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Meaningful Aspects of Change as Novel Random Coefficients: A General Method for Reparameterizing Longitudinal Models

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A fundamental goal of longitudinal modeling is to obtain estimates of model parameters that reflect meaningful aspects of change over time. Often, a linear or nonlinear model may be sensible from a theoretical perspective, yet may have parameters that are difficult to interpret in a way that sheds light on substantive hypotheses. Fortunately, such models may be reparameterized to yield more easily interpretable parameters. This article has 3 goals. First, we provide theoretical background and elaboration on Preacher and Hancock's (2012) 4-step method for reparameterizing growth curve models. Second, we extend this method by providing a user-friendly modification of the structured latent curve model in the third step that enables fitting models that are not estimable with the original method. This modification also allows researchers to specify the mean structure without having to determine which parameters enter nonlinearly and without needing to solve complex matrix expressions. Third, we illustrate how this general reparameterization method allows researchers to treat the average rate of change, half-life, and knot (transition point) as random coefficients; these aspects of change have not before been treated as random coefficients in structural equation modeling. We supply Mplus code for illustrative examples in an online supplement. Our core message is that growth curve models are considerably more flexible than most researchers may suspect. Virtually any parameter can be treated as a random coefficient that varies across individuals. Alternative parameterizations of a given model may yield unique insights that are not available with traditional parameterizations.

Keywords: reparameterization, nonlinear models, structured latent curves, latent growth curve modeling

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Researchers in psychology and allied disciplines are faced with an important challenge: They must specify models in ways that meaningfully describe aspects of underlying theory and allow tests of key theory-driven hypotheses. But rather than facilitating tests of specific hypotheses of interest, existing methods often appear to restrict the range of hypotheses that researchers are able to assess. Fortunately, these restrictions can be illusory. Taking structural equation modeling (SEM) as an example, many believe that SEM is useful only for single-level (unclustered) data, yet there is now a sizable literature describing ways to apply SEM to clustered data (Bauer, 2003; Bovaird, 2007; Curran, 2003; B. Muthén & Asparouhov, 2011). Similarly, researchers using SEM may believe they are limited to fitting models that contain only linear relations, but there are ways to circumvent this limitation as well (e.g., Browne, 1993; Wall & Amemiya, 2007).

Researchers can greatly benefit from knowing how to parameterize a model such that its parameters reflect quantities of key theoretical interest. This can be important in research applications in which linear, or particularly nonlinear, change over time is the focus. In using the SEM-based latent growth curve modeling (LGM) framework, the most theoretically relevant aspects of change are often the intercept and slopes describing some process, or possibly the effects of person-level predictors on those aspects of change. Once the researcher has decided that it is desirable to model nonlinear trajectories, the following critical question must be answered: How can models be specified and fit in such a way that theoretically relevant aspects of change are parameterized directly in the model rather than ignored entirely or derived post hoc?

Parameterization is the mathematical expression of the functional form of a model in terms of a set of known and unknown parameters. These parameters dictate the particular form the model will take (the "parameterization"). There are generally an infinite number of parameterizations for a given model, but only a small number may be useful in practice. *Reparameterization* is the translation of a given model from one parameterization to another. A *target function* is defined as one parameterization of the hypothesized trajectory function used in a model. In the present context, reparameterization is the reexpression of a target function so that parameters of the reexpressed function more closely align with questions of scientific interest. Generally, a reparameterized function will contain the same number of estimated parameters as the original function and, in the growth modeling context, will describe an identical trajectory. A simple example concerns the familiar quadratic curve, whose typical parameters reflect (a) the intercept (the model-implied value of y where $time = 0$), (b) the linear aspect of change (the amount by which y is expected to change

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per unit of time at *time* = 0), and (c) the quadratic aspect of change (half the amount by which the linear slope is expected to change per unit of time). These parameters, although able to describe the trajectories of change, may be completely uninteresting to the researcher. The researcher instead may be interested in the point in time at which a quadratic curve reaches its maximum or minimum (respectively, the *maximizer* or *minimizer*) and the predicted value of *y* at that point in time; the model can be reparameterized to estimate these parameters (Cudeck & du Toit, 2002; Cudeck & Harring, 2007).

A practical knowledge of reparameterization can be very useful to researchers for several reasons, as described by Preacher and Hancock (2012). First, it is often more convenient to directly estimate a parameter (e.g., the maximizer in the reparameterized quadratic model) than it is to compute it post hoc from other parameters. If the parameter is estimated directly in the model, it is simple to obtain its estimated standard error and confidence interval (CI). Second, with reparameterization, it is straightforward to investigate whether the new aspect of change is moderated or predicted by other variables or even by other aspects of change. For example, a researcher may wish to know what background variables best predict the minimizer of a quadratic trajectory. Third, it is desirable for researchers to have the option of treating a parameter as a fixed, known value; as an estimated parameter; or in some cases—central to this article—as a random coefficient reflecting individual differences.[1]

A number of researchers have independently used reparameterization of growth models in psychology applications. B. Muthén (2000) recentered time at different occasions to gauge the effect of background predictors at different points along a developmental trajectory; each recentering amounts to a different parameterization of the same model. Rausch (2004, 2008) reparameterized a negative exponential (NE) growth model to estimate *proportion of change* or *units from asymptote* parameters. These parameters bear potentially more interesting interpretations than those of the standard version of the NE growth model. Preacher and Hancock (2012) reparameterized a linear latent growth curve model to directly yield the *aperture*—the point in time at which the intercept–slope covariance is zero—as a model parameter. Choi, Harring, and Hancock (2009) reparameterized a logistic growth model to treat lower and upper asymptotes, surge points, and jerk points as parameters. To distinguish ordinal from disordinal interactions, moderated multiple regression or growth models can be reparameterized to contain as parameters the *crossover point* (*C*) and the predicted value of *y* at $x = C$ (Widaman et al., 2012). These examples have in common that they begin with a standard model whose parameters may not be particularly interesting, and reexpress the model such that the parameters bear direct substantive interpretations or help test a key scientific hypothesis.

Despite this variety of existing reparameterization applications, until recently, no guidance had been given to researchers regarding how to develop parameterizations of linear or nonlinear latent growth curve models that might be different from those previously used. To begin filling this gap, Preacher and Hancock (2012) recently proposed and illustrated a four-step strategy. First, a target function is reparameterized to contain substantively important parameters. Second, the new target function is linearized for specification in SEM. Third, the model is specified using the SEM-based structured latent curve modeling (SLCM) approach for modeling nonlinear trajectories (Blozis, 2004, 2007a, 2007b; Browne, 1993; Browne & du Toit, 1991). The SLCM framework permits converting almost any aspect of change into a fixed or estimated model parameter or random coefficient. Finally, the model is fit to data, yielding parameter estimates and CIs.

The current article has three goals. The first is to provide theoretical background and elaboration of Preacher and Hancock's (2012) strategy to frame it as a general method. Preacher and Hancock's general description of their steps was brief (pp. 28–29), and implementation details were specific to examples. We also build on this previous work by offering a more extensive discussion of the logic, utility, and interpretational issues associated with reparameterized trajectory models (e.g., population-average vs. subject-specific models, dynamic consistency, and error covariance structures). We contextualize the general method in the broader class of nonlinear growth curve modeling methods discussed by Meredith and Tisak (1990), Browne and du Toit (1991), Browne (1993), and Rovine and Molenaar (1998, 2000, 2003).

The second goal of this article is to extend this four-step strategy by providing a user-friendly modification of the structured latent curve model in the third step that makes such models easier to specify. This modification (a) allows researchers to specify the mean structure of a growth curve model without having to determine which parameters enter linearly or nonlinearly, and without being obliged to solve complex matrix expressions; and (b) enables fitting models for which traditional SLCM cannot be used (i.e., models in which all parameters are nonlinear).

The third goal of this article is to illustrate, in the context of two empirical examples, how this general reparameterization method allows researchers to treat the knot (transition point), the average rate of change (ARC), and the half-life as random coefficients, as reflecting individual differences in the targeted aspects of change. Importantly, these aspects of change have not before been treated as random coefficients in SEM. In the first example, we demonstrate how to specify and predict individually varying knot points (random knots) in piecewise linear spline models. Using an example drawn from Zerbe (1979) on plasma phosphate reuptake, we show how to predict individual differences in the timing of the knot point using person-level obesity data. In the second example, we model the ARC (the mean instantaneous slope between two points in time) and the half-life (the time necessary for a function to cover half the distance to an asymptote from any point) as random coefficients, making use of verbal and quantitative skill acquisition data. We provide an extensive online supplemental appendix containing annotated Mplus syntax, annotated output, and data files so that researchers can learn from and adapt our code to other contexts. We conclude with a broader discussion about this general method, including when to use reparameterization, variations and extensions of the models presented herein, and notes about implementation within current SEM software.

Strategic Reparameterization and Model Specification Within the SLCM Framework

To start, we draw a distinction between a target function and a model. A *target function* is a parametric function of time describ-

[1] In addition to these benefits, reparameterization has secondary uses. Sometimes reparameterization is used to stabilize estimation; often, a model will not converge under one parameterization, but will under another. Reparameterization also may be used to impose constraints on a model. For example, Davidian and Giltinan (1995, p. 146) use exponentials to force certain parameters to be positive.

ing a trajectory that is followed by the means. We thus use "target function" in the same sense as Browne (1993). A *model*, on the other hand, is a formal mapping of the target function onto the data themselves. As such, in addition to representing the mean trend, the model typically will have one or more stochastic terms, and may express some of the target function's parameters as random coefficients that vary across individuals.

Assuming one has identified a suitable linear or nonlinear target function, a general approach for obtaining interpretable reparameterizations was outlined by Preacher and Hancock (2012). It is presented here to more fully illustrate the procedure and to provide groundwork for further extensions, including our introduction of a modified SLCM method and the specification of novel random coefficients. Briefly, the procedure involves the following steps:

1. (Re)parameterize the target function to contain substantively important parameters.
2. Linearize the new target function to render it specifiable using SEM.
3. Specify the model using a modified version of the SLCM approach.
4. Estimate the model parameters (point and interval estimates).

In order to provide a framework for the general procedures presented in this article, we elaborate upon each of these steps using a simple nonlinear growth model as a running example. In the section following, we apply these general principles to two real-data examples.

(Re)parameterize the Target Function to Contain Substantively Important Parameters

First, the researcher needs to identify a suitable target function. For example, if the study concerns growth in task-specific procedural knowledge over an extended period of time, a logistic or Gompertz curve might provide a suitable approximation (Grimm, Ram, & Estabrook, 2010). If physical growth since birth is being modeled, the Jenss-Bayley function might be a good candidate (Jenss & Bayley, 1937). For illustrative purposes, we use the inverse second-order polynomial function (also called the inverse quadratic [Qinv] or Hailwood-Horrobin function; Hailwood & Horrobin, 1946; Nelder, 1966). The Qinv target function can be expressed as

$$y = \frac{t}{\theta_0 + \theta_1 t + \theta_2 t^2}, \tag{1}$$

where t is the variable *time*, and is depicted in Figure 1 for $\theta_0 = 2$, $\theta_1 = 2$ through 4, and $\theta_2 = 2$. The parameters of this function are quite difficult to interpret. Generally speaking, θ_0 and θ_2 control, respectively, the ascent to and descent from the maximum; θ_1 controls the height of the maximum, but does not directly quantify the maximum. The maximum occurs at $t = \sqrt{\theta_0/\theta_2}$, and the value of y at that maximum is $[2\sqrt{\theta_0\theta_2} + \theta_1]^{-1}$. In physiological or psychological research, the Qinv function might be suitable for modeling rapid response to some stimulus (e.g., blood pressure in response to pain, or blushing in response to a social stimulus), followed by a gradually diminishing response.

Once a target function is identified, the researcher specifies an aspect of change that it is desirable to quantify as a fixed or

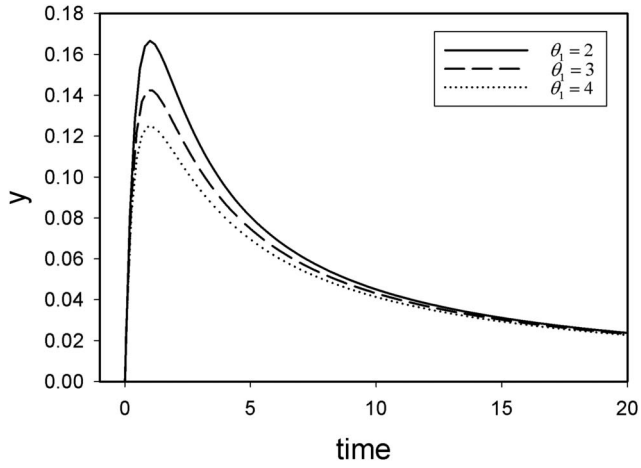

Figure 1. The inverse quadratic function plotted for $\theta_0 = 2$, $\theta_1 = 2$ through 4, and $\theta_2 = 2$.

estimated parameter or as a random coefficient. If the parameter or coefficient is not already explicitly part of the model expression, then reparameterization is necessary. For example, it might be of interest to estimate the time at which the Qinv function reaches its maximum, or to model individual differences in the maximum itself as a function of person characteristics (e.g., intensity of blushing as a function of trait anxiety). The most important step—and perhaps the most difficult—is to determine how this interesting aspect of change could be expressed in terms of existing model parameters, and to formulate such an expression. This step often requires recourse to basic calculus. The resulting expression can be solved algebraically for an existing model parameter that is of less interest, and then substituted into the original target function.

Consider the Qinv function in Equation 1. The time at which the function reaches its maximum (the *maximizer*) can be derived by noting that the instantaneous rate of change is zero at the point in time at which the trajectory reaches its maximum. That is, the maximum occurs where the first derivative of y with respect to *time* is zero. From elementary calculus, this derivative is

$$y' = \frac{\theta_0 - \theta_2 t^2}{(\theta_0 + \theta_1 t + \theta_2 t^2)^2}.$$

This expression can be set equal to zero and solved for an existing parameter that is of less interest (say, θ_0). Labeling the maximizer parameter θ_{max},

$$\begin{aligned} y' &= \frac{\theta_0 - \theta_2 \theta_{max}^2}{(\theta_0 + \theta_1 \theta_{max} + \theta_2 \theta_{max}^2)^2} \\ 0 &= \theta_0 - \theta_2 \theta_{max}^2 \\ \theta_0 &= \theta_2 \theta_{max}^2 \end{aligned}.$$

The result can be substituted back into the target function, yielding the reparameterized target function

$$y = f(\boldsymbol{\theta}, t) = \frac{t}{\theta_1 t + \theta_2(\theta_{max}^2 + t^2)}, \tag{2}$$

where $\boldsymbol{\theta}$ denotes the collection of model parameters to be estimated. If more than one new parameter is desired, this process can

be repeated. For example, we may also want to treat the maximum y at *time* $= \theta_{max}$ as a parameter. Once complete, the reparameterized target function is fundamentally the same as the original target function, in the sense that they describe the same mean trajectory and have the same number of free parameters. However—and herein lies the benefit—the less focal parameters have been sacrificed in order to estimate parameters of greater scientific interest.

Linearize the New Target Function to Render It Specifiable Using SEM

In many cases, reparameterization will result in an *intrinsically nonlinear* function. For example, some parameters may enter the target function embedded in reciprocals, radicals, trigonometric terms, exponents, or logarithms. Generally, it is not possible to algebraically reexpress intrinsically nonlinear functions in a linear form without transforming the outcome variable.[2] This intrinsic nonlinearity poses a practical obstacle for the SEM user because SEM is a fundamentally linear framework. As such, it may be necessary to *linearize* the target function to enable its conversion into a statistical model that is estimable in SEM software.

To linearize a target function, we employ a Taylor series expansion. A Taylor series is based on an infinite sum of derivatives of a function about a single point; a finite version of this sum is often used to represent a function. Here we use a first-order Taylor series that consists of the target function itself, evaluated at the population point θ, plus the sum of mean-deviated coefficients in the target function (e.g., intercepts, asymptotes) each multiplied by partial first derivatives of the target function with respect to each coefficient. For example, consider the reparameterized target function in Equation 2. The maximizer (θ_{max}) cannot be directly included as a random coefficient in SEM software. However, Equation 2 can be linearized with the following first-order Taylor series expansion:

$$\begin{aligned}\tilde{y} = {} & f(\boldsymbol{\theta},t) + (\theta_1 - \mu_1)\frac{\partial f}{\partial \theta_1}\bigg|_{\mu_1} + (\theta_2 - \mu_2)\frac{\partial f}{\partial \theta_2}\bigg|_{\mu_2} + (\theta_{max} - \mu_{max})\frac{\partial f}{\partial \theta_{max}}\bigg|_{\mu_{max}} \\ = {} & \frac{t}{\mu_1 t + \mu_2(\mu_{max}^2 + t^2)} + (\theta_1 - \mu_1)\frac{-(t^2)}{(\mu_1 t + \mu_2(\mu_{max}^2 + t^2))^2} \\ & + (\theta_2 - \mu_2)\frac{-t(\mu_{max}^2 + t^2)}{(\mu_1 t + \mu_2(\mu_{max}^2 + t^2))^2} + (\theta_{max} - \mu_{max})\frac{-2\mu_2\mu_{max}t}{(\mu_1 t + \mu_2(\mu_{max}^2 + t^2))^2}\end{aligned}, \tag{3}$$

where $\tilde{y}$ denotes a Taylor series expansion, $\boldsymbol{\theta}$ is again the collection of target function parameters, and the μs are parameters to be estimated as part of the fitted model. The $\boldsymbol{\theta}_{max}$ term is no longer "trapped" inside a reciprocal; thus, it can be specified (in mean-deviated form) as a latent variable in the SEM framework.

Taylor series expansions have long been used in fitting nonlinear regression models and nonlinear mixed models (e.g., Davidian & Giltinan, 1995). They are also integral to the SLCM approach proposed by Browne and du Toit (1991) and Browne (1993), described next.

Specify the Model Using an SLCM-Based Approach

In the third step, we employ an SLCM-based approach (Blozis, 2004, 2007a, 2007b; Browne, 1993; Browne & du Toit, 1991; Grimm et al., 2010; Neale & McArdle, 2000) to convert the reparameterized target function into a model that is estimable within the linear SEM context. In SLCM, the mean trend is assumed to follow the target function, which may be linear or nonlinear, although the potential of SLCM is fully realized for intrinsically nonlinear functions. SLCM involves treating the derivatives obtained in the linearization step as elements of a factor loading matrix, and the corresponding mean-deviated coefficients as latent variables.

For an arbitrary three-parameter target function, the first-order Taylor series[3] is represented as follows for a generic individual j, T-dimensional outcome vector $\mathbf{y}_j$, and T-dimensional time vector $\mathbf{t}$ (slightly modified from Blozis, 2004):

$$\mathbf{y}_j = \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \eta_{1j}\mathbf{f}'_1(\boldsymbol{\theta},\mathbf{t}) + \eta_{2j}\mathbf{f}'_2(\boldsymbol{\theta},\mathbf{t}) + \eta_{3j}\mathbf{f}'_3(\boldsymbol{\theta},\mathbf{t}), \tag{4}$$

where $\mathbf{f}'_k(\boldsymbol{\theta},\mathbf{t})$ is a vector containing the first partial derivative of the target function with respect to the kth growth parameter for several different values of *time* ($t = 1 \ldots T$), and the ηs are individual-level deviations from the growth parameters in $\boldsymbol{\theta}$ with means equal to zero. Because the means of the ηs are zero, $E[\mathbf{y}_j] = \mathbf{f}(\boldsymbol{\theta},\mathbf{t})$; that is, the average response curve corresponds exactly to the target function, although individual model-implied curves, except in some special cases, may only resemble the target function. The partial derivatives are then used to populate a factor loading matrix $\boldsymbol{\Lambda}$:

$$\boldsymbol{\Lambda} = \begin{bmatrix} f'_1(\boldsymbol{\theta},0) & f'_2(\boldsymbol{\theta},0) & \cdots & f'_k(\boldsymbol{\theta},0) \\ f'_1(\boldsymbol{\theta},1) & f'_2(\boldsymbol{\theta},1) & \cdots & f'_k(\boldsymbol{\theta},1) \\ \vdots & \vdots & \ddots & \vdots \\ f'_1(\boldsymbol{\theta},T) & f'_2(\boldsymbol{\theta},T) & \cdots & f'_k(\boldsymbol{\theta},T) \end{bmatrix}.$$

The columns of this matrix are termed *basis functions* (Browne, 1993; Meredith & Tisak, 1990) or *basis curves* (Blozis, 2004). Note that Equation 4 is not, strictly speaking, a model. According to the standard approach to SLCM, the model can be expressed in matrix form as

$$\begin{aligned}\mathbf{y}_j &= \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \eta_{1j}\mathbf{f}'_1(\boldsymbol{\theta},\mathbf{t}) + \eta_{2j}\mathbf{f}'_2(\boldsymbol{\theta},\mathbf{t}) + \eta_{3j}\mathbf{f}'_3(\boldsymbol{\theta},\mathbf{t}) + \boldsymbol{\varepsilon}_j \\ &= \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j\end{aligned}, \tag{5}$$

where $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ is the target function expressed as a function of parameters $\boldsymbol{\theta}$ and time vector $\mathbf{t}$, and $\boldsymbol{\varepsilon}_j$ is a vector of error terms.[4]

Equation 5 does not follow the typical LGM form, so we need to find a way to dispense with the $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ term. According to the traditional SLCM approach (e.g., Blozis, 2004, 2007a, 2007b; Browne, 1993; Browne & du Toit, 1991), if it can be assumed that $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ is invariant to a constant scaling factor, the target function can be decomposed into a matrix of its basis curves and the factor mean vector $\boldsymbol{\alpha}$:

$$\mathbf{f}(\boldsymbol{\theta},\mathbf{t}) = \boldsymbol{\Lambda}\boldsymbol{\alpha} \tag{6}$$

Then, the model is parameterized as

$$\begin{aligned}\mathbf{y}_j &= \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j \\ &= \boldsymbol{\Lambda}\boldsymbol{\alpha} + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j\end{aligned}, \tag{7}$$

[2] An example of a linearizing transformation exists for the Type I exponential function, $y = a\exp(bx)$. Taking the natural logarithm of each side yields the linearized function $\ln(y) = \tilde{a} + bx$, where $\tilde{a} = \ln(a)$.

[3] In theory, a Taylor series may be derived to an arbitrary order of polynomial complexity to more closely approximate the nonlinear target function. However, in SLCM, there have been no published attempts to utilize those beyond the first order, and there may be important practical impediments to doing so. We therefore limit attention to the customary first order.

[4] The model in Equation 5 is thus equivalent to the first-order linear component of the Taylor series initially suggested by Beal and Sheiner (1982), but approached from within a latent curve modeling framework.

where $E[\mathbf{y}_j] = \boldsymbol{\Lambda\alpha}$, and the vector $\boldsymbol{\varepsilon}$ contains occasion-specific errors. The elements of $\boldsymbol{\alpha}$ are a mix of estimated factor means and zeroes, with the zeroes corresponding to the means of growth coefficients that enter the target function nonlinearly. The matrix product $\boldsymbol{\Lambda\alpha}$, the loading matrix $\boldsymbol{\Lambda}$ multiplied by the factor mean vector $\boldsymbol{\alpha}$, reproduces the target model evaluated at the population point.

The matrix product $\boldsymbol{\Lambda\eta}_j$ represents the deviation of a typical individual's trajectory from the mean implied by $\boldsymbol{\Lambda\alpha}$. Thus, the vector $\boldsymbol{\eta}_j$ contains factor scores on several growth factors. The model-implied mean structure and covariance structure are thus

$$\begin{aligned}\boldsymbol{\mu} &= \boldsymbol{\Lambda\alpha} \\ \boldsymbol{\Sigma} &= \boldsymbol{\Lambda\Psi\Lambda}' + \boldsymbol{\Theta},\end{aligned} \tag{8}$$

where $\boldsymbol{\Psi}$ is the random effect covariance matrix and $\boldsymbol{\Theta}$ is the covariance matrix of occasion-specific errors.

The key feature of SLCM is the specification of columns of $\boldsymbol{\Lambda}$ to contain partial derivatives of the target function with respect to parameters of the target function. Just as in linear LGM (a special case of SLCM), individual cases' factor scores on the growth factors act as weights determining the degree to which each basis curve contributes to that case's modeled trajectory. The primary difficulty in applying SLCM, in our view, is determining which elements of $\boldsymbol{\alpha}$ are to be estimated and which are to be fixed to zero. The standard approach is to solve the matrix expression in Equation 6 for $\boldsymbol{\alpha}$ so that $E[\mathbf{y}] = E[\boldsymbol{\Lambda\alpha}] + E[\boldsymbol{\Lambda\eta}] = \mathbf{f}(\boldsymbol{\theta},\mathbf{t})$. Another approach is to fix to zero the means of the factors corresponding to the parameters that enter the target function nonlinearly, and estimate those that enter linearly, although it is not always immediately apparent which parameters are linear versus nonlinear.[5]

For example, briefly consider the target function $f(\boldsymbol{\theta},t) = \theta_1\,\theta_2^t + \theta_3 t$. The partial derivatives of $f(\boldsymbol{\theta},t)$ with respect to θ_1, θ_2, and θ_3 are, respectively, θ_2^t, $\theta_1\theta_2^{t-1}t$, and t. Because the partial derivative of $f(\boldsymbol{\theta},t)$ with respect to θ_2 contains θ_2, this parameter is said to enter the target function nonlinearly. Thus, the corresponding element of $\boldsymbol{\alpha}$ is set to zero, whereas the other two elements are estimated. It can be seen that the target function is reproduced by postmultiplying $\boldsymbol{\Lambda}$ by $\boldsymbol{\alpha}$ (for an arbitrary row t of $\boldsymbol{\Lambda}$):

$$\begin{aligned}\left[\boldsymbol{\Lambda\alpha}\right]_t &= \begin{bmatrix} f_1'(\boldsymbol{\theta},t) & f_2'(\boldsymbol{\theta},t) & f_3'(\boldsymbol{\theta},t)\end{bmatrix}\begin{bmatrix}\theta_1 \\ 0 \\ \theta_3\end{bmatrix} \\ &= \begin{bmatrix}\theta_2^t & \theta_1\theta_2^{t-1}t & t\end{bmatrix}\begin{bmatrix}\theta_1 \\ 0 \\ \theta_3\end{bmatrix} \\ &= \theta_1\theta_2^t + \theta_3 t\end{aligned}.$$

However, often it can be challenging to obtain $\boldsymbol{\alpha}$ by solving a matrix expression or by determining which parameters enter the function nonlinearly. Importantly, with the Qinv function it is not possible to use the $\boldsymbol{\Lambda\alpha}$ parameterization for the mean trend because all three parameters are nonlinear, and thus $\boldsymbol{\alpha} = \mathbf{0}$.

In the spirit of the present article, we utilize a reparameterization of the standard SLCM that we think renders the approach easier to understand and apply. In some cases, this modification makes it possible to specify some models that otherwise would not be possible to specify using the standard SLCM approach. This modification of the SLCM approach (see also Browne, 1993, Equation 4.7) takes the form

$$\mathbf{y}_j = \boldsymbol{\tau} + \boldsymbol{\Lambda\eta}_j + \boldsymbol{\varepsilon}_j. \tag{9}$$

Equation 9 differs from Equation 7 in two important ways. First, the factor mean vector is absent from the model specification in Equation 9. In the standard approach to SLCM, $\boldsymbol{\alpha}$ contains a mix of estimated means and zeroes so that it can capture the mean trend, that is, so that $E_j[\mathbf{y}_j] = \mathbf{f}(\boldsymbol{\theta},\mathbf{t})$. In the modified approach, on the other hand, $\boldsymbol{\alpha}$ is set to $\mathbf{0}$. Second, we include the item intercept vector $\boldsymbol{\tau}$, constrained to $\boldsymbol{\tau} = \mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ in order to capture the target function as the mean trend. Thus, $E_j[\mathbf{y}_j] = E_j[\boldsymbol{\tau}] + E_j[\boldsymbol{\Lambda\eta}_j] + E_j[\boldsymbol{\varepsilon}_j] = \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \mathbf{0} + \mathbf{0}$.

Alternatively, the model may be parameterized by again omitting $\boldsymbol{\tau}$, and including an extra fixed factor whose loadings are constrained equal to the target function $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ and whose mean is constrained to 1. This parameterization owes its inspiration to an insight of Rovine and Molenaar (1998, 2000, 2003), who described how the general linear mixed model of Laird and Ware (1982) can be parameterized within covariance structure modeling. This is done by (a) partitioning the design matrix (i.e., $\boldsymbol{\Lambda}$) into parts corresponding to fixed effects and random effects, (b) estimating the means of the fixed effect latent variables but constraining their variances and covariances to zero, and (c) estimating the (co)variances of the random effect latent variables but constraining their means to zero. The end result is the same—the model-implied mean and covariance structures for the SLCM method, our modified method, and Rovine and Molenaar's method are identical (see Equation 8). We adopt Equation 9 in what follows. Representationally, our modified method is not, strictly speaking, a special case either of latent curve modeling or of Rovine and Molenaar's method, because we make use of the item intercept vector $\boldsymbol{\tau}$.

There are two main advantages associated with using the modified approach instead of the traditional SLCM. First, the target function is parameterized directly into the item intercept vector $\boldsymbol{\tau}$, and not reconstructed as a function of loadings multiplied by factor means and summed across factors. Because the researcher is relieved from having to solve the linear equation $\mathbf{f}(\boldsymbol{\theta},\mathbf{t}) = \boldsymbol{\Lambda\alpha}$ for $\boldsymbol{\alpha}$, we find this approach easier to understand and more straightforward to implement within standard SEM software. Second, and more importantly, some target functions contain only parameters that are intrinsically nonlinear, such that the factor mean vector $\boldsymbol{\alpha}$—and hence $\boldsymbol{\Lambda\alpha}$—would be zero, making it impossible to recover the target function. For example, all three parameters in the Qinv target function are intrinsically nonlinear, in the sense that partial derivatives of the target function with respect to each of these parameters themselves contain the parameters. Simply replacing $\boldsymbol{\Lambda\alpha}$ with $\boldsymbol{\tau}$ and setting $\boldsymbol{\alpha} = \mathbf{0}$ solves this problem while preserving the ability to fit models that contain a mix of linear and nonlinear parameters. Furthermore, columns of $\boldsymbol{\Lambda}$ that correspond to fixed coefficients (i.e., those whose associated factors have no variance) can be removed from the model entirely because these loadings would be associated with a latent variable with zero mean and zero variance. Finally, if model convergence proves difficult, one can usually revert

[5] A nonlinear model is one in which at least one partial derivative of the model with respect to a parameter contains at least one of the parameters (Bates & Watts, 1988). Sometimes one parameterization of a model is nonlinear, but another is linear (e.g., the traditional vs. reparameterized quadratic model; Cudeck & du Toit, 2002). Even in a nonlinear model, not all parameters are considered "nonlinear"—only those parameters for which the partial derivative contains that parameter. As an example, the function $y = \exp(a + bx)$ has two parameters entering nonlinearly, yet it can be reexpressed as $y = \tilde{a}\exp(bx)$, which is linear in $\tilde{a}$.

back to the standard SLCM to improve the probability of convergence, unless the model contains only intrinsically nonlinear parameters.

Revisiting the linearized Qinv function from Equation 3, it can be seen that the first term is a constant function of *time*, and the remaining terms all take the form of a mean-centered stochastic variable multiplied by additional constant functions of *time*. Therefore, Equation 3 has a form similar to that of Equation 4, and the model may be specified in the confirmatory factor analysis framework with the following $\boldsymbol{\tau}$ and $\boldsymbol{\Lambda}$ (for five occasions of measurement, with all three aspects of growth specified as random coefficients):

$$\boldsymbol{\tau} = \begin{bmatrix} t_1/[\mu_1 t_1 + \mu_2(\mu_{max}^2 + t_1^2)] \\ t_2/[\mu_1 t_2 + \mu_2(\mu_{max}^2 + t_2^2)] \\ t_3/[\mu_1 t_3 + \mu_2(\mu_{max}^2 + t_3^2)] \\ t_4/[\mu_1 t_4 + \mu_2(\mu_{max}^2 + t_4^2)] \\ t_5/[\mu_1 t_5 + \mu_2(\mu_{max}^2 + t_5^2)] \end{bmatrix}$$

$$\boldsymbol{\Lambda} = \begin{bmatrix} \frac{-(t_1^2)}{(\mu_1 t_1 + \mu_2(\mu_{max}^2 + t_1^2))^2} & \frac{-t_1(\mu_{max}^2 + t_1^2)}{(\mu_1 t_1 + \mu_2(\mu_{max}^2 + t_1^2))^2} & \cdots & \frac{-2\mu_2\mu_{max}t_1}{(\mu_1 t_1 + \mu_2(\mu_{max}^2 + t_1^2))^2} \\ \frac{-(t_2^2)}{(\mu_1 t_2 + \mu_2(\mu_{max}^2 + t_2^2))^2} & \frac{-t_2(\mu_{max}^2 + t_2^2)}{(\mu_1 t_2 + \mu_2(\mu_{max}^2 + t_2^2))^2} & \cdots & \frac{-2\mu_2\mu_{max}t_2}{(\mu_1 t_2 + \mu_2(\mu_{max}^2 + t_2^2))^2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{-(t_5^2)}{(\mu_1 t_5 + \mu_2(\mu_{max}^2 + t_5^2))^2} & \frac{-t_5(\mu_{max}^2 + t_5^2)}{(\mu_1 t_5 + \mu_2(\mu_{max}^2 + t_5^2))^2} & \cdots & \frac{-2\mu_2\mu_{max}t_5}{(\mu_1 t_5 + \mu_2(\mu_{max}^2 + t_5^2))^2} \end{bmatrix}.$$

We provide an example in the Appendix, using Cudeck and du Toit's (2002) reparameterized quadratic curve as the target function, of how a function may be modeled using both SLCM and our modified approach. We also provide Mplus syntax for fitting the Qinv function to example data in an online supplemental appendix.[6]

In many cases, different parameterizations of the same functional form will yield identical model fit in SLCM (Browne, 1993; Browne & du Toit, 1991). Browne (1993) proved that these models are insensitive to reparameterization as long as the latent variable covariance matrix is left freely estimated. This implies that researchers are free to reparameterize the model in any way they see fit without fear that they are changing something fundamental about the model.

Estimate the Model Parameters (Point and Interval Estimates)

Once the target function has been reparameterized and linearized, it can be specified and fit as a model using SEM software. The chosen software must be capable of imposing nonlinear constraints (e.g., Mplus, Mx, OpenMx, LISREL, SAS PROCs CALIS and TCALIS, and lavaan). Precisely how this is done will depend on the chosen software package, so we do not elaborate on it here. We illustrate specific examples in the next section.

Summary

Thus far we have described four steps that can be taken to proceed from the conventional use of growth curve modeling with less interpretable parameters to the use of reparameterized growth curve modeling with more interpretable parameters. The first step is to reparameterize the target function so that the new parameters or random coefficients have direct substantive interpretations. The second step is to linearize the reparameterized target function using a first-order expansion so that it can be specified as a model using SEM software. The third step is to specify the model using either the standard structured latent curve model or the modified version. The fourth step is to estimate the model parameters using SEM software. The ability to treat coefficients as fixed values, estimated parameters, or random coefficients derives from the SEM analyst's freedom to estimate or constrain these latent variables' means and variances. Virtually any aspect of growth may be treated in this fashion. Now that the groundwork has been laid, we present concrete details in the context of two examples.

Illustrative Examples

Example 1: Random Knot

Our first example is from the field of metabolism biochemistry, focusing on how chemicals are absorbed and metabolized by the body. Specifically, we reexamine data published by Zerbe (1979) related to the dynamics of plasma phosphate concentration upon the ingestion of carbohydrates. Broadly speaking, ingestion of carbohydrates signals the liver to harvest phosphates from the blood to aid in metabolizing the carbohydrates. Phosphates depleted from the blood are diverted to the liver, and then returned to the blood as digestion proceeds. High liver phosphate levels signal satiety to the brain. However, compared with normal-weight individuals, obese persons' livers have low baseline phosphate levels, take longer to uptake phosphate from blood plasma, and do not uptake as much phosphate. How much food, and how much time, it takes for the liver to signal satiety is associated with weight-related problems, such as heart disease (Obeid, Dimachkie, & Hlais, 2010).

Changes in liver phosphate levels can be measured indirectly by noting the inversely related phosphate concentration in blood plasma;

[6] This is available at http://quantpsy.org; see online supplemental Appendices 1 and 9 for Mplus syntax and output, respectively.

as plasma phosphates decline, it can be assumed that liver phosphate concentration increases. Zerbe (1979) provided measurements of plasma phosphate (mg/dl) for 33 participants (20 obese, 13 control) after a glucose challenge. Figure 2 depicts group means for eight measurement occasions.

An appropriate model for Zerbe's (1979) data may be the segmented linear spline with two phases. In such a model, the first phase (here, phosphate depletion) is fit with a linear model, and the second phase (recovery) is fit with a different linear model. The point at which one line changes into the next (here, when depletion turns into recovery) is commonly called the *knot*, *joint*, *change point*, or *transition point*. Often the knot is known in advance; other times it is treated as an estimated parameter. Additionally, the knot is not always expected to be the same for all individuals. Recognizing this, Cudeck and Klebe (2002) fit a segmented spline to Zerbe's data using multilevel modeling, showing that the knot may be treated as a fixed quantity, an estimated parameter, or even a random coefficient. Random knots are relatively novel, but have been modeled successfully using traditional (Cudeck, 1996; Cudeck & du Toit, 2003) and Bayesian (Dominicus, Ripatti, Pedersen, & Palmgren, 2008; McArdle & Wang, 2008; Muniz Terrera, van den Hout, & Matthews, 2011; Wang & McArdle, 2008) mixed effects models and growth mixture models (Kohli, 2011; Kohli, Harring, & Hancock, 2013; Li, Duncan, Duncan, & Hops, 2001). Here, we use the LGM framework and Steps 1 through 4 to reparameterize the traditional segmented spline. In the LGM context, knots have been treated as fixed, known quantities (Bollen & Curran, 2006; Flora, 2008) or as estimated parameters (Harring, Cudeck, & du Toit, 2006; Kohli et al., 2013), but not as random coefficients. Clearly, it would be beneficial to treat knots as randomly varying across individuals to more accurately mirror individual differences in the timing of phosphate rebound, and in many other contexts as well. Additionally, the ability to specify random knots in SEM makes available many of the advantages of latent variable modeling.

We begin with the traditional mixed-model expression of a two-segment linear spline target function:

$$y = \begin{cases} \theta_1 + \theta_2 t & t \le \theta_\kappa \\ \theta_3 + \theta_4 t & t > \theta_\kappa \end{cases} \tag{10}$$

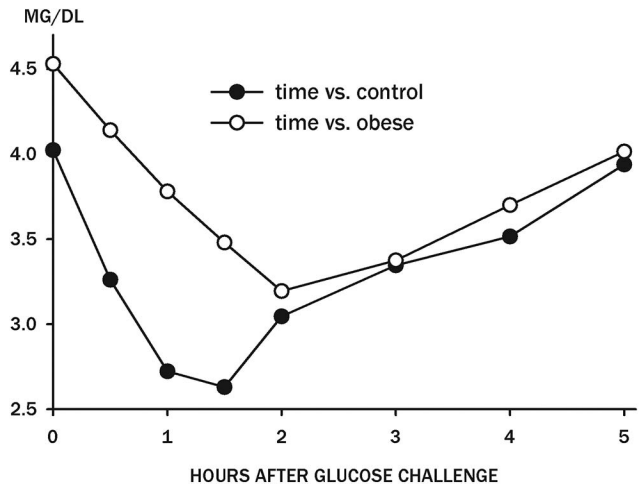

Figure 2. Obese and normal-weight group means for plasma phosphate concentration at eight unequally spaced occasions.

where θ_1 and θ_2 are the intercept and slope for the first segment, θ_3 and θ_4 are the intercept and slope for the second segment, and θ_κ is the knot. The segments are assumed to join at the knot, so there are effectively only four growth coefficients rather than the apparent five; that is, once any four of the θs are known, the fifth is determined. Cudeck and Klebe (2002) approached the problem from a mixed model perspective, treating the four free parameters as random effects, with separate means for the two groups but a common Level 2 covariance matrix. We would like to treat the knot as a random coefficient using LGM. However, it is not possible to specify this parameterization of the target function in SEM directly in a way that permits treating the knot as a random coefficient.

The first step will be to reparameterize the model, but the purpose of doing so is to render the model in such a way that it can be linearized and fit using SEM while preserving θ_κ as a parameter. Harring et al. (2006), Kohli and Harring (2013), and Kohli et al. (2013) reparameterized the target function in Equation 10 in a way that makes it possible to specify in SEM as a partially nonlinear model.[7] That is, the unknown change point θ_κ can be estimated, but must be treated as a fixed rather than random coefficient. Their parameterization[8] is

$$y = f(\boldsymbol{\theta}, t) = \omega_1 + \omega_2 t + \omega_3 \sqrt{(t - \theta_\kappa)^2}. \tag{11}$$

(Note that if we suspect $\theta_2 > \theta_4$, we would subtract rather than add the ω_3 term.)

In the now reparameterized Equation 11, the three ω coefficients are functions of the original growth coefficients θ_1 through θ_4. They still represent aspects of change (respectively, the average intercept across segments, the average slope across segments, and half the difference between the two slopes).[9] However, we are more concerned with the knot. It is important to note that θ_κ survived the reparameterization intact, and bears the same interpretation as in the original parameterization in Equation 10. Crucially, Equation 11 is in a form that can be linearized and modeled using SEM, whereas Equation 10 is not.

The second step is to linearize the reparameterized target function to express it in a form that will be more palatable to SEM software. Anticipating that all parameters in the target function will be treated as random coefficients, the first partial derivatives of Equation 11 with respect to each coefficient, evaluated at the population point, are

$$\partial f / \partial \omega_1 = 1$$

$$\partial f / \partial \omega_2 = t$$

$$\partial f / \partial \omega_3 = \sqrt{(t - \mu_\kappa)^2}$$

$$\partial f / \partial \theta_\kappa = \mu_3 (\mu_\kappa - t) / \sqrt{(t - \mu_\kappa)^2}$$

Thus, the linearized target function is

[7] A partially (or conditionally) nonlinear model is one in which only those parameters that enter the model linearly may be treated as random coefficients (Blozis, 2012; Blozis & Cudeck, 1999).

[8] A similar but slightly different model was used for estimating random knots in the mixed effects modeling framework by Crockett, Harvey, Guo, Francis, and Brouwers (2005).

[9] We can express the original model coefficients in terms of these new ones: $\theta_1 = \omega_1 + \omega_3 \theta_\kappa$, $\theta_2 = \omega_2 - \omega_3$, $\theta_3 = \omega_1 - \omega_3 \theta_\kappa$, $\theta_4 = \omega_2 + \omega_3$, and $\theta_\kappa = \theta_\kappa$. See Harring et al. (2006) and Kohli and Harring (2013) for more complete details, and see online supplemental Appendix 8 for the derivation of Equation 11.

$$\tilde{y} = f(\boldsymbol{\theta},t) + (\omega_1 - \mu_1)\frac{\partial f}{\partial \omega_1}\bigg|_{\mu_1} + (\omega_2 - \mu_2)\frac{\partial f}{\partial \omega_2}\bigg|_{\mu_2} + (\omega_3 - \mu_3)\frac{\partial f}{\partial \omega_3}\bigg|_{\mu_3} + (\theta_\kappa - \mu_\kappa)\frac{\partial f}{\partial \theta_\kappa}\bigg|_{\mu_\kappa}$$
$$= \left[\mu_1 + \mu_2 t + \mu_3\sqrt{(t-\mu_\kappa)^2}\right] + (\omega_1 - \mu_1)(1) + (\omega_2 - \mu_2)t$$
$$+ (\omega_3 - \mu_3)\sqrt{(t-\mu_\kappa)^2} + (\theta_\kappa - \mu_\kappa)\mu_3(\mu_\kappa - t)/\sqrt{(t-\mu_\kappa)^2}$$

In the third step, we use the derivatives obtained in Step 2 as factor loadings,[10] substituting values of $t = 0, \ldots, T$:

$$\boldsymbol{\Lambda} = \begin{bmatrix} 1 & 0 & \sqrt{(0-\mu_\kappa)^2} & \mu_3(\mu_\kappa - 0)/\sqrt{(0-\mu_\kappa)^2} \\ 1 & 1 & \sqrt{(1-\mu_\kappa)^2} & \mu_3(\mu_\kappa - 1)/\sqrt{(1-\mu_\kappa)^2} \\ \ldots & \ldots & \ldots & \ldots \\ 1 & T & \sqrt{(T-\mu_\kappa)^2} & \mu_3(\mu_\kappa - T)/\sqrt{(T-\mu_\kappa)^2} \end{bmatrix}.$$

The linearized model can then be expressed in matrix form as

$$\mathbf{y}_j = \boldsymbol{\tau} + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j, \tag{12}$$

where $\boldsymbol{\tau}$, the intercept vector, represents the target model evaluated at the population point, and $\boldsymbol{\Lambda}\boldsymbol{\eta}_j$ represents the deviation of individual j's trajectory from the mean implied by $\boldsymbol{\tau}$. The vector $\boldsymbol{\varepsilon}_j$ contains occasion-specific errors for individual j; for simplicity, we assume $\boldsymbol{\varepsilon}_{ij} \sim \mathrm{N}(0, \sigma^2_{\varepsilon})$ with time-homoscedastic variance.

We make use of our modification of SLCM to specify the model in Equation 12. Recall that in the modified method, $\boldsymbol{\alpha} = \mathbf{0}$ and can be omitted, and $\boldsymbol{\tau}$ is set equal to the desired mean trajectory at the parameter estimates. The model is depicted graphically in Figure 3, Panel A, and is an *unconditional* model that does not consider obesity (we will include obesity next in a conditional model, shown in Panel B). Symbols for elements of the random coefficient covariance matrix are omitted from the figure for simplicity, but can be represented as

$$\boldsymbol{\Psi} = \begin{bmatrix} \psi_1 & & & \\ \psi_{2,1} & \psi_2 & & \\ \psi_{3,1} & \psi_{3,2} & \psi_3 & \\ \psi_{\kappa,1} & \psi_{\kappa,2} & \psi_{\kappa,3} & \psi_\kappa \end{bmatrix}.$$

Fitting the model to data using Mplus 7.2 (L. K. Muthén & Muthén, 1998–2014) yields

$$\begin{aligned} \hat{\mu}_1 &= 3.400\ (.128) \\ \hat{\mu}_2 &= -.258\ (.034) \\ \hat{\mu}_3 &= .539\ (.040)\text{'} \\ \hat{\mu}_\kappa &= 1.588\ (.112) \end{aligned}$$

and

$$\hat{\boldsymbol{\Psi}} = \begin{bmatrix} .457\ (.135) & & & \\ -.030\ (.028) & .013\ (.010) & & \\ -.024\ (.030) & -.009\ (.009) & .027\ (.013) & \\ -.008\ (.085) & .018\ (.026) & .001\ (.027) & .254\ (.110) \end{bmatrix},$$

with $\boldsymbol{\varepsilon}_{ij} \sim \mathrm{N}[0, .103(.013)]$.[11] The model fits poorly ($\chi^2_{29} = 68.163$, $p < .001$; root mean square error of approximation [RMSEA] = .202, 90% CI [.140, .265]; non-normed fit index [NNFI] = .849), so the results of this example should be understood only in a didactic spirit and should not be taken to reflect on the substantive domain of plasma phosphate dynamics. The mean knot is estimated to occur 1.588 hr after the glucose challenge, with a standard deviation of approximately one half hour ($\hat{\psi}_\kappa = .254$). That is, even though phosphate levels begin to rebound on average just after the 1.5-hr mark, there exists considerable individual variability around this mean.

Regarding this individual variability, recall that the goal of this example was not only to show how the knot may be treated as a random coefficient within the SEM/LGM framework but also to predict individual differences in the knot using obesity status as a Level 2 predictor. The structural equation for the random coefficients $\boldsymbol{\eta}_j$ in the *conditional* model may be written as

$$\boldsymbol{\eta}_j = \boldsymbol{\Gamma}\mathbf{x}_j + \boldsymbol{\zeta}_j$$

where $\boldsymbol{\Gamma}$ contains structural coefficients (γs) linking growth factors to exogenous measured variables in $\mathbf{x}_j$. Regressing the growth factors on obesity status yields

$$\begin{aligned} \hat{\mu}_1 &= 3.553\ (.160) \\ \hat{\mu}_2 &= -.212\ (.042) \\ \hat{\mu}_3 &= .490\ (.050)\text{'} \\ \hat{\mu}_\kappa &= 1.951\ (.123) \end{aligned} \tag{13}$$

$$\hat{\boldsymbol{\Psi}} = \begin{bmatrix} .421\ (.126) & & & \\ -.041\ (.027) & .010\ (.009) & & \\ -.013\ (.028) & -.006\ (.008) & .024\ (.013) & \\ -.084\ (.077) & -.001\ (.023) & .011\ (.023) & .076\ (.082) \end{bmatrix},$$

and

[10] The Taylor series expansion used in SLCM and our modification of SLCM requires the target function to be differentiable with respect to its parameters in the neighborhood of the point of expansion. However, the derivatives of Equation 11 with respect to ω_3 and θ_κ are undefined where $t = \mu_\kappa$. The range in which most subjects' random knots are expected to fall may be inferred using $\hat{\boldsymbol{\psi}}_\kappa$ (e.g., $\hat{\mu}_\kappa \pm 1.96\hat{\boldsymbol{\psi}}_\kappa^{1/2}$). When such a range includes a known singularity, such as those occurring at the points of measurement in the current model, then the quality of the Taylor series expansion may become compromised and inference regarding parameter estimates tenuous.

[11] We used bootstrapping to obtain standard errors because we encountered unstable estimation in both the unconditional and conditional models arising from the small sample size; standard errors are based on 2,367 converged solutions out of 3,000 requested for the unconditional model, and on 2,105 out of 3,000 for the conditional model.

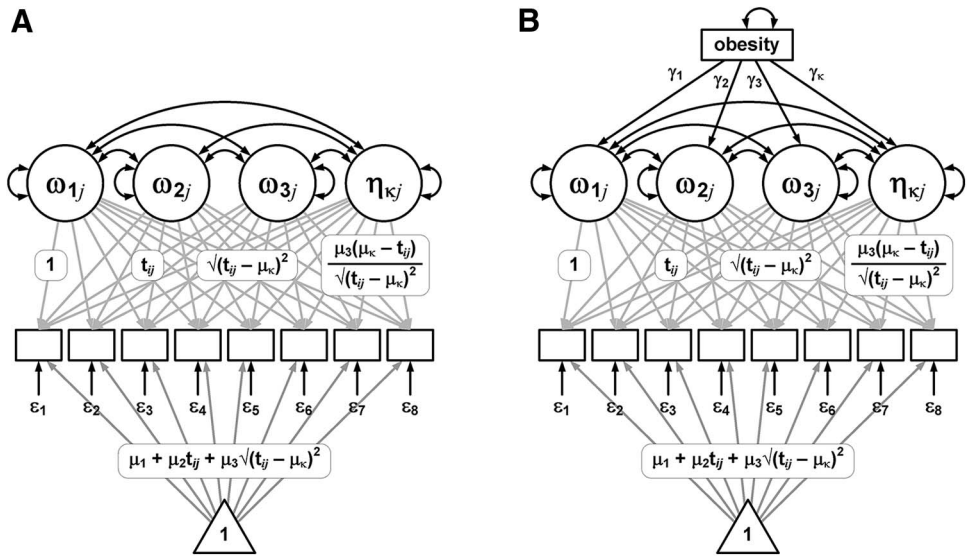

Figure 3. (A) A two-segment linear spline model for plasma phosphate depletion and recovery. The mean knot is represented by μ_κ, whereas the variance of the $\eta_{\kappa j}$ factor represents variability in the knot. (B) The same model is represented with obesity as a Level 2 predictor of growth coefficients. Because obesity is coded (0 = obese, 1 = normal), μ_κ represents the model-implied knot for the obese group, and the coefficient γ_κ represents the group mean difference (in units of hours) between normal-weight and obese groups.

$$\hat{\boldsymbol{\Gamma}} = \begin{bmatrix} -.387\ (.254) \\ -.117\ (.067) \\ .124\ (.079) \\ -1.013\ (.253) \end{bmatrix},$$

with $\boldsymbol{\varepsilon}_{ij} \sim \mathrm{N}[0, .103(.013)]$. The model fits poorly ($\chi^2_{33} = 70.711$, $p < .001$; RMSEA = .186, 90% CI [.126, .246], NNFI = .849), so the results of this example again should be treated only didactically. Because the obese group was coded "0" and the normal weight group was coded "1," the means in Equation 13 reflect model-implied values of the growth coefficients for the obese group. The negative effect of obesity status on the knot latent variable conveys the finding that normal weight individuals' mean knot occurred approximately an hour before the obese group's mean knot ($\hat{\gamma}_4 = -1.013$ hr), a result that tallies well with the means plotted in Figure 2. Mplus syntax is provided in the online supplemental appendix to reproduce results for both the unconditional and conditional models.[12]

Using these reparameterized models, we were able to predict individual differences in the timing of a metabolic event: the point in time at which plasma phosphates cease to be absorbed by the liver and begin to be returned to the blood. The advantages of specifying the segmented linear spline model with a random knot in SEM are clear.

Example 2: Average Rate of Change (ARC) and Half-Life

Our second example is drawn from a procedural learning study concerning verbal and quantitative skill acquisition, using data originally collected by Scott Chaiken of Armstrong Laboratory, Brooks Air Force Base (for a thorough description of these data, see Blozis, 2004).[13] The dependent measures are verbal and quantitative accuracy scores, consisting of aggregated response times within 12 trial blocks. Individual and mean-level data based on 228 cases are illustrated in Figure 4.

In this example, we reparameterize a common learning function to contain random coefficients for two relatively novel parameters, one reflecting an absolute learning rate and another reflecting scale-free learning rate. The first of these is the ARC—an individual's mean instantaneous linear slope across the full span of a trajectory (Kelley, 2009; Kelley & Maxwell, 2008). This mean derivative is simply $\Delta y_i / \Delta t_i$, regardless of the functional form of change, but as Kelley and Maxwell (2008) emphasized, the ARC is distinct from the mean slope in all but the simplest models of change. In repeated measures scenarios, every individual has his or her own ARC. Thus, it would be useful to treat the ARC as a random coefficient.[14] Kelley and Maxwell did not specify the ARC as a parameter or coefficient of the model, but they did suggest that the model's functional form may be considered by fitting a functional form of change and using predicted values of y to obtain the ARC. This would avoid ignoring intermediate occasions and increase accuracy when estimating the ARC.

The second parameter of interest is the *half-life*, defined as the amount of time necessary for a function to cover half the distance from any point to its asymptote (Rausch, 2004, 2008; Willett, 1989). Certain exponential models are characterized by a constant half-life parameter. As with the ARC, each individual can have his or her own half-life parameter. We suggest that the half-life can be a useful metric of learning rate. It reflects not the final level or

[12] See online supplemental Appendices 2 and 3 for Mplus syntax, and see Appendices 10 and 11 for annotated output.

[13] These data are included in installations of LISREL.

[14] Models involving ARC parameters are similar to, but distinct from, the *growth rate models* discussed by Zhang, McArdle, and Nesselroade (2012), which involve reparameterizing a target growth function in terms of a first derivative at a given occasion, such that the derivative (growth rate) can be treated as a model parameter or random coefficient. The ARC, in contrast, is a parameter representing the average of these growth rates over a given span of time.

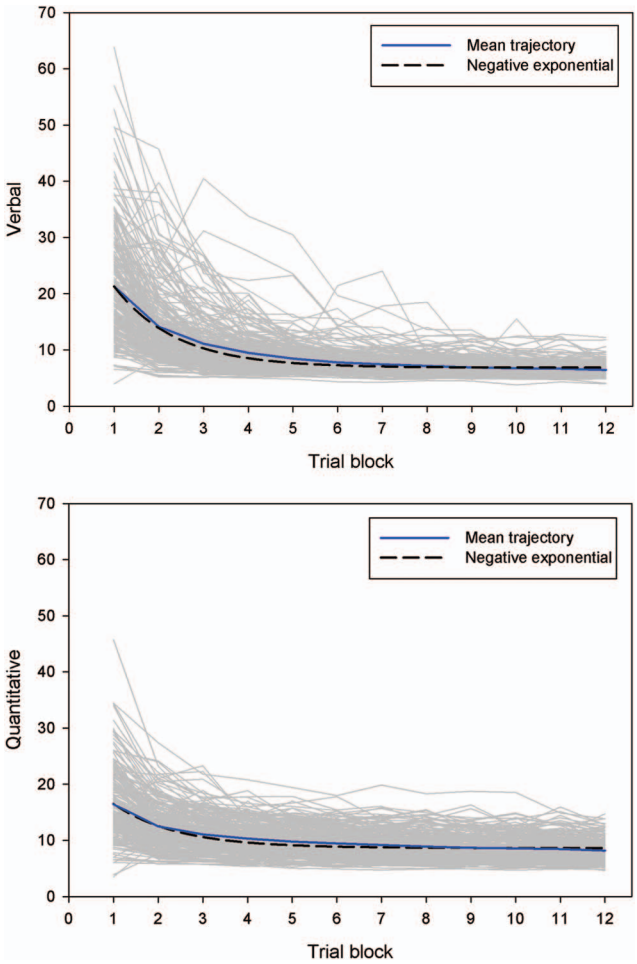

Figure 4. Verbal and quantitative skill acquisition response times from Chaiken's data. See the online article for the color version of this figure.

overall amount of learning, but rather the rapidity with which it is approached. Because half-life parameters are on a common metric (time), they can be used to compare learning rates for variables in different domains, even if they are measured on different scales.

Our first task was to choose an appropriate functional form to describe change in Chaiken's skill acquisition data. We used a three-parameter negative exponential (NE) function previously used by Blozis (2004) with the same data:

$$y = \theta_1 - (\theta_1 - \theta_2)\exp(-\theta_3[t-1]). \tag{14}$$

Here, θ_1 is the horizontal asymptote, θ_2 is the model-implied value of y at the initial trial, and θ_3 governs the rate of change. The rate parameter θ_3 governs how quickly the curve falls toward its horizontal asymptote at $y = \theta_1$. Importantly, although the NE function contains a parameter reflecting rate of change, it does not contain parameters that directly describe the ARC or half-life. Thus, our second task was to reparameterize the model such that the ARC and half-life are treated as random coefficients.

To reparameterize the NE function to contain a half-life parameter, we must find a way to express the half-life in terms of existing model parameters. We want the time at which the proportion of total change equals 1/2. Assuming negative growth (i.e., $\theta_2 > \theta_1$), the half-life will be

$$\begin{aligned}\frac{1}{2} &= \frac{\theta_2 - \left[\theta_1 - (\theta_1 - \theta_2)\exp(-\theta_3(\theta_h - 1))\right]}{\theta_2 - \theta_1} \\ &= 1 - \exp(-\theta_3(\theta_h - 1)).\end{aligned}$$

That is, θ_h is the value of t for which the distance between the initial value of y (θ_2) and the value of y at θ_h is exactly one half the total distance between θ_2 and the asymptote θ_1. Expressing the rate parameter as a function of θ_h yields

$$\theta_3 = \frac{\ln(1/2)}{1 - \theta_h}.$$

Substitution into the target function yields

$$\begin{aligned}y &= \theta_1 - (\theta_1 - \theta_2)\exp\left(-\frac{\ln(1/2)}{1-\theta_h}(t-1)\right) \\ &= \theta_1 - (\theta_1 - \theta_2)(1/2)^{\frac{t-1}{\theta_h - 1}}.\end{aligned} \tag{15}$$

This half-life parameterization can be further parameterized to trade the initial value parameter θ_2 for an ARC parameter. The ARC is formally defined as (Kelley & Maxwell, 2008)

$$\text{ARC} = \frac{1}{t_T - t_1}\int_{t_1}^{t_T} f'(y)dt = \frac{y_{t=t_T} - y_{t=t_1}}{t_T - t_1}.$$

That is, the ARC is the difference between the model-implied values of y at the beginning and end of the desired span of time, divided by that span. Substituting the model expression for the two instances of y yields

$$\begin{aligned}\theta_{\text{ARC}} &= \frac{\theta_1 - (\theta_1 - \theta_2)(1/2)^{\frac{t_T - 1}{\theta_h - 1}} - \left(\theta_1 - (\theta_1 - \theta_2)(1/2)^{\frac{t_1 - 1}{\theta_h - 1}}\right)}{t_T - t_1} \\ &= \frac{(\theta_2 - \theta_1)\left((1/2)^{\frac{t_T - 1}{\theta_h - 1}} - (1/2)^{\frac{t_1 - 1}{\theta_h - 1}}\right)}{t_T - t_1}.\end{aligned}$$

Therefore,

$$\theta_2 = \frac{\theta_{\text{ARC}}(t_T - t_1)}{(1/2)^{\frac{t_T - 1}{\theta_h - 1}} - (1/2)^{\frac{t_1 - 1}{\theta_h - 1}}} + \theta_1.$$

Substitution into Equation 15 yields the fully reparameterized target function:

$$\begin{aligned}y &= f(\boldsymbol{\theta}, t) \\ &= \theta_1 - (\theta_1 - \theta_2)(1/2)^{\frac{t-1}{\theta_h - 1}} \\ &= \theta_1 + \frac{\theta_{\text{ARC}}(t_T - t_1)(1/2)^{\frac{t-1}{\theta_h - 1}}}{(1/2)^{\frac{t_T - 1}{\theta_h - 1}} - (1/2)^{\frac{t_1 - 1}{\theta_h - 1}}}.\end{aligned} \tag{16}$$

The third step is to linearize Equation 16. We theorize that each individual may have a different half-life and a different ARC, reflecting individual differences in learning rates. It is also natural to expect individual differences in asymptote. Thus, all three parameters of the

reparameterized target function will be treated as random coefficients. Moreover, we wish to model both verbal and quantitative skill acquisition simultaneously in a bivariate trajectory model, which requires asymptote, half-life, and ARC coefficients for each domain.

The derivatives of Equation 16 with respect to each coefficient, evaluated at the population point, are

$$\frac{\partial f}{\partial \theta_1} = 1,$$

$$\frac{\partial f}{\partial \theta_{\text{ARC}}} = \frac{(t_T - t_1)(1/2)^{\frac{t-1}{\theta_h - 1}}}{(1/2)^{\frac{t_T - 1}{\theta_h - 1}} - (1/2)^{\frac{t_1 - 1}{\theta_h - 1}}}, \text{ and}$$

$$\frac{\partial f}{\partial \theta_h} = \frac{(1/2)^{\frac{t}{\theta_h - 1}}\theta_h\left((1/2)^{\frac{t_1}{\theta_h - 1}}(t - t_1) + (1/2)^{\frac{t_T}{\theta_h - 1}}(t_T - t)\right)(t_T - t_1)\ln(1/2)}{(\theta_h - 1)^2\left((1/2)^{\frac{t_T - 1}{\theta_h - 1}} - (1/2)^{\frac{t_1 - 1}{\theta_h - 1}}\right)^2}.$$

Two sets of these derivatives exist—one for verbal and one for quantitative.

In the next step, these derivatives are used as loadings in the 24×4 block diagonal matrix $\boldsymbol{\Lambda}$ (with parameters associated with V and Q superscripted as such),

$$\boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}^{\text{V}} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Lambda}^{\text{Q}} \end{bmatrix},$$

with columns of $\boldsymbol{\Lambda}^{\text{V}}$ (12×2) containing $\partial f/\partial \eta_1^{\text{V}}$, $\partial f/\partial \eta_{\text{ARC}}^{\text{V}}$ and $\partial f/\partial \eta_h^{\text{V}}$ columns of $\boldsymbol{\Lambda}^{\text{Q}}$ (12×2) containing $\partial f/\partial \eta_1^{\text{Q}}$, $\partial f/\partial \eta_{\text{ARC}}^{\text{Q}}$, and $\partial f/\partial \eta_h^{\text{Q}}$. Values of $t = 1, \ldots, 12$ are substituted within both $\boldsymbol{\Lambda}^{\text{V}}$ and $\boldsymbol{\Lambda}^{\text{Q}}$. The linearized model can then be expressed in the form of Equation 9, where $\boldsymbol{\Lambda}\boldsymbol{\eta}_j$ represents the deviation of individual j's verbal and quantitative trajectories from the respective mean trajectories implied by $\boldsymbol{\tau}$. The vector $\boldsymbol{\varepsilon}_j$ again contains occasion-specific errors for individual j. Errors for each outcome will have homoscedastic variances over time and autoregressive covariance structures determined by parameters ρ^{V} and ρ^{Q}, as in Blozis (2004).

We next specify the linearized model, the diagram for which is depicted in Figure 5. The asymptote, half-life, and ARC parameters for verbal and quantitative domains are estimated as

$$\begin{aligned} \hat{\theta}_1^{\text{V}} &= 6.845\ (.100) & \hat{\theta}_1^{\text{Q}} &= 8.629\ (.143) \\ \hat{\theta}_{\text{ARC}}^{\text{V}} &= -1.312\ (.058) & \hat{\theta}_{\text{ARC}}^{\text{Q}} &= -.715\ (.031). \\ \hat{\theta}_h^{\text{V}} &= 1.962\ (.026) & \hat{\theta}_h^{\text{Q}} &= 1.993\ (.033) \end{aligned}$$

The ARC parameters indicate statistically significant negative average rates of change for each domain, whereas the half-life parameters indicate that the time that elapses for typical individuals to reach a point halfway between their current status and their learning level is comparable for the verbal and quantitative tasks. A Wald test of $(\theta_h^{\text{V}} - \theta_h^{\text{Q}})$ indicated no statistically significant difference in the domain-specific half-life parameters ($p = .454$).

The random coefficient covariance matrix is

$$\hat{\boldsymbol{\Psi}} = \begin{bmatrix} \hat{\psi}_{1(\text{V})} & & & & & \\ \hat{\psi}_{\text{ARC(V)},1(\text{V})} & \hat{\psi}_{\text{ARC(V)}} & & & & \\ \hat{\psi}_{h(\text{V}),1(\text{V})} & \hat{\psi}_{h(\text{V}),\text{ARC(V)}} & \hat{\psi}_{h(\text{V})} & & & \\ \hat{\psi}_{1(\text{Q}),1(\text{V})} & \hat{\psi}_{1(\text{Q}),\text{ARC(V)}} & \hat{\psi}_{1(\text{Q}),h(\text{V})} & \hat{\psi}_{1(\text{Q})} & & \\ \hat{\psi}_{\text{ARC(Q)},1(\text{V})} & \hat{\psi}_{\text{ARC(Q)},\text{ARC(V)}} & \hat{\psi}_{\text{ARC(Q)},h(\text{V})} & \hat{\psi}_{\text{ARC(Q)},1(\text{Q})} & \hat{\psi}_{\text{ARC(Q)}} & \\ \hat{\psi}_{h(\text{Q}),1(\text{V})} & \hat{\psi}_{h(\text{Q}),\text{ARC(V)}} & \hat{\psi}_{h(\text{Q}),h(\text{V})} & \hat{\psi}_{h(\text{Q}),1(\text{Q})} & \hat{\psi}_{h(\text{Q}),\text{ARC(Q)}} & \hat{\psi}_{h(\text{Q})} \end{bmatrix}$$

$$= \begin{bmatrix} 1.652(.207) & & & & & \\ -.193(.084) & .712(.069) & & & & \\ -.131(.051) & .025(.030) & .216(.023) & & & \\ 1.664(.235) & -.597(.126) & -.183(.071) & 4.187(.423) & & \\ -.035(.046) & .122(.028) & .015(.016) & -.293(.068) & .208(.021) & \\ -.037(.025) & -.021(.014) & .016(.008) & -.064(.036) & -.031(.008) & .046(.006) \end{bmatrix}$$

All of the random coefficient variances and most of the covariances exceed chance levels, indicating that the coefficients reflecting learning rate vary significantly from person to person, and often covary with each other and with the final level of learning (asymptote). The verbal and quantitative ARC coefficients were positively related, as were the verbal and quantitative half-life coefficients. The model does not fit well by conventional criteria ($\chi^2_{293} = 2435.191$, $p < .001$, RMSEA = .179, 90% CI [.173, .186], NNFI = .745), so results should be taken in a didactic spirit and do not reflect on the substantive domain of verbal and quantitative skill acquisition. Mplus syntax is provided in the online supplemental appendix to reproduce these results.[15]

Recall that Browne (1993) showed that if no restrictions are placed on the random effect covariance matrix, reparameterization

[15] See online supplemental Appendices 5 and 13 for Mplus syntax and annotated output, respectively.

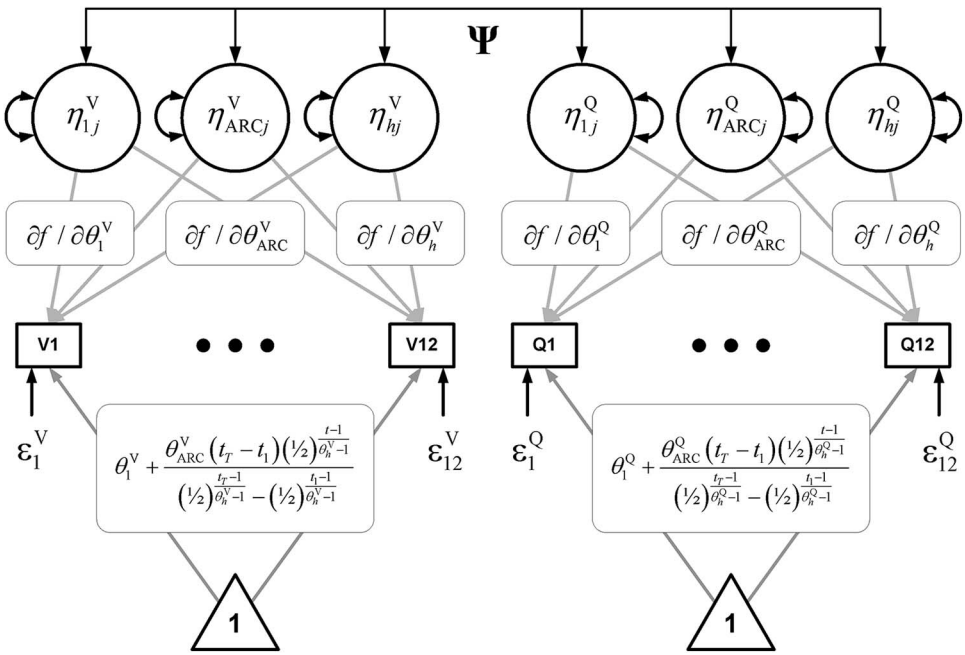

Figure 5. A bivariate trajectory model for verbal (V) and quantitative (Q) skill acquisition, in which each trajectory is a negative exponential curve with asymptote (θ_1), average rate of change (θ_{ARC}), and half-life (θ_h) random coefficients. Not depicted are the occasion-specific errors, which have an autoregressive covariance structure within each domain.

yields an equivalent model. For completeness, and to illustrate the equivalence of the reparameterized target function to the original target function in Equation 14, we also fit a model using the original parameterization. Following all the preceding steps, but with this other target function in mind, we obtain identical model fit (χ^2_{293} = 2435.191, $p < .001$, RMSEA = .179, 90% CI [.173, .186], NNFI = .745). Estimates of the target function parameters are

$$\begin{aligned}
\hat{\theta}_1^{V} &= 6.845(.100) & \hat{\theta}_1^{Q} &= 8.629(.143)\\
\hat{\theta}_2^{V} &= 21.278(.661) & \hat{\theta}_2^{Q} &= 16.492(.404)\,.\\
\hat{\theta}_3^{V} &= .721(.020) & \hat{\theta}_3^{Q} &= .698(.023)
\end{aligned}$$

These are the estimated horizontal asymptotes, intercepts, and rate of change parameters for verbal and quantitative skill acquisition. The random coefficient covariance matrix is

$$\hat{\boldsymbol{\Psi}} = \begin{bmatrix}
\hat{\psi}_{1(V)} & & & & & \\
\hat{\psi}_{2(V),1(V)} & \hat{\psi}_{2(V)} & & & & \\
\hat{\psi}_{3(V),1(V)} & \hat{\psi}_{3(V),2(V)} & \hat{\psi}_{3(V)} & & & \\
\hat{\psi}_{1(Q),1(V)} & \hat{\psi}_{1(Q),2(V)} & \hat{\psi}_{1(Q),3(V)} & \hat{\psi}_{1(Q)} & & \\
\hat{\psi}_{2(Q),1(V)} & \hat{\psi}_{2(Q),2(V)} & \hat{\psi}_{2(Q),3(V)} & \hat{\psi}_{2(Q),1(Q)} & \hat{\psi}_{2(Q)} & \\
\hat{\psi}_{3(Q),1(V)} & \hat{\psi}_{3(Q),2(V)} & \hat{\psi}_{3(Q),3(V)} & \hat{\psi}_{3(Q),1(Q)} & \hat{\psi}_{3(Q),2(Q)} & \hat{\psi}_{3(Q)}
\end{bmatrix}$$

$$= \begin{bmatrix}
1.652(.207) & & & & & \\
3.783(.976) & 92.144(8.816) & & & & \\
-.147(.059) & -.468(.391) & .272(.044) & & & \\
1.664(.235) & 8.242(1.468) & -.205(.082) & 4.187(.423) & & \\
2.051(.606) & 23.425(4.200) & -.392(.232) & 7.414(.985) & 35.773(3.456) & \\
-.072(.049) & .371(.318) & .036(.018) & -.126(.073) & .540(.204) & .179(.030)
\end{bmatrix}$$

Note that the horizontal asymptote parameter estimates are the same across parameterizations; this parameter was preserved in the reparameterization process. Mplus syntax is provided in the online supplemental appendix to reproduce these results.[16]

Discussion

We had three goals in this article. First, we aimed to provide theoretical background for Preacher and Hancock's (2012) four-step method for reparameterizing and fitting linear and nonlinear growth curve models, and elaborated on it. Second, we described a modification to the traditional structured latent curve model that enables fitting a broader class of nonlinear growth models and renders model specification easier. Third, we presented two examples illustrating the specification of several aspects of change as random coefficients, some new to the SEM literature. We further supplied extensive Mplus syntax in an online supplemental appendix to make the application of such models more feasible for applied researchers. Our core message is that growth curve models may be considerably more flexible than most researchers suspect, and that strategic reparameterization is one practical way to unlock that flexibility.

Good model specification requires a model's parameters to have direct, substantive interpretations that are meaningful within the research context. Many models used by social scientists are already parameterized such that their parameters are readily interpretable. For example, multiple regression models contain, by default, intercepts and linear slopes that bear directly on questions of scientific interest. Item response models contain parameters that correspond directly to item difficulty and discrimination, which are of direct interest to researchers and test constructors. However, many models, despite providing accurate descriptive matches to observed data, do not contain directly interpretable parameters. In such cases, more interesting parameters must be derived through often-cumbersome second-stage analyses, and treating the new parameters as random coefficients is beyond most researchers' abilities. Still other models contain parameters that are interpretable, yet not as interesting as other quantifiable aspects of the model might be.

In such cases, we advocate strategic reparameterization as a general approach to model specification. Learning the basic approach to reparameterization will enable researchers to think creatively about how they specify models to directly test hypotheses of scientific interest and substantive importance. In this article, we described how to reparameterize a growth model such that aspects of change are represented as fixed values, as estimated parameters, or as random coefficients, and how to fit such reparameterized models within the SEM framework. In the process, we also described a slight modification of the standard SLCM method that facilitates model specification for many nonlinear models, and, in some cases, makes it possible to specify models that were not specifiable under standard SLCM.

We illustrated these steps using two examples involving empirical data. The first involved fitting a reparameterized spline model to a sample of obese and normal-weight individuals, treating the knot point as a predictable random coefficient. The second involved fitting parallel NE growth curves to verbal and quantitative skill acquisition data, treating the ARC and half-life as random coefficients.

When to Use Reparameterization

We noted that reparameterization enables the researcher to treat an aspect of change as a known, fixed constant. We did not illustrate this capability, but it could be used to render a model more parsimonious by incorporating known information. For example, if the knot point in our first example had been known a priori and did not vary over individuals, it could be fixed to that known value. Using reparameterization to treat an aspect of change as an estimated parameter or random coefficient, on the other hand, enables the researcher to investigate whether the aspect of change is predicted (moderated) by person-level predictors. We see this as the most important use of reparameterization, although there are others, as we mentioned earlier. These include (a) *convenience*—it is often more straightforward to estimate a parameter directly, and therefore to obtain a standard error and CI for it, than to compute it post hoc as a function of parameter estimates; (b) *stability*—if one parameterization has difficulty converging, sometimes another parameterization will not; and (c) *imposing constraints*—parameterizing a model such that only certain values are permissible is a way of constraining its range.

We have found reparameterization to be particularly useful in models of growth or change. In such models it is useful to consider (a) those aspects of change that are missing from the model but which we would like to treat as parameters or random coefficients, given the opportunity; and (b) which existing parameters we could live without. Usually it will be possible to sacrifice the latter for the former through reparameterization. For example, models of learning processes often contain an intercept parameter and one or more parameters linked to change over time. However, the intercept parameter (as in ordinary regression) is rarely of substantive interest. Rate of growth or change is of key interest. Additional parameters of interest in the learning context might include the total amount learned over the course of the study, or how long it takes to learn a subject to some criterion amount. Parameters or random coefficients reflecting the level of learning at the end of a study, or the time it takes an individual to reach a certain criterion of learning, would seem to be of far greater interest to education researchers than parameters related to students' starting points. In this article, we examined two examples of parameterizing novel aspects of change: treating the knot point in a segmented spline model as a random coefficient, and treating two measures of learning rate as random coefficients. But the basic idea of strategic reparameterization extends easily to other settings.

Comments on the Modeling Framework

A key distinction that should be borne in mind is the one between *marginal* or *population-average* (PA) and *subject-specific* (SS) models (Davidian & Giltinan, 1995, 2003; Demidenko, 2004; Lindstrom & Bates, 1990; Serroyen, Molenberghs, Verbeke, & Davidian, 2009; Zeger, Liang, & Albert, 1988). All applications of SLCM are PA models in the sense that only the mean trend is required to follow the functional form specified in the target function. This is ensured by the explicit requirement that $E[\mathbf{y}_j] = \mathbf{f}(\boldsymbol{\theta},\mathbf{t})$. Individual differences are accommodated by the inclusion

[16] See online supplemental Appendices 4 and 12 for Mplus syntax and annotated output, respectively.

of random effects for some or all aspects of change. However, PA models do not require individuals to follow the same functional form as the means, although model-implied subject-specific trajectories often will resemble the mean trend.[17] Thus, PA models tend to be used in situations in which the primary questions are about the mean trend. SS models, in contrast, require individuals to follow the target function, but make no such requirement for the mean trend. In SS models (termed *random-effects models* by Serroyen et al., 2009), the means do not necessarily follow a (simple) known functional form, although it is possible to aggregate the individual trajectories to get an idea of how the means change over time. Thus, SS models tend to be used when the primary focus is on modeling individuals' response trajectories. By and large, SLCM models (and our modification) are PA models, not SS models (Blozis, 2007a; Blozis, Conger, & Harring, 2007; Cudeck & Harring, 2007; Harring, 2009). However, when the model is linear in the random effects, the model is both PA and SS (Serroyen et al., 2009; Vonesh & Chinchilli, 1997). This property has been termed *dynamic consistency* (Singer & Willett, 2003; Vandergrift, 2004; Willett, 1989). Dynamically consistent models include linear and polynomial growth models and, more generally, *partially nonlinear* or *conditionally nonlinear* models, in which the intrinsically nonlinear parameters are treated as fixed coefficients but the linear parameters may vary across persons. We refer the reader to lucid discussions of the distinctions between PA and SS models by Cudeck and Harring (2007), Davidian and Giltinan (1995, 2003), Lindstrom and Bates (1990), and Vonesh and Chinchilli (1997).

Error Covariance Structures

We have been largely silent on how the error covariance structure is specified. With few exceptions (e.g., Blozis, 2004), the SLCM literature typically assumes errors to be independent over time (Blozis, 2007a; Blozis et al., 2007), more out of a desire for simplicity, not necessity. It has been repeatedly argued and shown that misspecification of the Level 1 error covariance structure translates into biased random effect parameters and biased standard errors elsewhere in the model (Grimm & Widaman, 2010; Gurka, Edwards, & Muller, 2011; Harring & Blozis, 2014). Cudeck and Harring (2007, p. 623) described the list of options for the error covariance structure as "truly dizzying." Guidance in parameterizing error covariance structures can be found in our Example 2 syntax, as well as in Rovine and Molenaar (1998, 2000), Blozis and Cudeck (1999), Harring and Blozis (2014), and Davidian and Giltinan (1995, Section 4.2).

Comments on Software Implementation

There are two points at which specialized software is relevant to our discussion. First, Steps 1 and 2 often will involve recourse to calculus. Many users will find it convenient to use software capable of symbolic calculus, such as Maple or Mathematica. We used the latter, and provide some example code in the online supplemental appendix.[18] Calculus is commonly used at two points. First, such software can be a great help in reparameterizing the target function. Reparameterizations that involve locating the maximum, minimum, or point of greatest change require locating points at which derivatives equal zero or themselves reach a maximum or minimum; in these cases, calculus is essential. Second, once the reparameterized target function has been identified, linearizing the function requires computing partial derivatives with respect to the function's coefficients. These actions are possible to do by hand, but the process can be quite tedious and error-prone.

The second point at which specialized software becomes indispensable is the model-fitting stage. Not all SEM software is capable of imposing the constraints required as part of the SLCM approach and our modification of it. We have found Mplus particularly useful in this regard, although LISREL, Mx, OpenMx, SAS PROCs CALIS and TCALIS, and lavaan all have constraint capabilities that vary in flexibility. Grimm and Ram (2009) provided code for a number of nonlinear models in Mplus and SAS, Blozis (2007a) provided code in LISREL and Mx, and Grimm et al. (2010) provided code for SLCM mixture models in Mplus and OpenMx. We include Mplus syntax for each of our examples, including the motivating inverse quadratic function example. Similar models can be fit using nonlinear mixed effects modeling. Nonlinear extensions of multilevel (random coefficients) modeling are very powerful and flexible when the goal is to estimate interindividual differences in intraindividual change that follows a nonlinear trajectory. Such models are commonly implemented using SAS PROC NLMIXED (e.g., Grimm & Ram, 2009), the R package lme4, OpenBUGS, Mx, and, to a limited extent, the MULTILEV module of LISREL.

Conclusion

We end by urging psychological researchers to make greater use of nonlinear trajectory models. Nonlinear models have a long history in psychology (see McArdle & Nesselroade, 2003, for an overview of early uses in psychology), but seem to have fallen somewhat out of fashion despite being more appropriate than linear growth curves in most situations (Cudeck & Harring, 2007). In our opinion, with rare exceptions, nonlinear trajectory models remain remarkably underutilized relative to their clear potential for psychological research. In other fields, a rich variety of nonlinear functions have been proposed to describe diverse phenomena. Gompertz (1825) proposed a sigmoidal function to describe the relationship between mortality and age (Winsor, 1932). Nonlinear functions potentially useful for the social sciences can be drawn from a surprising variety of sources, including biology (Karkach, 2006), botany (Hunt, 1982), oncology (Tabatabai, Williams, & Bursac, 2005), forestry (Leech & Ferguson, 1981; Sweda, 1984; Yang, Kozak, & Smith, 1978), and pharmacokinetics (Davidian & Giltinan, 1995, 2003). Many examples can be seen in treatments by Bates and Watts (1988), Davidian and Giltinan (1995), Huet, Bouvier, Poursat, and Jolivet (2004), Leech and Ferguson (1981), Mead and Pike (1975), Nelder (1966), Pinheiro and Bates (2000), Ratkowsky (1983, 1990), Seber and Wild (1989), Singer and Willett (2003), Sit and Poulin-Costello (1994), and Vonesh and Chinchilli (1997).

[17] Because random effects are treated as latent variables in this context, it is possible to estimate individual trajectories by obtaining factor scores and explicitly including them in Equation 12.

[18] See online supplemental Appendix 6 for Mathematica code for obtaining partial derivatives of an exponential function.

To date, only a few nonlinear functions have been modeled using SLCM, and only one or two parameterizations of each have been attempted. These are the *logistic curve* (Browne, 1993), various *exponential curves* (Blozis, 2004, 2007b; Blozis, Harring, & Mels, 2008; Browne, 1993; Grimm, Ram, & Hamagami, 2011), the *Gompertz curve* (Browne, 1993; Browne & du Toit, 1991), a modified *two-parameter logistic curve* (Blozis, 2007a), the *Michaelis-Menten curve* (Harring, Kohli, Silverman, & Speece, 2012), the *Preece-Baines model* (Grimm et al., 2011), and the *negative exponential curve* (Ghisletta, Kennedy, Rodrigue, Lindenberger, & Raz, 2010). In fact, there are several kinds of logistic and exponential curves, and potentially many different ways to parameterize each of these curves. Further development and application of SLCM and related methodology offers clear potential for both applied and methodological work. We hope our exposition of these issues will make researchers in psychology more willing, and more able, to employ nonlinear models in their own work.

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Appendix

Specification of a Reparameterized Quadratic Curve

Consider the common quadratic curve

$$y = \theta_0 + \theta_1 t + \theta_2 t^2. \tag{A1}$$

Many authors have noted the difficulty of lending meaning to the parameters of traditional polynomial functions. Cudeck and du Toit (2002) suggest a reparameterization of Equation A1 that contains more easily interpretable parameters. The reparameterized model is

$$y = \alpha_y - (\alpha_y - \alpha_0)\left(\frac{t}{\alpha_t} - 1\right)^2. \tag{A2}$$

Here, $\boldsymbol{\alpha}_0$ is the value of y when $t = 0$ (the intercept), $\boldsymbol{\alpha}_t$ is the value of t that lies at the minimum or maximum of the curve, and $\boldsymbol{\alpha}_y$is the value of y at that value of t.

Here, we show how to specify this model in SEM using both the structured latent curve approach and our modification of it. We might hypothetically fit the model in Equation A2 to Kanfer and Ackerman's (1989) air traffic controller learning task data, consisting of nine equally spaced repeated measures. First, the derivatives of y with respect to each parameter, evaluated at the population point, are

$$\begin{aligned} \partial y/\partial \alpha_0 &= (t/\mu_t - 1)^2 \\ \partial y/\partial \alpha_t &= 2t(\mu_y - \mu_0)(t - \mu_t)/\mu_t^3 \\ \partial y/\partial \alpha_y &= 1 - (t/\mu_t - 1)^2 \end{aligned} \tag{A3}$$

The linearized model may then be expressed in matrix form as

$$\begin{aligned} \mathbf{y}_j &= \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j \\ &= \boldsymbol{\Lambda}\boldsymbol{\alpha} + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j \end{aligned}$$

where $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ is the target function and the elements of $\boldsymbol{\Lambda}$ are the derivatives in Equation A3, with time values substituted for t:

(*Appendix continues*)

$$\boldsymbol{\Lambda} = \left[\frac{\partial \mathbf{y}}{\partial \alpha_0} \quad \frac{\partial \mathbf{y}}{\partial \alpha_t} \quad \frac{\partial \mathbf{y}}{\partial \alpha_y}\right]\Bigg|_{\boldsymbol{\mu}}$$

$$= \begin{bmatrix} (0/\mu_t - 1)^2 & 2(0)(\mu_y - \mu_0)(0 - \mu_t)/\mu_t^3 & 1 - (0/\mu_t - 1)^2 \\ (1/\mu_t - 1)^2 & 2(1)(\mu_y - \mu_0)(1 - \mu_t)/\mu_t^3 & 1 - (1/\mu_t - 1)^2 \\ (2/\mu_t - 1)^2 & 2(2)(\mu_y - \mu_0)(2 - \mu_t)/\mu_t^3 & 1 - (2/\mu_t - 1)^2 \\ (3/\mu_t - 1)^2 & 2(3)(\mu_y - \mu_0)(3 - \mu_t)/\mu_t^3 & 1 - (3/\mu_t - 1)^2 \\ (4/\mu_t - 1)^2 & 2(4)(\mu_y - \mu_0)(4 - \mu_t)/\mu_t^3 & 1 - (4/\mu_t - 1)^2 \\ (5/\mu_t - 1)^2 & 2(5)(\mu_y - \mu_0)(5 - \mu_t)/\mu_t^3 & 1 - (5/\mu_t - 1)^2 \\ (6/\mu_t - 1)^2 & 2(6)(\mu_y - \mu_0)(6 - \mu_t)/\mu_t^3 & 1 - (6/\mu_t - 1)^2 \\ (7/\mu_t - 1)^2 & 2(7)(\mu_y - \mu_0)(7 - \mu_t)/\mu_t^3 & 1 - (7/\mu_t - 1)^2 \\ (8/\mu_t - 1)^2 & 2(8)(\mu_y - \mu_0)(8 - \mu_t)/\mu_t^3 & 1 - (8/\mu_t - 1)^2 \end{bmatrix}$$

In the traditional SLCM approach (Browne, 1993), the researcher determines what elements of the factor mean vector $\boldsymbol{\alpha}$ are estimated or fixed to zero by solving the linear equation $E[\mathbf{y}_j] = \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) = \boldsymbol{\Lambda}\boldsymbol{\alpha}$:

$$\begin{aligned} &\mathbf{f}(\boldsymbol{\theta},\mathbf{t}) = \boldsymbol{\Lambda}\boldsymbol{\alpha} \\ &(\boldsymbol{\Lambda}'\boldsymbol{\Lambda})^{-1}\boldsymbol{\Lambda}'\mathbf{f}(\boldsymbol{\theta},\mathbf{t}) = (\boldsymbol{\Lambda}'\boldsymbol{\Lambda})^{-1}\boldsymbol{\Lambda}'\boldsymbol{\Lambda}\boldsymbol{\alpha} \\ &\boldsymbol{\alpha} = (\boldsymbol{\Lambda}'\boldsymbol{\Lambda})^{-1}\boldsymbol{\Lambda}'\mathbf{f}(\boldsymbol{\theta},\mathbf{t}) \end{aligned} \tag{A4}$$

Even though all the elements of $\boldsymbol{\Lambda}$ and $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ are known, Equation A4 often is intractably complex because of the nonlinear expressions in the elements of $\boldsymbol{\Lambda}$ and $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$. An easier way to determine what elements of $\boldsymbol{\alpha}$ to fix to zero is to note which parameters in Equation A2 enter the function nonlinearly and fix the corresponding factor means to zero. This can be accomplished by noting which derivatives in Equation A3 contain the parameter with respect to which the derivative was taken. Only $\partial y/\partial \alpha_t$ meets this criterion because it contains μ_t, so the second element of $\boldsymbol{\alpha}$ is fixed to zero and the other two are estimated:

$$\boldsymbol{\alpha} = [\,\mu_0\ 0\ \ \mu_y]'.$$

As a check, note that evaluating the product $\boldsymbol{\Lambda}\boldsymbol{\alpha}$ yields the target function

$$\begin{aligned} \boldsymbol{\Lambda}\boldsymbol{\alpha} &= \left[\frac{\partial \mathbf{y}}{\partial \alpha_0} \quad \frac{\partial \mathbf{y}}{\partial \alpha_t} \quad \frac{\partial \mathbf{y}}{\partial \alpha_y}\right]\Bigg|_{\boldsymbol{\mu}} \begin{bmatrix} \mu_0 \\ 0 \\ \mu_y \end{bmatrix} \\ &= \mu_0 \frac{\partial \mathbf{y}}{\partial \alpha_0}\Bigg|_{\boldsymbol{\mu}} + \mu_y \frac{\partial \mathbf{y}}{\partial \alpha_y}\Bigg|_{\boldsymbol{\mu}} \\ &= \mu_0(t/\mu_t - 1)^2 + \mu_y(1 - (t/\mu_t - 1)^2) \\ &= \mu_y - (\mu_y - \mu_0)\left(\frac{t}{\mu_t} - 1\right)^2. \end{aligned}$$

Alternatively, the linearized model may be expressed in matrix form as

$$\begin{aligned} \mathbf{y}_j &= \mathbf{f}(\boldsymbol{\theta},\mathbf{t}) + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j \\ &= \boldsymbol{\tau} + \boldsymbol{\Lambda}\boldsymbol{\eta}_j + \boldsymbol{\varepsilon}_j, \end{aligned}$$

There is no need to determine what elements of $\boldsymbol{\alpha}$ should be fixed to zero because $\boldsymbol{\alpha}$ is not in the model. Rather, the target function $\mathbf{f}(\boldsymbol{\theta},\mathbf{t})$ is coded directly into the intercept vector $\boldsymbol{\tau}$.

For the quadratic function applied to Kanfer and Ackerman's (1989) data, it does not matter which specification is used; both yield identical results. We include Mplus code in the online supplemental appendix for readers to demonstrate the equivalence of these methods.[19] The modified approach arguably is easier to implement and to understand, and it can be used in situations in which the classic approach cannot (e.g., the Qinv function considered earlier).

[19] See online supplemental Appendix 7 for Mplus syntax, and see online Appendices 14 and 15 for annotated output.

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