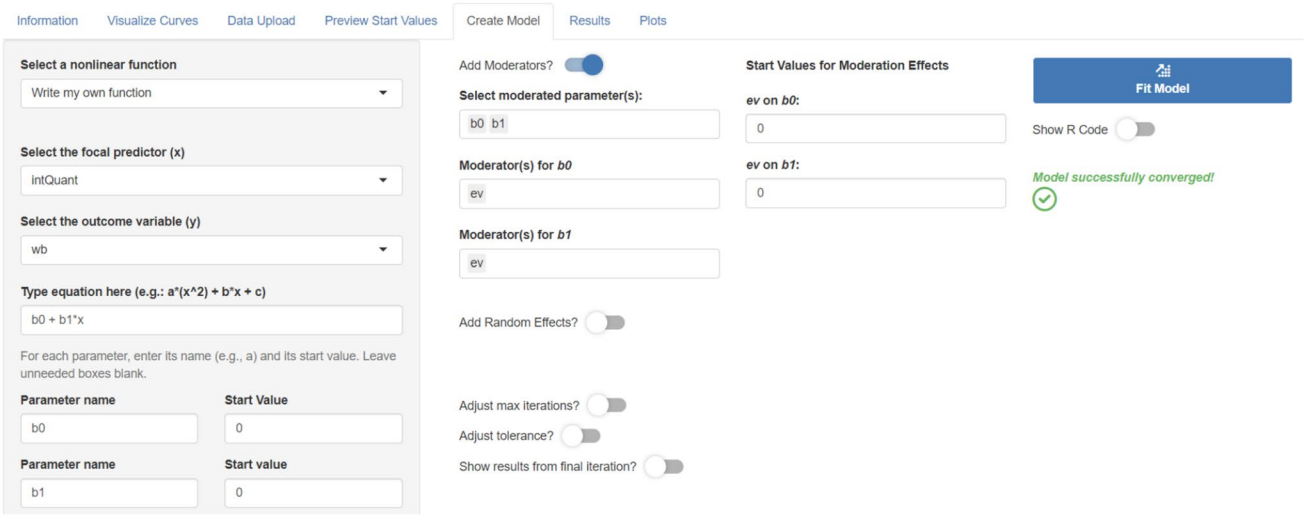

Fig. 13 Fitting the moderated linear model in the *Create Model* tab

In *Results* (Fig. 14), parameter names have been updated like they were in the MM model; *b0* has been replaced with *b00* and *b01 (Effect of ev on b0)*, and *b1* has been replaced with *b10* and *b11 (Effect of ev on b1)*. The model converged after 1 iteration because iterative estimation is not necessary for linear models. We also see that AIC = 28,662 and BIC = 28,698, which 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.

Following similar steps in *Create Model*, we can again use the custom function feature to fit a moderated quadratic model consistent with the Inverted U hypothesis. For this model, AIC = 28,476 and BIC = 28,526, meaning the quadratic model fits better than the linear model, but worse than the MM model. Overall, we obtain support for the Diminishing Returns hypothesis. We proceed with the moderated MM model for further evaluation and interpretation. As shown in Fig. 12, 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

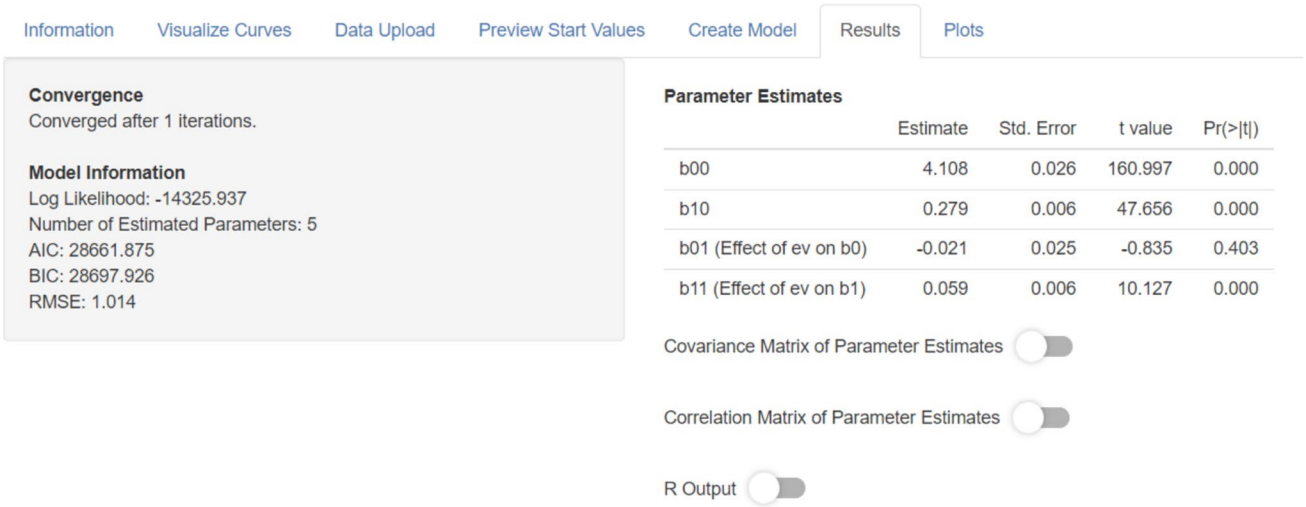

Fig. 14 *Results* tab for the moderated linear model

these estimates, note that *ev* has been centered, meaning *ev* = 0 is equivalent to *ev* at its mean.

Parameter *a0* = 2.80, and parameter *a* is the intercept. For individuals with mean extraversion, we expect a psychological well-being score of about 2.80 when social interaction frequency is zero. Parameter $a1 = -0.49$, indicating that as extraversion increases, the intercept decreases by about 0.49. In other words, more extraverted people are less happy when interaction frequency is zero. Next, parameter *b0* = 4.15, and parameter *b* is the vertical distance between the intercept and asymptote. At average extraversion, frequent social interaction results in a well-being score that is about 4.15 points higher than the intercept. 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 well-being relative to its maximum. At average extraversion, the halfway point of well-being occurs at an interaction frequency of about 2.6. Additionally, $c1 = -0.42$, meaning as extraversion increases, the halfway point of well-being occurs at a smaller *x*-value. In other words, more extraverted people require fewer social interactions to reach their relative halfway point of well-being.

Step 5: Plots

We can begin with *Model Evaluation* plots (Fig. 15) to assess how well the moderated MM model characterizes our data. *Residuals vs. Fitted Y-Values* shows no patterns in terms of residual mean or variance. *Residual Autocorrelation* shows correlations near zero for lag = 1 and beyond. The *Histogram* and *QQ Plot of Residuals* both indicate that residuals are normally distributed. In summary, all plots indicate good model-data fit.

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 indicates satisfactory model-data fit. To prepare this plot for publication, we can edit the *x*- and *y*-axis labels as desired (Fig. 16).

Next, we use pick-a-point and JN plots to better understand how extraversion moderates the relation between interaction quantity and well-being. 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. To help the user choose moderator values to plot, CurveBuilder displays the mean and SD of the moderator in this tab. Because *ev* has been standardized, its mean is about zero and its *SD* is about 1. Therefore, we select −2, −1, 0, 1, and 2 as the *ev* values at which to plot the curve.

Using toggles and label editors, we can view the curves with or without the observed data, and we may display *ev* values with either color or paneling. After toggling off the observed data layer, displaying the curves by color, and editing the legend and axis labels as desired, we obtain the plot shown in Fig. 17. Another way to declutter the plot—without sacrificing the observed data—is to use paneling. Using this option and editing panel labels, we obtain Fig. 18.

To create color-coding and paneling, the data are binned according to moderator value. Cut points are the halfway points between each entered value (e.g., if two entered moderator values are 1 and 2, a cut point is created at 1.5). For more detail, see pp. 21–22 of the CurveBuilder documentation (https://osf.io/7gkny/). Additionally, there is an option to add

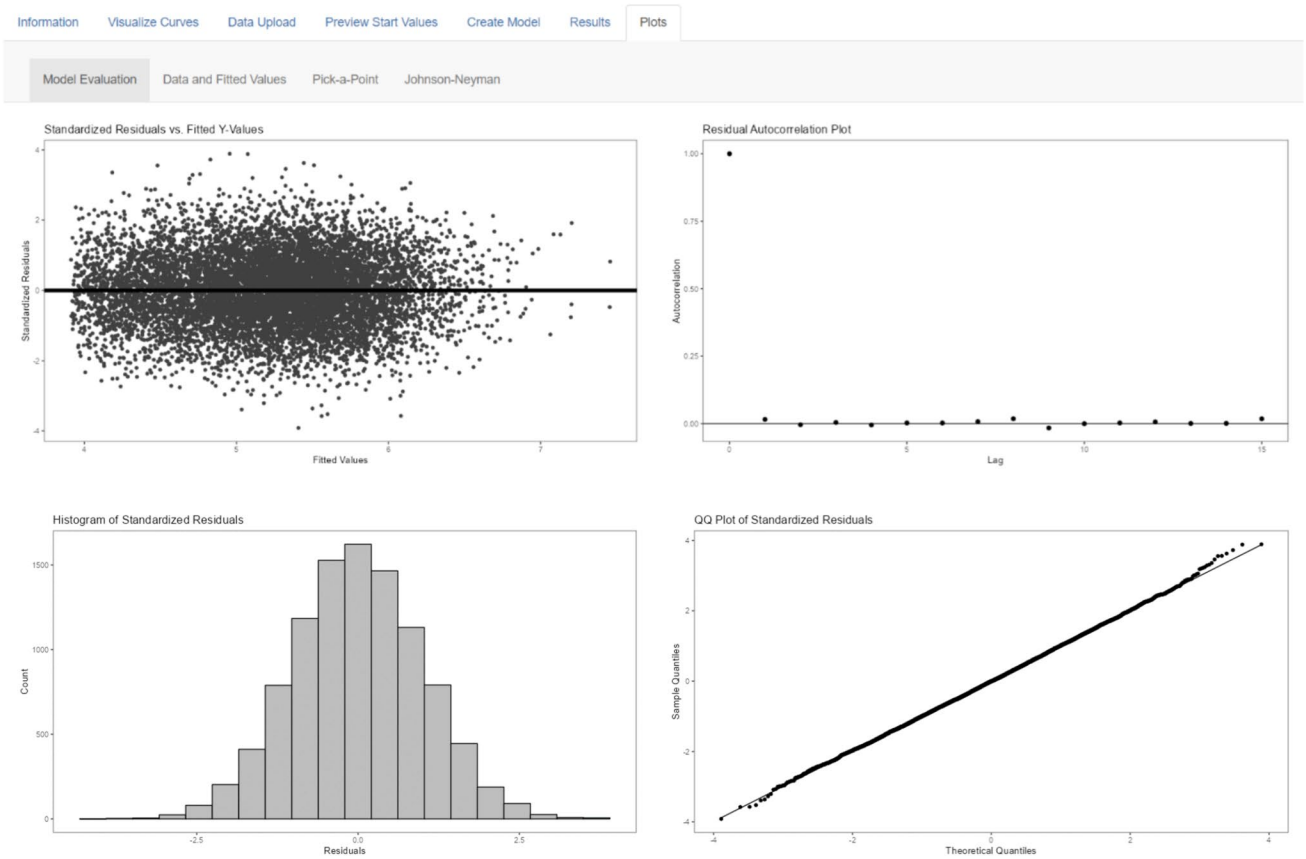

Fig. 15 *Model Evaluation* plots for the moderated MM model

Fig. 16 *Data and Fitted Values* plot for the moderated MM model

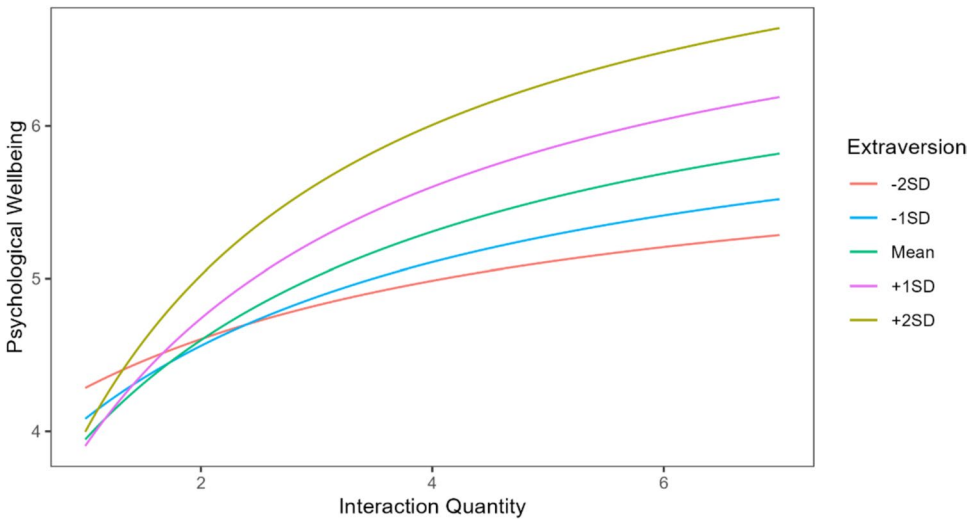

Fig. 17 CurveBuilder *Pick-a-Point* plot with color

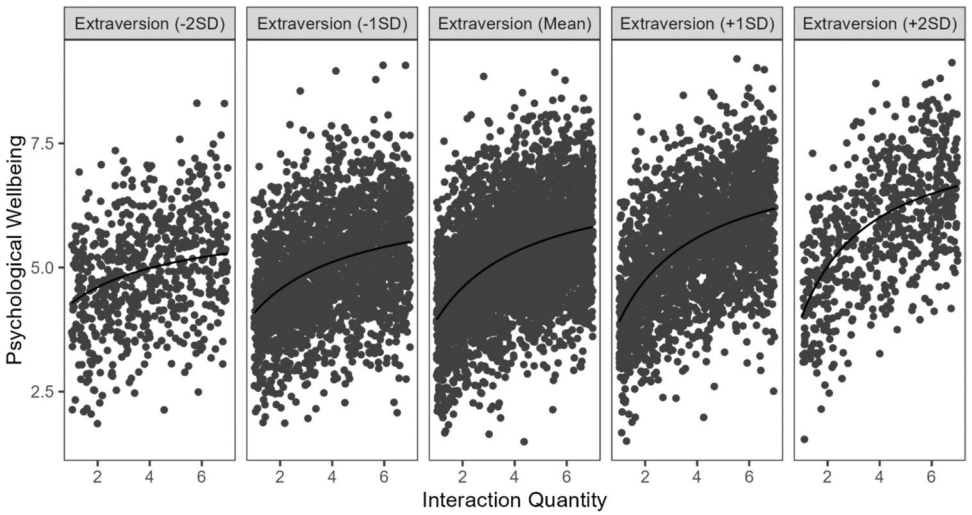

Fig. 18 CurveBuilder *Pick-a-Point* plot with paneling

confidence bands around the predicted values in the pick-a-point plot; these bands are simulation based. For more detail about how they are obtained, see p. 22 of the documentation.

Even more detailed information about our moderation results can be gained by creating a JN plot. 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 we focus our attention here. Again, using toggles and editors similar to those shown in Fig. 13, when creating the JN plot we can edit axis labels, opt to show observed values of the moderator with a rug plot, choose from grayscale versus color, and importantly, change the null value used to compute significance boundaries.

For our purposes, a null value of zero may be nonsensical for parameter *b*. We likely expect that more frequent social interaction will be related to greater well-being for all people in our study, so parameter *b* being greater than zero is not interesting. Instead, we may want to know at what levels of extraversion parameter *b* is significantly greater than 1—in other words, at what levels of extraversion does frequent social interaction result in a greater than one-point boost to psychological well-being. Since our well-being scale ranges from 0 to 10, this would reflect a 10% change. After indicating 1 as the null value, CurveBuilder produces Fig. 19.

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

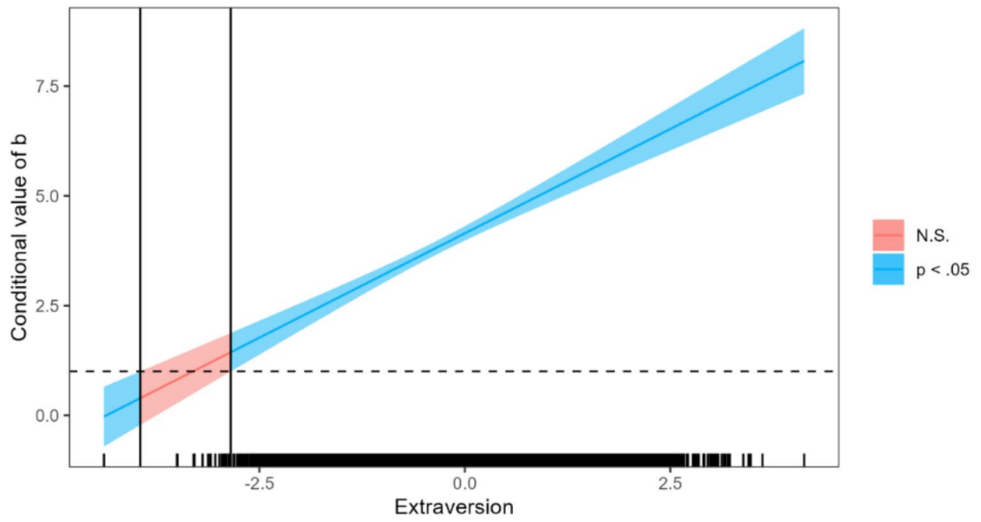

Fig. 19 JN plot of the conditional value of parameter *b* versus extraversion

observed range of extraversion. The rug plot along the *x*-axis shows observed values of extraversion.

Many components of the plot are informed by the null value. 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 boundaries—denoted by vertical lines—are the moderator values at which parameter *b* goes from being nonsignificant to significantly different from 1. Under the plot, CurveBuilder provides more detailed information about these boundaries; a sentence below the plot reads: "When $ev = -3.95$ and -2.85, 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 be interpreted with caution. Focusing on the second boundary, when extraversion is greater than -2.85, parameter *b* is significantly greater than 1. In other words, for individuals whose standardized extraversion score is greater than -2.85, frequent social interaction leads to a boost in psychological well-being that is significantly greater than one point. Only the individuals with extremely low extraversion experience a well-being boost that is not significant according to our definition.

Conclusions

In this example, we compared the MM, linear, and quadratic models to characterize the relation between social interaction quantity and psychological well-being. 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; 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. We gained more nuanced information about this moderation by creating pick-a-point and JN plots.

Example 2: Jenss-Bayley function and random effects

Next, we demonstrate how to use CurveBuilder to fit a NLME model. In this example, we work with height data collected in the Berkeley Growth Study (Jones & Bayley, 1941) and presented by Grimm et al. (2016). The study tracked the heights 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 dataset is freely available for download (Grimm et al., 2016) at https://www.guilford.com/companion-site/Growth-Modeling/9781462526062.

Here we implement the Jenss-Bayley function, which was created to approximate changes in human height over time (Jenss & Bayley, 1937) and models growth in two 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: $y = a + bx - exp(c + dx)$, where y is the outcome variable (height), x is the predictor (age in months), a is the intercept of the linear asymptote, b is the slope of the linear asymptote, $exp(c)$ is the vertical distance between the observed intercept and the intercept of the linear asymptote, and $exp(d)$ is the ratio of acceleration of growth at time t relative to time $t-1$, where 1 is a one-unit change in x. In this example, since age was measured in

months, *exp*(*d*) reflects the ratio of growth acceleration at 2 months relative to 1 month, and at 8 months relative to 7 months, etc.

Step 1: Data Upload

Because we have a priori knowledge about the nonlinear model to be used for these data, we bypass *Visualize Curves* and proceed to *Data Upload*, which shows a summary of the variables: subject ID, gender, age, and height. (Figure not shown.)

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 Fig. 20.

Steps 3: Create Model

In *Create Model*, we select the Jenss-Bayley function and import the start values that were found in Step 2. To add random effects to the model, select *ID* as the grouping variable, and then indicate 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 fails to converge, to progressively remove random terms (e.g., McNeish & Bauer, 2022; McNeish et al., 2020). Therefore, we may begin by specifying parameters a, b, c, and d as random; however, this model fails to converge. (Results not shown.) In this example, which parameter(s) 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 fails to converge, but if we remove parameter d from the random effects, the model converges.

Step 4: Results

Results for this model (Fig. 21) indicate that, in our sample, the average 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

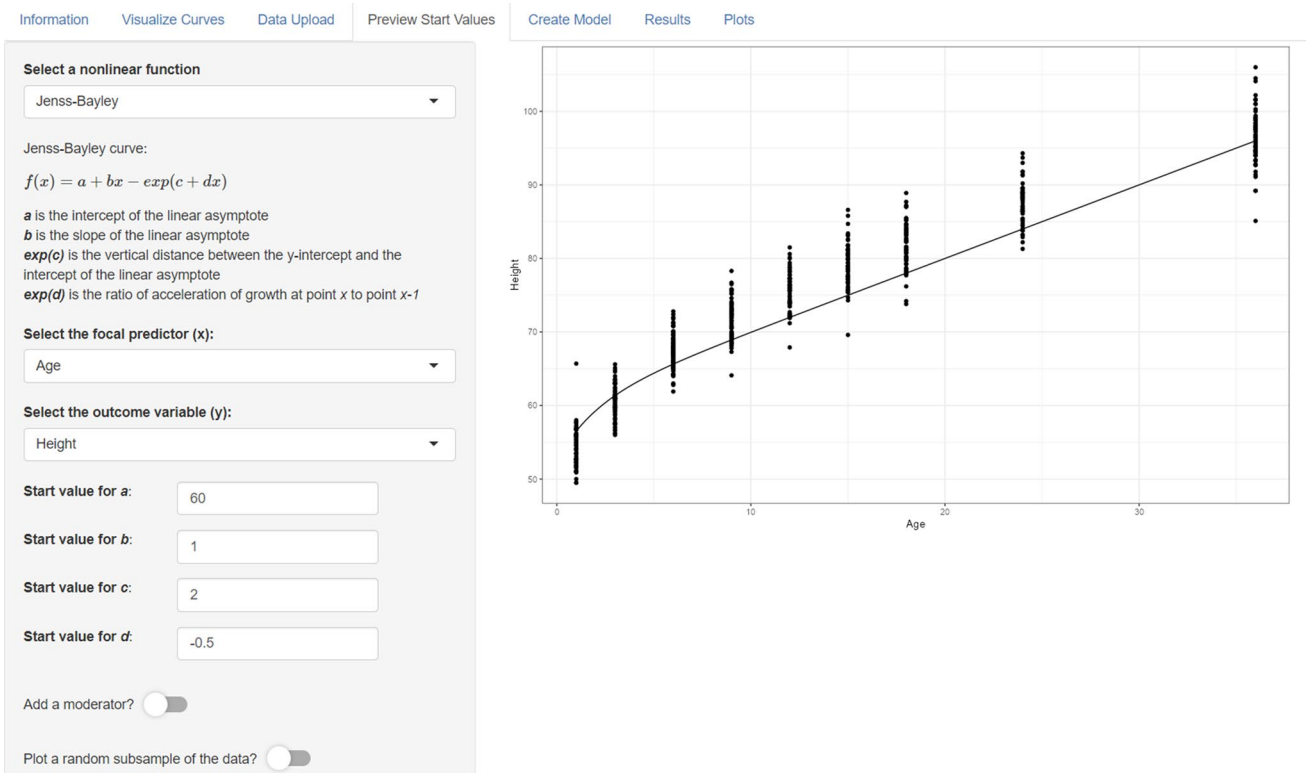

Fig. 20 *Preview Start Values* tab for the Jenss-Bayley model

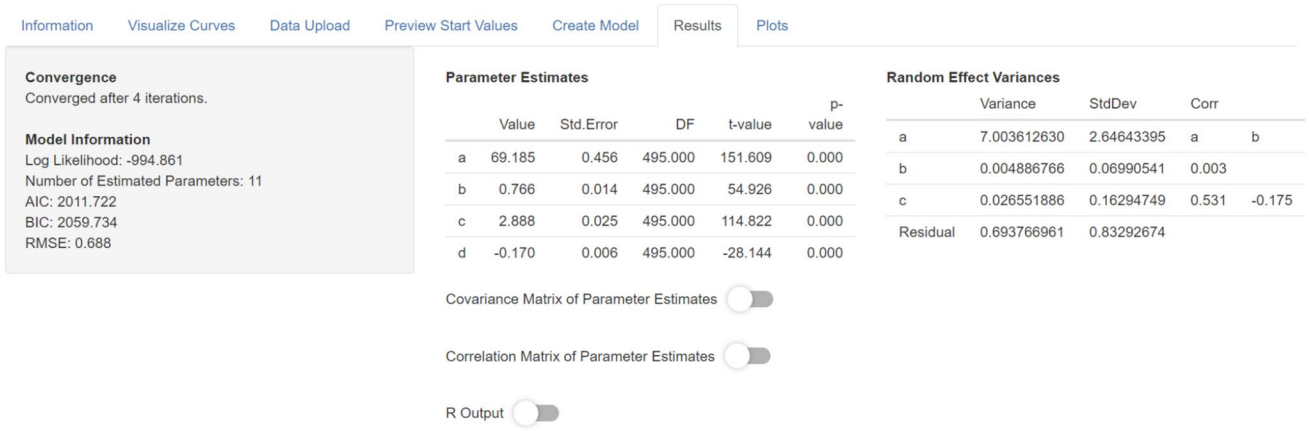

Fig. 21 *Results* tab for the NLME Jenss-Bayley model

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.

Step 5: Plots

Beginning with *Model Evaluation* (not shown), diagnostic plots indicate that this model fits the data well. Next, the plot produced under *Data and Fitted Values* (Fig. 22) indicates that the model-implied values correspond well with the observed data. Because this model does not contain moderators, the *Pick-a-Point* and *Johnson-Neyman* tabs are not available.

Conclusions

In this example, we used CurveBuilder to fit a NLME model to characterize changes in height over the course of infancy and toddlerhood. 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 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.

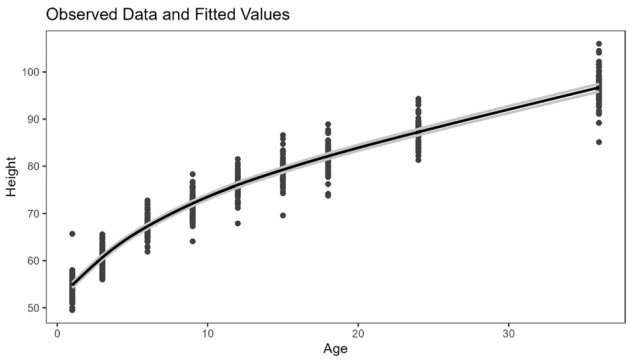

Fig. 22 *Data and Fitted Values* plot for the NLME Jenss-Bayley model

Discussion

The aims of the current paper were twofold. First, we presented novel extensions of the JN technique—both conceptual and mathematical—to enable its application to moderated parameters within nonlinear models. The potential need for nonzero null values was discussed, and the technique was extended such that significance boundaries can be calculated for both zero and nonzero null values. Second, we introduced a new Shiny app called CurveBuilder, wherein researchers can carry out all steps of the (moderated) nonlinear modeling process. Next, we discuss potential extensions and future directions with respect to each of these objectives.

A variety of nuanced issues arise when applying the JN technique to probe moderation within nonlinear models, raising interesting questions to be pursued in future work. For example, 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, 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 should not be smaller than the minimum observable *y*-value (e.g., the minimum 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 all parameter estimates follow a normal sampling distribution (Motulsky & Christopoulos, 2004). This assumption underlies the computation of a simple parameter's SE, and subsequently, the confidence bands that are a hallmark feature of the JN plot. Thus, the JN technique rests on the assumption that parameter estimates follow a normal sampling distribution (Aiken & Bauer & Curran, 2005; West, 1991). Therefore, multiple questions will be worthwhile to pursue in future work. For example, 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? Similar questions arise for models created via reparameterization; the normality of parameters in one parameterization does not necessarily imply the normality of parameters in a reparameterization of the same model (Johnson & Hancock, 2019). Finally, 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. Indeed, because the assumption of normal sampling distributions underlies the estimators themselves, simulation studies to address these questions will have broad impact.

Additionally, the scope of this work 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. 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.

The primary goal of CurveBuilder is to simplify and unify each stage of the nonlinear modeling process, and there are many areas in which future work may enable the expansion of CurveBuilder to further accomplish this goal. First, CurveBuilder offers a few utilities for troubleshooting nonconvergence. The user may easily adjust the model specification by selecting a simpler functional form or by graphically identifying different starting values, increase the iteration cap for the maximum likelihood estimator, adjust the convergence tolerance, or print the results obtained in the final iteration of the estimation algorithm. While these approaches are often suggested (e.g., Bates & Watts, 1988; Gallant, 1987; Ritz & Streibig, 2008), they may not always work. More advanced approaches, such as reparameterizing the random effects covariance matrix via a Cholesky decomposition (Lindstrom & Bates, 1988; McNeish & Bauer, 2022), and decomposing the random effects covariance matrix via factor analysis (McNeish & Bauer, 2022), have been proposed for NLME models. The latter method may be carried out in SAS and SPSS; however, extensions to the R environment have yet to be developed.

Second, an important aspect of nonlinear modeling is (re)parameterization, and there are many opportunities for future work to enable easier reparameterization of nonlinear models. For example, the sigmoidal models provided in CurveBuilder contain parameters for the (1) lower asymptote, (2) total growth/decline, (3) rate of change, and (4) *x*-location of the inflection point. However, in some contexts it is more useful to estimate the upper asymptote itself rather than total change, or to estimate jerk points (i.e., locations along the *x*-axis where the surge area begins and ends) rather than the inflection point. CurveBuilder does not offer extensive utilities for reparameterization; if a user wishes to implement a model with a parameterization that differs from the prespecified offering, they must manually create it as a custom function. Preacher and Hancock (2012, 2015) describe the steps for reparameterizing a nonlinear model, which may involve algebra and/or calculus. Extant software does not enable automated reparameterization of nonlinear models; however, such resources would be a valuable focus for future work. Tools to ease and/or simplify the process of reparameterization will be helpful for ensuring that nonlinear models offer maximal substantive utility.

A final limitation of CurveBuilder is that it requires users to interface with R to incorporate certain advanced model specifications. First, to obtain a well-fitting NLME model, it is often necessary to model autocorrelation, 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, in longitudinal data, heteroscedasticity may need to be modeled explicitly, which may involve treating residual variance as a function of the predictor(s) (Blozis & Harring, 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, CurveBuilder currently does not provide functionality to do so. To incorporate these components, the user may 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. (Of note, the same process may be followed for incorporating other advanced model specifications, such as non-default estimators like weighted least squares or sandwich.)

The aims of this paper were to (1) both conceptually and mathematically extend the Johnson-Neyman technique such that it can now be applied to moderated parameters in nonlinear models, and to (2) introduce CurveBuilder, a Shiny app which unifies the process of selecting, specifying, fitting, visualizing, and probing moderated nonlinear models in a code-free interface. Given the enhanced insight into psychological phenomena that intrinsically nonlinear models provide, alongside the importance of moderation for psychological theory testing, these developments will ideally provide researchers with better tools for modeling and visualizing their data in optimal ways.

Authors' contributions Both authors contributed to study conception and design. HY carried out derivations, designed and developed the app, generated and analyzed example data in the app, and wrote the first draft. Both authors contributed to editing, reading, and approving the final manuscript.

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Data availability The datasets generated and analyzed for the current paper are available in the OSF repository, https://osf.io/7gkny/.

Code availability Code underlying the software application in the current paper is available in the OSF repository, https://osf.io/7gkny/.

Declarations

Conflicts of interest The authors have no relevant financial or non-financial interests to disclose.

Ethics approval Not applicable.

Consent to participate Not applicable.

Consent for publication Not applicable.

Open practices statement All data, materials, and documentation for CurveBuilder are available at https://osf.io/7gkny/. None of the work described in this paper was preregistered.

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