

# **Alternative covariance structures in mixed‑efects models: Addressing intra‑ and inter‑individual heterogeneity**

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#### **Abstract**

Mixed-effects models for repeated measures and longitudinal data include random coefficients that are unique to the individual, and thus permit subject-specific growth trajectories, as well as direct study of how the coefficients of a growth function vary as a function of covariates. Although applications of these models often assume homogeneity of the within-subject residual variance that characterizes within-person variation after accounting for systematic change and the variances of the random coefficients of a growth model that quantify individual differences in aspects of change, alternative covariance structures can be considered. These include allowing for serial correlations between the within-subject residuals to account for dependencies in data that remain after ftting a particular growth model or specifying the within-subject residual variance to be a function of covariates or a random subject efect to address between-subject heterogeneity due to unmeasured influences. Further, the variances of the random coefficients can be functions of covariates to relax the assumption that these variances are constant across subjects and to allow for the study of determinants of these sources of variation. In this paper, we consider combinations of these structures that permit fexibility in how mixed-efects models are specifed to understand within- and between-subject variation in repeated measures and longitudinal data. Data from three learning studies are analyzed using these diferent specifcations of mixed-efects models.

**Keywords** Autocorrelation · Procedural learning · Response latency · Working memory · Mixed-efects location scale models · Nonlinear mixed-efects models

Repeated measures and longitudinal data are essential in studies of growth or change in human behavior. Data collected across repeated occasions, whether the occasions are closely spaced (e.g., studies of human learning or ecological momentary assessments to understand variation in mood) or span across a relatively long period of time (e.g., longitudinal studies of human growth and development), are necessary to understand if, when, or how behaviors change and how other variables might infuence the process.

Mixed-efects models are widely applied for the analysis of repeated measures and longitudinal data. These models emphasize the individual by specifying a growth model at the subject level and provide a framework to study within- and between-subject variation in measured behaviors. In specifying a model, a function, typically assumed to be common to

 $\boxtimes$  Shelley A. Blozis sablozis@ucdavis.edu all individuals, is selected to describe the response, but one or more of the function coefficients are subject-specific to allow for individual diferences in certain aspects of change or development. In this way, the subject-specifc model can be used to account for variation in scores within individuals, and the subject-specific coefficients permit the study of how individuals difer in aspects of change. An appealing quality of these models is that the coefficients of a function can vary according to covariates at the subject level to study how specifc aspects of change or development depend on covariates.

Careful selection of a growth function that efectively summarizes a large collection of data by a relatively small number of parameters can aid in the analysis and interpretation of repeated measures and longitudinal data, especially when the form of change is complex (Cudeck & Harring, [2007](#page-18-0)). Further, if the chosen function is efective in capturing variation within individuals, then the occasion-specifc residuals will be independent within subjects. In other words, it is typically reasonable to assume that scores within subjects are correlated, and a mixed-efects model accounts

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for these correlations with the random coefficients of the growth model. If, however, a function is inefective in fully accounting for this variation, some dependencies between residuals will remain.

Previous work has documented the impact on model ft and statistical inference of poorly specifed residual covariance structures at the frst level of a mixed-efects model. It is well known that applications of mixed-efects models that erroneously assume that the residuals are independent with constant variance across occasions have consequences for the estimates of the variances of the random coefficients of the subject-level model (Baek et al., [2020](#page-18-1); Baek & Ferron, [2020](#page-18-2); Blozis & Harring, [2021;](#page-18-3) Chi & Reinsel, [1989](#page-18-4); Ferron et al., [2002](#page-18-5); Harring & Blozis, [2014](#page-18-6); Joo et al., [2019](#page-18-7); Sivo et al., [2005](#page-19-0)). Thus, in ftting a mixed-efects model, the analyst faces a need to balance parsimony and interpretability in selecting a growth model with the need to adequately address dependencies of scores within subjects.

A special class of mixed-efects models, known as mixedefects location scale models, have expanded the ways in which to model intra- and inter-individual diferences by including submodels for the variance of the residuals at the frst level of the model, as well as for the variances of the random coefficients at the second level (for three-level models, see Lin et al., [2018;](#page-18-8) Nestler et al., [2018](#page-18-9)). Importantly, these extensions provide a framework to relax assumptions of homogeneity of the covariance structure at each model level, in addition to providing a means to study the determinants of these sources of variation in data. These models grew from the need to model repeated-measures data that generally did not involve growth or change, and the residuals at level 1 were assumed to be independent (see Hedeker et al., [2008](#page-18-10)), but their application to growth and change processes (e.g., McNeish, [2021](#page-18-11); Williams et al., [2019](#page-19-1)) have not consistently incorporated this earlier literature that has emphasized the importance of considering alternative residual covariance structures when the assumption of independence between the level-1 residuals is not tenable. Shown to be useful in applications of linear growth models (Nestler, [2021,](#page-18-12) [2022\)](#page-18-13), this paper joins these two methodological areas within the context of ftting nonlinear mixed-efects models, thus broadening their use in problems involving relatively complex forms of change.

To accomplish this, data from three learning experiments are utilized to motivate researchers to expand their thinking about how they might formulate the covariance structure of a mixed-efects model to study within- and between-individual diferences in repeated measures that follow complex forms of change. We frst develop a general framework to increase options in how one specifes the covariance structure of a mixed-efects model with special attention to how covariates may be incorporated into the structure. The examples are then presented. We develop syntax for using maximum likelihood (ML) estimation of models using SAS PROC NLMIXED by expanding on the developments of Harring and Blozis ([2014\)](#page-18-6). A discussion follows with implications and directions for future research.

## **Mixed‑efects models for repeated measures and longitudinal data**

Resources on mixed-efects models are numerous. Among the many published materials on mixed-efects models are books that serve a range of purposes, with some providing a general resource (Wu, [2010](#page-19-2)) or focus on a particular software program (Rabe-Hesketh & Skrondal, [2012\)](#page-18-14) or area of application (Brown & Prescott, [2015\)](#page-18-15), and others emphasizing specifc topics, such as nonlinear mixed-efects models (Fiedler-Kelly & Owen, [2014\)](#page-18-16) or autoregressive mixedeffects models (Funatogawa & Funatogawa, [2018\)](#page-18-17). We assume readers are familiar with common formulations of a mixed-efects model, including linear and nonlinear models. We give a brief description of the model that serves as a starting point for our developments here.

Let  $y_{ii}$  be the observed measure for individual *i* at time *j*, where  $i = 1,..., N$  and  $j = 1,..., n_i$ , letting *N* denote the number of subjects and  $n_i$  the number of measures for individual *i*. Let  $t_{ii}$  be the time when  $y_{ii}$  was observed. A mixed-effects model for  $y_{ii}$  is

<span id="page-1-0"></span>
$$
y_{ij} = f(t_{ij}, \mathbf{X}_{ij}, \mathbf{\theta}_i, \mathbf{W}_i, \gamma) + \varepsilon_{ij}
$$
 (1)

where  $f(\cdot)$  is a function (e.g., linear, quadratic, logistic) assumed to characterize the growth or developmental trend of the response. In ([1\)](#page-1-0),  $y_{ii}$  is a function of  $t_{ii}$ , a set of covariates  $\mathbf{X}_{ii}$ (that usually includes 1 for the intercept of the model) that vary with  $y_{ij}$ , a set of subject-specific coefficients  $\theta_i$  that link  $\mathbf{X}_{ij}$  and *y*ij, a set of between-subject covariates **𝐖**<sup>i</sup> , a set of fxed coefficients  $\gamma$  that link  $W_i$  and  $y_{ij}$ , and a time- and subject-specific residual  $\varepsilon_{ij}$ . Coefficients in  $\theta_i$  can be fixed, random, or the sum of a fixed and a random effect. That is, for the q<sup>th</sup> coefficient in  $\theta_i$ ,  $\theta_{qi} = \alpha_q + u_{qi}$ , where  $\alpha_q$  is the fixed effect and  $u_{qi}$  is the corresponding random efect. The random efects are assumed to be independently and identically distributed (i.i.d.) as normal across subjects with mean  $\bf{0}$  and covariance matrix  $\bf{\Phi}$ , where the dimensions of  $\Phi$  depend on the number of random effects in  $\theta_i$ . The residual  $\varepsilon_{ij}$  is the response not accounted for by the subject-specific model given by  $f(t_{ij}, \mathbf{X}_{ij}, \theta_i, \mathbf{W}_i, \gamma)$ . The set of residuals  $\varepsilon_i = (\varepsilon_{i1},...,\varepsilon_{in_i})'$  is assumed to be i.i.d. normal across subjects with mean **0** and covariance matrix  $\mathbf{\Theta}_{\varepsilon}$ , where the dimensions of  $\Theta_{\varepsilon}$  depends on  $n_i$ .

#### **Within‑subject covariance structure**

The residual covariance matrix characterizes the variation and between-occasion covariation of the deviations of observations from their expected values. For a growth model that fully accounts for the within-subject dependencies of scores between occasions and given that the residual variances are equal across time, a simple structure for the covariance matrix is appropriate:  $\mathbf{\Theta}_{\varepsilon} = \sigma_{\varepsilon}^2 \mathbf{I}_{n_i}$ . Other options ought to be considered, however, if within-subject dependencies between scores remain, even after accounting for covariates, or if the variances of the residuals are not equal across occasions. The assumption of homogeneity of the residual covariance structure between subjects can be relaxed by specifying a model in which the covariance structure differs between groups, such as by allowing the variance of a simple covariance structure to differ between groups:  $\mathbf{\Theta}_{\varepsilon k} = \sigma_{\varepsilon k}^2 \mathbf{I}_{n_{ik}}$ , where *k* denotes group membership. The variance itself could also be a function of measured covariates (Stroup et al., [2018](#page-19-3)), similar to linear regression models that use an exponential function to model the residual variance to address heterogeneity (Aitkin, [1987](#page-18-18); Cook & Weisberg, [1983](#page-18-19); Harvey, [1976](#page-18-20); Carroll & Ruppert, [1988](#page-18-21)). In such cases, between-subject heterogeneity of the residual variance is assumed to be due to measured covariates.

An alternative is a mixed-efects location scale model in which the residual variance is assumed to be due to unmeasured covariates, in addition to possibly being due to measured covariates, by including a random subject efect in a model for the residual variance (Hedeker et al., [2008;](#page-18-10) Hedeker & Nordgren, [2013\)](#page-18-22). For example, in a model that assumes independent residuals between occasions, an exponential function (that ensures the result is positive) can be used to model the residual variance (cf. Hedeker et al., [2008\)](#page-18-10):

$$
\sigma_i^2 = exp(\tau_0 + v_i)
$$

where the exponentiated value of  $\tau_0$  is the within-person variance for a person whose random effect  $v_i$  is equal to 0. The random effect  $v_i$  is assumed to be i.i.d. lognormal across subjects. Similar to earlier work (e.g., Harvey, [1976](#page-18-20)), the model for the residual variance can be expanded to include measured covariates. For example, let  $X_{ij}$  and  $W_i$  denote a time-varying covariate and a between-subjects covariate, respectively, a model for  $\sigma_{ij}^2$  that is assumed to vary by individual and according to the two covariates is

$$
exp\Bigl(\tau_0+\tau_1X_{ij}+\tau_2W_i+\nu_i\Bigr),\,
$$

where  $\tau_0$ , when exponentiated, is the within-person variance for a person whose random effect  $v_i$ , within-subject covariate  $X_{ij}$ , and between-subject covariate  $W_i$  are equal to 0. The coefficients  $\tau_1$  and  $\tau_2$  are the effects of the within- and betweensubject covariates, respectively, on the residual variance, with a positive efect indicating that a higher level of a covariate corresponds to greater within-subject variation and a negative effect indicating that a higher level of a covariate corresponds to a lower degree of within-subject variation. For

example, using a mixed-efects location scale model, Blozis et al. [\(2020](#page-18-23)) reported greater between-subject heterogeneity of the within-subject variance of daily time spent engaged in leisure activities on weekends versus weekdays and for women versus men. The random effect  $v_i$  is the residual from the regression and is assumed to be independent and lognormally distributed between subjects. Importantly, the variance of the random scale effect  $v_i$ , if different from zero, reflects an additional source of between-subject variation due to unobserved sources, conditional on the observed covariates.

As mentioned previously, earlier reports have documented the impact of mis-specifying the level-1 residual covariance structure of a mixed-effects model, including reports of relatively poor model ft, and perhaps more importantly, consequences for the estimated variances of the random subject effects at the second level. Ignoring correlations between residuals at the occasion level has, for example, been shown to result in overestimation of the variances of the random efects at the second level of a linear mixed-effects model (Chi & Reinsel, [1989;](#page-18-4) Ferron et al., [2002](#page-18-5); Sivo et al., [2005](#page-19-0)). Thus, the connection between how the occasion-level covariance structure is specifed and its impact on the subject-level covariance structure deserves attention when ftting a mixed-efects model to understand between-subject differences in a behavior studied over time. This point may be of particular importance when considering more advanced versions of a mixed-efects model, namely a mixed-efects location scale model. The implication is that ignoring serial correlations between the residuals at the occasion level may have consequences for the estimated variances of the random efects at the subject level, including the between-subject random scale variance that is a key component of a mixed-efects location scale model.

#### **Between‑subject covariance structure**

Mixed-effects models are subject-specific models because one or more of the coefficients of a growth function are assumed to vary between subjects. The between-subject covariance matrix of the random coefficients characterizes the degree to which individuals differ in the coefficients, as well as the extent to which the coefficients covary with one another. A useful aspect of a mixed-efects model is that it is possible to test if the random coefficients are related to subject-level covariates. This could be done to test if features of a growth or developmental process are associated with individual diference measures. If subject-level covariates are included in the regression equation of a random efect, the residual of that equation is a conditional random effect, and the variance of the conditional random effect represents variation in the random effect left unaccounted for.

As stated earlier, the variance of a random coefficient may be studied as a function of occasion- and subject-level covariates (Hedeker & Nordgren, [2013](#page-18-22)). In this way, it is possible to study the determinants of the variances of the random coefficients. To illustrate this, let  $\phi_0^2$  denote the variance of a random intercept that is modeled as a function of an occasionand a subject-level covariate. Using an exponential function to model the variance (cf. Hedeker & Nordgren, [2013](#page-18-22)),

$$
\phi_0^2 = exp(\alpha_{00} + \alpha_{01}X_{ij} + \alpha_{02}W_i)
$$

where the exponentiated value of  $\alpha_{00}$  is the variance of the random intercept when the covariates  $X_{ij}$  and  $W_i$  are equal to 0, and  $\alpha_{01}$  and  $\alpha_{02}$  are the effects of  $X_{ii}$  and  $W_i$ , respectively, on the variance. A positive covariate efect would indicate greater between-subject variation in the random intercept with an increase in the covariate, and a negative efect would indicate a decrease in between-subject variation with an increase in the covariate. In a study of positive afect in adolescent cigarette smokers, for example, Hedeker et al. [\(2008](#page-18-10)) reported greater between-subject variation in a random intercept for individuals identifed as loners relative to others and less variation among novelty seekers and 10th grade students relative to others.

#### **Estimation**

Estimation of linear mixed-efects models can be conducted using statistical software programs that use methods applicable to the estimation of other linear multivariate models, such as linear structural equation models with latent variables (Blozis, [2007](#page-18-24)). In a mixed-efects location scale model, the variances at the occasion level and the variances of the random coefficients at the subject level are typically expressed using exponential functions, and thus involve the estimation of nonlinear parameters, and more generally, estimation of a nonlinear mixed-efects model. Among the software packages developed for maximum likelihood (ML) estimation of nonlinear mixed-efects models, SAS PROC NLMIXED (Wolfnger, [1999](#page-19-4)) has been widely used to estimate mixedefects location scale models. PROC NLMIXED is well suited for the estimation of these models because the procedure makes it convenient to include the nonlinear models for the variance of a random effect at the subject level and the variance of the residual at the occasion level to model heterogeneity of variance at both levels (Hedeker et al., [2008\)](#page-18-10).

PROC NLMIXED is also adaptable for ML estimation of the mixed-efects location scale models developed here in which the residual covariance structures do not conform to the procedure's default model specifcations. Specifcally, we consider models in which the residual covariance structure assumes an first-order autoregressive  $(AR(1))$  structure to help address the possibility of correlation between adjacent residuals at the frst level of a model, a possible indication that the explanatory portion of a growth model does not fully account for the within-subject variation. The default residual covariance structure in PROC NLMIXED is one in which the residuals are assumed to be independent between occasions

with constant variance across occasions and subjects. The GENERAL model statement option permits a user-defned likelihood function of a given model. Using this option, it is possible to specify alternative residual covariance structures, such as an  $AR(1)$  structure with a fixed variance and autocorrelation coefficient (Harring & Blozis,  $2014$ ) or a structure with a random scale and autocorrelation as discussed in this paper.

PROC NLMIXED offers ML estimation using Gaussian quadrature and a dual quasi-Newton optimization routine (SAS Institute Inc., [2015\)](#page-18-25). To ft the models presented in this paper, we relied on guidance provided by Kiernan et al. [\(2012](#page-18-26)) by providing reasonable starting values. For each of the data sets, we started by fitting a fixed-effects model to obtain estimates of the fxed efects of the growth curve and the effects of the covariates on growth parameters. We then built up models by adding random effects, one at a time, and updating the starting values for each model based on estimates obtained for previous models. Syntax for ftting models to the fight simulation data (the second example) is in the Appendix. Tests were carried out using a type 1 error rate of .05.

In the examples that follow, SAS PROC NLMIXED was used for estimation. The default method of estimation in this procedure involves approximating the marginal loglikelihood using an adaptive Gaussian quadrature method (Pinheiro & Bates, [1995\)](#page-18-27). In a given problem, a good approximation requires an adequate number of quadrature points and appropriate centering and scaling of the abscissas for the random efects. The adaptive method has the advantage of requiring fewer quadrature points and has been shown to perform well when good starting values are provided and the number of ran-dom effects is not large (Pinheiro & Bates, [1995](#page-18-27)). For some of the models considered here, estimation using adaptive Gaussian quadrature (including the Laplace approximation) stopped with a report that no valid parameter points were found. We instead used Gaussian–Hermite quadrature that approximates each integral by a weighted average of the integrand that is evaluated at specifc points over a grid centered at 0. Following guidance by Carlin et al. [\(2001](#page-18-28)) to use a high number of quadrature points when using nonadaptive Gaussian quadrature, models were estimated using 30 quadrature points. Although an increase in the number of grid points can increase the precision of the approximation of the integral, an increase can result in a computationally intensive analysis. We observed increasing stability in the parameter estimates as the number of quadrature points was increased, but recommend caution when ftting such complex methods using this method of estimation.

# **Examples**

The frst of three data sets is analyzed using models that test possible autocorrelation and between-subject heterogeneity of the residual covariance structure at the frst level of a model.

This frst example is one in which covariates are not available for study; thus the example illustrates the utility of considering alternative residual covariance structures at the frst level of the model. The second and third data sets include individual diference measures that are studied in relation to learning. These two examples include individual diference measures that are used to study how such measures may serve as determinants of the diferent aspects of variation in responses at the subject level.

Each of the three examples involves response data that tend to follow nonlinear trends. One of the appealing aspects of ftting a growth model to repeated measures is that a large number of data values per subject may be summarized using a function that is parameterized by a relatively small number of coefficients. With the addition of random coefficients, the corresponding covariance structure imposed by a mixed-efects model is a parsimonious representation of the variances and covariances of the data. It may not be reasonable, however, to assume that conditional on the subject-specifc growth model that the residuals are independent. That is, although a given growth model may do well in summarizing trends in the individual-level responses, it may not be reasonable to assume that it completely addresses within-subject dependencies, especially given that a function based on a small number of parameters is used to summarize a relatively large number of data points. With a need to balance parsimony and interpretability in selecting a growth model, it may be reasonable to consider alternative covariance structures at the frst level of the model with the sensible acknowledgement that the imposed structure, including AR(1), is not assumed to be the specifc structure that generated the dependencies in the data, but rather, that the AR(1) process may help to better represent the correlation structure of the data.

### **Example 1: Performance on a complex procedural learning task**

Data from a procedural learning task described in Woltz [\(1988\)](#page-19-5) represent response latencies for 393 participants on 11 learning trial blocks (64 trials per block) (henceforth referred to as "trials") that occurred in one session. Data from the frst trial are excluded from analysis because it is assumed that these scores refect participants' adjustments to the task. Supplemental Table S1 gives descriptive statistics for trials 2–11. A plot of scores for 16 selected participants in Fig. [1](#page-5-0) suggests that response latencies decrease at a nonconstant rate as trials progress, with scores leveling off towards the latter part of the session. We fit a series of models to these scores while making diferent assumptions about the residual covariance structure at the trial level, including the addition of an  $AR(1)$  structure and heterogeneity of the residual variance.

Analysis of the frst data set began by ftting an exponential and a logistic growth function to the scores to test

which best accounted for the data while assuming that the trial-level residuals were independent, with constant variance across trials and subjects. Each function included three subject-specifc parameters representing the initial level, a lower asymptote, and a learning rate parameter. Responses were positively skewed within trials due to a subset of participants having relatively long response times. Given this, each function was applied to the data assuming that scores followed one of three response distributions— normal, gamma, or lognormal—with the latter two being continuous and positively skewed distributions. Based on the Akaike information criterion (AIC) and Bayesian information criterion  $(BIC)^{1}$  $(BIC)^{1}$  $(BIC)^{1}$  fit indices, the exponential growth function that assumed that the residuals were lognormal provided the best ft. Using log-transformed (base 10) scores (assumed to be normally distributed), this model was provisionally taken as the best ftting and used to test diferent assumptions about the residual covariance structure.

The exponential growth model for response  $y_{ii}$  was specifed as

<span id="page-4-1"></span>
$$
y_{ij} = \beta_{1i} - (\beta_{1i} - \beta_{0i})exp{-\beta_{2i}t_{ij}} + \varepsilon_{ij},
$$
\n(2)

where  $t_{ij}$  denotes the *j*<sup>th</sup> trial for subject *i*. For subject *i*,  $\beta_{0i}$ is the performance score at the first trial,  $\beta_{1i}$  is the potential performance level (lower asymptote), and  $\beta_{2i}$  is the rate parameter that combines with  $t<sub>ij</sub>$  to represent the learning rate. At the subject level, each coefficient was a function of a fxed and random efect:

$$
\beta_{0i} = \gamma_{00} + u_{0i},\tag{3a}
$$

<span id="page-4-2"></span>
$$
\beta_{1i} = \gamma_{10} + u_{1i},\tag{3b}
$$

<span id="page-4-3"></span>
$$
\beta_{2i} = \gamma_{20} + u_{2i},\tag{3c}
$$

where  $\gamma_{00}$ ,  $\gamma_{10}$ , and  $\gamma_{20}$  are the response level at the first trial, the potential performance level, and the rate parameter, respectively, for a subject whose random efects are equal to 0.

Next, we ft two sets of models using the exponential growth function in ([2](#page-4-1)). These are summarized here, followed by more detailed descriptions. Models in the first set were mixed-efects models and those in the second were mixed-efects location scale models. The frst model in each set assumed that the residuals were independent between trials, and the second in each set assumed that the residuals were correlated between trials. All three growth coefficients in the frst and second models of each set were random, as in  $(3a)$ – $(3c)$  $(3c)$ . The third model in each set assumed that the

<span id="page-4-0"></span> $1$  Singer and Willett [\(2003](#page-18-29)) recommend using the level 1 sample size in calculating the BIC =  $-2$ loglikelihood + ln(N)k, where *N* is the number of units at level 1.



<span id="page-5-0"></span>**Fig. 1** Response latencies on a procedural learning task for a selection of 16 participants

residuals were correlated between trials but that the rate parameter of the growth model was fxed. By ftting these particular models, we could test whether the growth function could be simplifed in terms of the number of random coefficients in exchange for using an  $AR(1)$  structure (cf. Chi & Reinsel, [1989](#page-18-4)) and whether there was evidence of heterogeneity of the residual variance across subjects. We next provide greater detail about these models.

In the first set of models, Model 1a assumed that the residuals in ([2](#page-4-1)) were i.i.d. normal and independent between trials with constant variance across the 10 trials:  $\mathbf{\Theta}_{\varepsilon} = \sigma_{\varepsilon}^2 \mathbf{I}_{10}$ , where  $\sigma_{\varepsilon}^2$  is the common variance. The covariance matrix of the random effects at the subject level was assumed to be homogeneous across subjects and specified as

$$
\Phi = \begin{bmatrix} \phi_{u_0}^2 \\ \phi_{u_1 u_0} & \phi_{u_1}^2 \\ \phi_{u_2 u_0} & \phi_{u_2 u_1} & \phi_{u_2}^2 \end{bmatrix},
$$
(4)

where  $\phi_{u_0}^2$ ,  $\phi_{u_1}^2$ , and  $\phi_{u_2}^2$  are the variances of the random intercept, asymptote, and rate parameter, respectively, and  $\phi_{u_1u_0}$ ,  $\phi_{u_2u_0}$ , and  $\phi_{u_2u_1}$  are their covariances.

In Model 1b, the residual covariance matrix was assumed to follow an AR(1) structure:

<span id="page-5-2"></span>
$$
\Theta_{\varepsilon} = \sigma_{\varepsilon}^{2} \begin{bmatrix} 1 & & & \\ \rho & 1 & & \\ \rho^{2} & \rho & 1 & \\ \vdots & \vdots & \vdots & \ddots \\ \rho^{9} & \rho^{8} & \rho^{7} & \cdots & 1 \end{bmatrix},
$$
(5)

<span id="page-5-1"></span>where  $\epsilon$  is a common variance assumed to be constant across trials and subjects and  $\rho$  is a fixed autocorrelation coefficient. The covariance matrix of the random effects of the growth model was assumed to have the same structure as in [\(4](#page-5-1)). Model 1c assumed the AR(1) residual structure in ([5\)](#page-5-2). The growth model assumed a random intercept and asymptote and a fxed rate parameter, thus reducing the dimensions of  $\Phi$ :

$$
\mathbf{\Phi} = \begin{bmatrix} \phi_{u_0}^2 \\ \phi_{u_1u_0} & \phi_{u_1}^2 \end{bmatrix}.
$$

The next set of models were mixed-efects location scale models. In Model 2a, the residuals were assumed to be independent between trials with constant variance across trials and between-subject heterogeneity of the residual variance:  $\mathbf{\Theta}_{\varepsilon_i} = \sigma_{\varepsilon_i}^2 \mathbf{I}_{10}$ , where

$$
\sigma_{\varepsilon_i}^2 = \exp(\tau_0 + \nu_i). \tag{6}
$$

The exponentiated value of  $_{\tau_0}$  is the residual variance for a subject whose random effect  $v_i$  is equal to 0. The random scale effect  $v_i$  accounts for heterogeneity of variance due to unmeasured sources and is assumed to be lognormally and independently distributed between subjects. Given the random scale effect in  $(6)$  $(6)$ , the covariance matrix of the random effects at the subject level includes the variance of the random scale effect and its covariances with the random growth coefficients:

$$
\Phi = \begin{bmatrix} \phi_{u_0}^2 & & \\ \phi_{u_1u_0} & \phi_{u_1}^2 & \\ \phi_{u_2u_0} & \phi_{u_2u_1} & \phi_{u_2}^2 \\ \phi_{vu_0} & \phi_{vu_1} & \phi_{vu_2} & \phi_{v}^2 \end{bmatrix},\tag{7}
$$

where  $\phi_{\nu}^2$  is the variance of the random scale effect. Its covariances with the random growth coefficients are the first three elements in the last row of the matrix.

In Model 2b, the covariance matrix of the residuals followed an AR(1) structure for which the residual variance could vary by subject:

$$
\Theta_{\varepsilon_{ij}} = \sigma_{\varepsilon_{ij}}^2 \begin{bmatrix} 1 & & & \\ \rho & 1 & & \\ \rho^2 & \rho & 1 & \\ \vdots & \vdots & \vdots & \ddots \\ \rho^9 & \rho^8 & \rho^7 & \cdots & 1 \end{bmatrix},
$$
(8)

where  $\sigma_{\varepsilon_{ij}}^2 = exp(\tau_0 + v_i)$ . The autocorrelation coefficient was assumed to be constant across subjects. In Model 2c, an AR(1) structure as specifed for Model 2b was assumed, and the rate parameter of the growth model was assumed to be fxed across subjects. The mean and covariance structures of Models 1a–1c and 2a–2c are summarized in Supplemental Table S4.

## **Results**

Point estimates and 95% confdence intervals (CI) for Models 1a–1c and 2a–2c are in Table [1](#page-7-0). When estimating these models, the variances at both levels were expressed by exponential functions, and so the calculated variances are provided in <span id="page-6-0"></span>the lower part of the table. Models are frst compared in terms of ft, and then conclusions are drawn. We frst compared Model 1a that assumed independence between the residuals and Model 1b that assumed an AR(1) structure. A deviance test comparing the models was significant  $(\chi^2(1 \text{ df}) = 148$ ,  $p < .001$ ), suggesting that dependencies in scores were not entirely accounted for by the growth function, and indeed, the estimated autocorrelation was .38. This result is consistent with a preference for Model 1b according to the AIC and BIC indices, where both indices are lower under Model 1b. We next compared the ft of Models 1a and 1c to test whether the number of random growth coefficients could be reduced in exchange for using an AR(1) structure (cf. Chi & Reinsel, [1989](#page-18-4)). That is, Model 1a is relatively complex due to the inclusion of three random growth coefficients, whereas Model 1c involves only two random growth coefficients and uses the AR(1) to help account for the dependencies of scores within subjects. Although the fit was better under Model 1c, suggesting that an  $AR(1)$  structure might be used to reduce the dimensionality of the model in terms of the number of random effects, the fit of Model 1b was best among the three, suggesting that the most complex model was preferred overall. Thus, assuming homogeneity of the residual variance across subjects, individuals difered in the three aspects of performance, but the subject-specifc growth model did not capture all of the within-subject dependencies in scores.

<span id="page-6-2"></span>Whereas Models 1a–1c are mixed-efects models that assumed homogeneity of the residual variance, Models 2a–2c are mixed-efects location scale models that permit between-subject heterogeneity of the residual variance. We compared the frst model of the two sets, Models 1a and 2a, which difer in that the former assumed homogeneity of the residual variance and the latter assumed between-subject heterogeneity. The deviance test<sup>[2](#page-6-1)</sup> was significant  $(\chi^2(4 \text{ d}t))$  $= 803, p < .001$ ), suggesting between-subject heterogeneity of the residual variance. Deviance tests between Models 1b and 2b and between 1c and 2c (not reported here) result in comparable conclusions about the need to permit heterogeneity of the residual variance.

We next compared the ft of Models 2a and 2c to test whether the number of random growth coefficients could be reduced in exchange for using an AR(1) structure. Similar to comparisons between models in the frst set, model ft according to the AIC and BIC values was better under Model 2c relative to 2a, suggesting again that an AR(1) structure might be used to reduce the dimensionality of the model in terms of the number of random effects. The ft of Model 2b, however, was the best (according to the AIC and BIC values) among the three, suggesting that

<span id="page-6-1"></span> $\overline{2}$  Here and where other deviance tests for a nonzero variance were carried out, a 50:50 mixture of  $\chi_q^2$  and  $\chi_{q+1}^2$ , where *q* is the number of random effects at the subject level, was used to calculate the *p*-value (Snijders & Bosker, [2012](#page-19-6)).



<span id="page-7-0"></span> $\mathcal{L}$  Springer

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the more complex model was preferred. Our overall conclusion about this performance measure is that there is evidence of individual diferences in the three aspects of performance, but the subject-specifc growth model did not fully capture the within-subject dependencies in scores, and there was signifcant within-subject variation about the subject-specifc performance trajectories.

For these data there were slight diferences in the estimated variances of the random growth coefficients between the models that allowed for autocorrelation between the level-1 residuals versus assuming independence and whether the model assumed heterogeneity of the residual variance or not (see Table [1\)](#page-7-0). More remarkable, however, was the difference in the estimated variance of the random scale effect, a value that indicates the extent to which individuals difer from each other with regard to the variance of the residuals about the subject-specifc trajectories. The estimated variance of the random scale efect was reduced from 2.63 under Model 2a that assumed independence of residuals between trials to 0.60 under Model 2b that assumed an AR(1) structure, suggesting the importance of considering an AR(1) structure when drawing inferences about the degree of between-subject heterogeneity of the residual variance. This result suggests that between-subject heterogeneity of the residual variance was due in part to dependencies between the residuals after accounting for systematic growth by the subject-specifc model, again illustrating the importance of accounting for autocorrelation in a growth process.

## **Example 2: Performance on a fight controller simulation task**

The second data set is from a study of motivation, cognitive abilities, and skill acquisition (Kanfer & Ackerman, [1989](#page-18-30)). For 140 participants, the set includes repeated measures on a fight controller simulation task and a battery of motivation and cognitive ability measures. The task was designed to measure skill acquisition during a 100-minute period. The repeated measures are the number of planes brought in safely every ten minutes. Scores for the frst trial are excluded from analysis, as it is assumed that participants used the frst trial to adjust to the task. Scores for trials 2–10 are analyzed here. Two individual diference measures, mathematics knowledge (MK) and coding speed (CS), are used to study how each is related to performance. The MK score refects general mathematical knowledge, including algebra and geometry. CS measures processing speed and accuracy by having subjects relate numbers in a list to information provided in a graph.

Descriptive statistics for the performance scores and individual diference measures are in Supplemental Table S2. The performance scores for 16 selected participants are displayed in Fig. [2](#page-9-0). In Harring and Blozis ([2014\)](#page-18-6), this set of scores was analyzed, and among the models tested, the

best ftting was one that assumed scores changed according to a negatively accelerated logistic function and the level 1 residuals followed an AR(1) structure, with the covariance structured assumed to be homogeneous across participants. Thus, from their analysis, the logistic function did not fully account for dependencies in the data, and as they showed, it was important to address this in the residual covariance structure by allowing scores between trials to correlate. This was especially important when drawing inferences about the variances of the random efects at the subject level because those estimates were impacted by the assumptions made about the residuals at the frst level.

For these data, we combine a mixed-efects model that includes an AR(1) structure with features of a mixed-efects location scale model. Specifcally, we use the same logistic function in Harring and Blozis ([2014](#page-18-6)) and add the betweensubject measures, MK and CS, to test their effects on specific aspects of learning. We relax the assumption of homogeneity of the residual covariance structure across subjects by including a random effect for the scale and autocorrelation coefficient, thus permitting the within-subject variance of the residuals and the autocorrelation coefficient to differ between subjects. Additionally, the variances of the random coefficients are studied as functions of the individual difference measures to test if the variances of the random growth coefficients are related to either of these measures.

A logistic growth function that included a random intercept  $\beta_{0i}$ , upper asymptote  $\beta_{1i}$  and rate parameter  $\beta_{2i}$  was applied to the performance measures:

<span id="page-8-3"></span>
$$
y_{ij} = \frac{\beta_{0i}\beta_{1i}}{\beta_{0i} + (\beta_{1i} - \beta_{0i})exp\{-\beta_{2i}(t_{ij} - 1)\}} + \varepsilon_{ij}.
$$
 (9)

For subject *i*,  $\beta_{0i}$  is the performance score at the first trial,  $\beta_{1i}$  is the potential performance level (upper asymptote), and  $\beta_{2i}$  is the rate parameter that, when combined with  $t_{ii}$ , governs the learning rate across trials. These coefficients were modeled as functions of MK and  $CS<sup>3</sup>$  $CS<sup>3</sup>$  $CS<sup>3</sup>$ :

<span id="page-8-1"></span>
$$
\beta_{0i} = \gamma_{00} + \gamma_{01} M K_i + \gamma_{02} C S_i + u_{0i}, \qquad (10a)
$$

$$
\beta_{1i} = \gamma_{10} + \gamma_{11} M K_i + \gamma_{12} C S_i + u_{1i}, \qquad (10b)
$$

<span id="page-8-2"></span>
$$
\beta_{2i} = \gamma_{20} + \gamma_{21} M K_i + \gamma_{22} C S_i + u_{2i},\tag{10c}
$$

where  $\gamma_{00}$ ,  $\gamma_{10}$ , and  $\gamma_{20}$  are the performance levels at the first trial, the potential level, and the rate parameter for a subject with MK and CS scores equal to their respective sample means. The coefficients  $\gamma_{01}$ ,  $\gamma_{11}$ , and  $\gamma_{21}$  are the effects of MK, holding constant the effects of CS, on the three learning coefficients, respectively. The coefficients  $\gamma_{02}$ ,  $\gamma_{12}$ , and  $\gamma_{22}$  are

<span id="page-8-0"></span><sup>&</sup>lt;sup>3</sup> MK and CS were centered about their respective sample means.



<span id="page-9-0"></span>**Fig. 2** Performance scores on a fight simulation task for a selection of 16 participants

the efects of CS, holding constant the efects of MK, on the three learning coefficients, respectively. The residuals of  $(10a)$ – $(10c)$  $(10c)$  $(10c)$ ,  $u_{0i}$ ,  $u_{1i}$ , and  $u_{2i}$ , are the respective subject-specifc efects that remain after accounting for the efects of MK and CS.

Four models were applied to the data using the growth function in ([9\)](#page-8-3) with the level-2 equations in  $(10a)$  $(10a)$ – $(10c)$  $(10c)$  $(10c)$ , with models differing according to the assumed covariance structure. The first two, Models 3a and 3b, were mixed-effects models that assumed homogeneity of the level 1 and level 2 covariance structures across subjects but differed in that Model 3a assumed that the residuals at the trial level were independent and Model 3b assumed that the residuals were correlated between trials (also see Harring & Blozis, [2014](#page-18-6)). The second two, Models 4a and 4b, were mixed-effects location scale models that assumed between-subject heterogeneity of the level 1 and level 2 covariance structures and differed in that Model 4a assumed that the residuals at the trial level were independent and Model 4b assumed that the residuals were correlated between trials. More details are given next.

Model 3a assumed that the residuals in ([9\)](#page-8-3) were i.i.d. normal and independent with constant variance across trials and subjects:  $\mathbf{\Theta}_{\varepsilon} = \sigma_{\varepsilon}^2 \mathbf{I}_9$ , where  $\sigma_{\varepsilon}^2$  is the common variance. The covariance matrix of the three conditional random efects in  $(10a)$  $(10a)$ – $(10c)$  $(10c)$  was assumed to be homogeneous across subjects, similar to  $(4)$  $(4)$  in the first example. In Model 3b, the residual covariance matrix at level 1 was assumed to follow an AR(1) structure similar to [\(5](#page-5-2)), assuming homogeneity of the residual variance and autocorrelation coefficient. Similar to Model 3a, the covariance matrix of the conditional random efects in  $(10a)$  $(10a)$ – $(10c)$  $(10c)$  was assumed to be homogeneous across subjects.

Model 4a was mixed-effects location scale model in which the level 1 residuals were assumed to be independent between trials with constant variance, but the variance could vary between subjects according to the measured covariates MK and CS and unmeasured sources:  $\mathbf{\Theta}_{\varepsilon_{ij}} = \sigma_{\varepsilon_i}^2 \mathbf{I}_9$ , where

$$
\sigma_{\varepsilon_i}^2 = exp(\tau_0 + \tau_1 MK_i + \tau_2 CS_i + v_i),
$$

where  $\tau_0$ , when exponentiated, is the residual variance for a subject whose MK and CS scores are each at their respective

sample mean, and  $v_i$  is equal to 0;  $\tau_1$  and  $\tau_2$  are the effects of MK and CS, respectively, on the exponent with each adjusted for the efect of the other. The random scale efect  $v_i$  is the residual that remains after accounting for the two measured variables and was assumed to be lognormally and independently distributed between subjects. Given the added random scale efect, the level 2 covariance matrix included the variance of the random scale and its covariances with the conditional random efects of the growth model, like that shown in ([7](#page-6-2)).

Model 4b was a mixed-efects location scale model that assumed correlated residuals at the trial level (similar to Model 3b) but allowed for between-subject heterogeneity of the covariance structures at levels 1 and 2. Specifcally, the covariance matrix of the residuals at level 1 was assumed to follow a random AR(1) structure:

$$
\mathbf{\Theta}_{\varepsilon_i} = \sigma_{\varepsilon_i}^2 \begin{bmatrix} 1 \\ \rho_i & 1 \\ \rho_i^2 & \rho_i & 1 \\ \vdots & \vdots & \vdots \\ \rho_i^8 & \rho_i^7 & \rho_i^6 & \cdots & 1 \end{bmatrix},
$$

 $\mathbf{r}$ 

where

$$
\sigma_{\varepsilon_i}^2 = exp(\tau_0 + \tau_1 MK_i + \tau_2 CS_i + v_i),
$$
  

$$
\rho_i = \rho + w_i,
$$

where the interpretation of the model for the within-subject variance  $\sigma_{\epsilon_i}^2$  was identical to that for Model 4a. The coefficient  $\rho$  is the autocorrelation coefficient for a subject whose random effect  $w_i$  is equal to 0;  $w_i$  is a random effect for the autocorrelation coefficient assumed to be approximated by a normal distribution. Given the random scale and random autocorrelation coefficient ( $v_i$  and  $w_i$ ) of the level 1 covariance structure and the three conditional random efects of the growth model  $(u_{0i}, u_{1i})$  and  $u_{2i}$  from [10a](#page-8-1) to [10c\)](#page-8-2), the covariance matrix at level 2 is as shown in (11) where, with the exception that the variance of each conditional random efect of the growth model is a function of the covariates, MK and CS:

$$
\Phi = \begin{bmatrix} \phi_{u_0}^2 \\ \phi_{u_1u_0} & \phi_{u_1}^2 \\ \phi_{u_2u_0} & \phi_{u_2u_1} & \phi_{u_2}^2 \\ \phi_{vu_0} & \phi_{vu_1} & \phi_{vu_2} & \phi_{vv}^2 \\ \phi_{wu_0} & \phi_{wu_1} & \phi_{wu_2} & \phi_{wv} & \phi_{w}^2 \end{bmatrix}
$$
(11)

$$
\phi_{u_0}^2 = exp\{\alpha_{00} + \alpha_{01}MK_i + \alpha_{02}CS_i\},
$$
  
\n
$$
\phi_{u_1}^2 = exp\{\alpha_{10} + \alpha_{11}MK_i + \alpha_{12}CS_i\},
$$
  
\n
$$
\phi_{u_2}^2 = exp\{\alpha_{20} + \alpha_{21}MK_i + \alpha_{22}CS_i\}.
$$

The mean and covariance structures of Models 3a, 3b, 4a, and 4b are summarized in Table S1.

### **Results**

The most complex of the four models was Model 4b. This model included a random scale efect and a random autocorrelation coefficient, thus allowing subjects to differ in the degree of variation of their residuals about their ftted trajectories and in the degree of autocorrelation between their residuals, respectively. For these data, the estimated variance of the random effect for the autocorrelation was very close to 0. From this, we concluded that subjects did not vary signifcantly in the autocorrelation parameter, and so Model 4b was simplified by assuming a fixed autocorrelation coefficient. Reports on Model 4b henceforth relate to this simplifed model. The estimates and 95% confdence intervals from the models are given in Table [2.](#page-11-0) As variances at both levels of each model were expressed using exponential functions, Table [2](#page-11-0) includes the calculated variances in the lower part of the table.

We frst examined the overall impact of including the autocorrelation residual structure in the mixed-efects models (Models 3a and 3b) and the mixed-efects location scale models (Models 4a and 4b). Models 3a and 4a assumed independence between the residuals and Models 3b and 4b assume an AR(1) structure. A deviance test comparing Mod-els 3a and 3b was significant<sup>[4](#page-10-0)</sup>, suggesting that dependencies in the scores were not entirely accounted for by the logistic growth function. The estimated autocorrelation under Model 3b was .39. Model 3b is also preferred to Model 3a according to the lower AIC and BIC indices under Model 3b. A significant deviance test comparing Models 4a and 4b ( $\chi^2(1)$  $df$  = 27.8,  $p$  < .001) and lower AIC and BIC values under Model 4b suggest that dependencies in the scores were not fully accounted for by the growth function. The estimated autocorrelation under Model 4b was .44. Thus, whether one is ftting a mixed-efects model or a mixed-efects location scale model, it can be important to test the assumption of independence between residuals at the frst level of a model.

Allowing for autocorrelation between the trial-level residuals impacted the estimated variances of the random efects at the subject level when comparing the mixedeffects models, as also documented elsewhere (e.g., Chi & Reinsel, [1989;](#page-18-4) Blozis & Harring, [2021](#page-18-3)). Under Models 3a and 3b, the estimated variance of the random intercept was 91.7 under Model 3a and increased to 137 under Model 3b. The variance of the random asymptote was 68.0 under Model 3a and decreased to 61.5 under Model 3b. The variance of the random rate parameter was 0.10 under both Models 3a and 3b. Despite diferences in the estimated

<span id="page-10-0"></span>
$$
^{4} \text{ (}\chi^{2} = 16.4, p = .5^{*}.004
$$

<span id="page-11-0"></span>**Table 2** ML estimates of a logistic growth model for flight simulation performance scores (n = 140)

	Mixed-effects model		Mixed-effects location scale model	
	Model 3a	Model 3b	Model 4a	Model 4b
Within-subject covariance structure	$\sigma_{\rho}^2 \mathbf{I}_9$	$AR(1)$ with $\sigma^2$	$\sigma_e^2 \mathbf{I}_9$	$AR(1)$ with $\sigma_{e_i}^2$
Fixed effects	MLE [95% CI]	MLE[95% CI]	<b>MLE[95% CI]</b>	MLE[95% CI]
Initial level, $\gamma_{10}$	18.4 [16.9, 19.8]	15.3 [14.1, 16.6]	16.2 [15.8, 16.7]	17.1 [16.1, 18.0]
$MK, \gamma_{11}$	$1.26$ [1.16, 1.36]	1.48 [1.35, 1.60]	$1.59$ [1.53, 1.65]	1.86 [1.69, 2.03]
$CS, \gamma_{12}$	$-0.26$ [ $-0.28$ , $-0.23$ ]	$-0.30[-0.34, -0.26]$	$-0.22$ [ $-0.26$ , $-0.20$ ]	$-0.19$ [ $-0.30$ , $-0.09$ ]
Asymptote, $\gamma_{20}$	39.5 [38.5, 40.5]	37.9 [36.4, 39.5]	39.1 [38.2, 39.9]	39.1 [37.6, 40.5]
MK, $\gamma_{21}$	0.59 [0.39, 0.79]	$0.62$ [0.29, 0.94]	$0.69$ [0.51, 0.87]	$0.65$ [0.30, 0.99]
CS, $\gamma_{22}$	$0.08$ [0.02, 0.15]	$0.05$ [ $-0.07, 0.17$ ]	$0.06$ [0.01, 0.11]	$0.09[-0.01, 0.19]$
Rate, $\gamma_{30}$	$0.69$ [0.62, 0.77]	$0.74$ [0.65, 0.82]	$0.72$ [0.67, 0.78]	$0.69$ [0.59, 0.78]
MK, $\gamma_{31}$	$-0.04$ [ $-0.04$ , $-0.03$ ]	$-0.04$ [ $-0.05$ , $-0.03$ ]	$-0.05$ [ $-0.06$ , $-0.04$ ]	$-0.04$ [ $-0.06$ , $-0.03$ ]
CS, $\gamma_{32}$	$0.003$ [0.002, 0.005]	$0.004$ [ $-0.002, 0.01$ ]	$0.003$ [0.0002, 0.01]	$0.001$ [-0.005, 0.007]
Within-subject covariance parameters				
$\tau_0$	2.22 [2.13,2.31]	2.55 [2.35, 2.74]	2.11 [1.94, 2.27]	2.54 [2.28, 2.79]
$MK, \tau_1$			$-0.04$ [ $-0.07$ , $-0.002$ ]	$-0.03$ [ $-0.06$ , 0.005]
CS, $\tau_2$			$0.01$ [ $-0.004$ , $0.02$ ]	$0.01$ [-0.01, 0.02]
ρ		.39		.44
Between-subject covariance parameters				
Intercept, $\alpha_{10}$	4.52 [4.37,4.67]	4.92 [4.75, 5.09]	4.50 [4.44, 4.55]	4.19 [4.05, 4.32]
$MK, \alpha_{11}$			$-0.08[-0.09, -0.07]$	$-0.12$ [ $-0.16$ , $-0.08$ ]
CS, $\alpha_{11}$			0.02[0.02, 0.03]	0.03[0.01, 0.04]
Asymptote, $\alpha_{20}$	4.22 [3.94,4.50]	4.12 [3.73, 4.50]	4.13 [3.94, 4.32]	3.85 [3.51, 4.20]
$MK, \alpha_{21}$			$-0.003$ [ $-0.04$ , 0.04]	$0.02$ [ $-0.05, 0.08$ ]
CS, $\alpha_{11}$			$0.01[-0.01, 0.02]$	$0.02$ [-0.01, 0.05]
Rate, $\alpha_{30}$	$-2.33$ [ $-2.56$ , $-2.10$ ]	$-2.27$ [ $-2.69$ , $-1.86$ ]	$-2.10[-2.29, -1.91]$	$-2.79[-3.36, -2.14]$
MK, $\alpha_{31}$			$-0.15$ [ $-0.18$ , $-0.13$ ]	$-0.25$ [ $-0.35$ , $-0.15$ ]
CS, $\alpha_{11}$			$-0.004$ [ $-0.01$ , 0.01]	$0.01$ [-0.01, 0.04]
Scale, $\alpha$ <sub>v</sub>			$-0.67$ [ $-1.07$ , $-0.26$ ]	$-1.13$ [ $-1.64$ , $-0.62$ ]
Corr $(u_2, u_1), \phi_{u_2u_1}$	.58	.67	.68	.59
Corr $(u_3, u_1)$ , $\phi_{u_3u_1}$	$-.56$	$-.63$	$-.60$	$-.46$
Corr $(u_3, u_2), \phi_{u_3u_2}$	$-.51$	$-.55$	$-.43$	$-.39$
Corr $(v, u_1)$ , $\phi_{vu_1}$			$-.32$	$-.31$
Corr $(v, u_2), \phi_{vu_2}$			$-.14$	$-.07$
Corr(v, $u_3$ ), $\phi_{vu_3}$			.19	.28
Additional variance estimates				
Residual, $\sigma_{e_0}^2$	9.21	12.7	7.9	12.7
Initial, $\phi_{u_1}^2$	91.7	137.	89.7	65.7
Asymptote, $\phi_{u_2}^2$	68.0	61.5	62.3	47.1
Rate, $\phi_{u_3}^2$	$0.10\,$	0.10	0.12	0.06
Scale, $\phi_v^2$			0.51	0.32
$-2lnL$	7346.3	7329.9	7291.8	7264.0
$\rm AIC$	7382.7	7369.0	7362.5	7337.9
$_{\rm BIC}$	7425.4	7414.0	7430.2	7407.4

MK = Math Knowledge, CS = Coding Speed (each centered to their respective sample mean). The within-subject covariance structures are as follows:  $\sigma_e^2 \mathbf{I}_9$  denotes independence between trials and homogeneity of variance across trial blocks and subjects;  $AR(1)$  with  $\sigma_e^2$  denotes a first-<br>order autocorrelation with constant variance across trial bloc across trial blocks and heterogeneity of variance between subjects;  $AR(1)$  with  $\sigma_{e_i}^2$  denotes a first-order autocorrelation with constant variance effects of MK and CS on the coefficients of the growth model, the general interpretations are similar.

Relative to Models 3a and 3b, Models 4a and 4b were far more complex because they permitted heterogeneity of the covariance structure at both levels of the model. We frst examined the estimates of the level 1 covariance structure for Models 4a and 4b. The estimated residual variance when both MK and CS were equal to their respective sample means was 7.9 under Model 4a and increased to 12.7 under Model 4b. The estimated effect of CS on the residual variance was close to 0 and not statistically signifcant under both Models 4a and 4b, and the efect of MK, also small in both models, was only signifcant under Model 4a. The most notable consequence of ignoring autocorrelation at the trial level was apparent when examining the point estimate of the variance of the random scale efect under Model 4a that assumed independence and Model 4b that assumed an AR(1) structure. The estimated variance of the random scale efect was reduced from 0.51 under Model 4a to 0.32 under Model 4b. Similar to the frst example presented in this paper, this result suggests that between-subject heterogeneity of the residual variance was due in part to dependencies between the residuals after accounting for growth by the subject-specifc model.

Unlike Models 3a and 3b that assumed homogeneity of the covariance structure at the subject level, Models 4a and 4b specifed that the variances of the conditional random growth coefficients to be functions of the measured covariates MK and CS, and consequently, the variances of the conditional random growth coefficients are the variances when both MK and CS are at their respective sample means. Given that the efects of MK and CS are signifcant, it is natural to expect that the estimated variances of the conditional coeffcients under Models 4a or 4b to difer from the estimates obtained under Models 3a or 3b, and indeed, the estimates do (see Table [2](#page-11-0)). Thus, we turn to study the impact of ignoring the autocorrelation in the trial-level residuals when interpreting the subject-level covariance structure.

We examined both the estimated variances of the conditional random growth coefficients and the effects of MK and CS on these variances. The estimated variance of the conditional random intercept was lower when the trial-level residuals are allowed to correlate: The estimated variance was 89.7 under Model 4a and was reduced to 65.7 under Model 4b. The estimated efects of MK and CS on this variance were also impacted by the trial-level covariance structure: The estimated effect of MK increased (in absolute value) from  $-0.08$  under Model 4a to  $-0.12$  under Model 4b; although slight, the estimated efect of MK increased from 0.02 under Model 4a to 0.03 under Model 4b. The degree of precision of the estimates decreased, however, when the trial-level residuals were allowed to correlate, as the estimated confdence intervals for the efects increased under Model 4b. Next, the estimated variance of the conditional asymptote was lower when the trial-level residuals

were allowed to correlate: The estimated variance was 62.3 under Model 4a and 47.1 under Model 4b. Although the estimated effects of MK and CS differed between Models 4a and 4b, neither were statistically signifcant under either model. Finally, the estimated variance of the conditional rate parameter was lower when the trial-level residuals were allowed to correlate: The estimated variance was 0.12 under Model 4a and 0.06 under Model 4b. The estimated effects of MK and CS also difered between Models 4a and 4b: the magnitude of the effect of MK increased from  $-0.15$  under Model 4a to  $-0.25$ under Model 4b, and although the estimated efect of CS differed between models, the efect was not statistically signifcant under either model. We again note the trade-off in fitting the more complex model by the decrease in the precision of the estimates evidenced by wider estimated confdence intervals.

### **Example 3: Performance on a quantitative skill acquisition task**

The third data set involves response latencies on a procedural learning task designed to measure quantitative skill acquisition<sup>[5](#page-12-0)</sup>. Participants were instructed to learn a set of declarative rules for evaluating characteristics of visual stimuli that were presented in a series of trials. Each of the 12 scores represents the median time to respond across a block of 32 trials. Scores for the frst trial block are not analyzed, assuming that participants were adapting to the task, leaving data for trials 2–12 for analysis. Included in a battery of individual diference measures was one of working-memory capacity obtained using a quantitative verifcation span paradigm. The quantitative working-memory capacity measure (QWM) is used to test how working memory capacity is related to learning acquisition.

Descriptive statistics for the response latencies and working-memory capacity are in Supplemental Table S3. Scores for 16 selected participants are displayed in Fig. [3.](#page-13-0) These scores were analyzed by applying a negatively accelerated exponential function, and like the preceding examples, alternative covariance structures are applied to understand the diferent sources of variation in performance scores, with working-memory capacity included in the models to test its relation to diferent aspects of learning and sources of score variation. We used the third data set to specifcally focus on the use of an AR(1) structure as a means for reducing the dimensionality of nonlinear mixed-efects and nonlinear mixed-efects location scale models. As the dimensionality of a mixed-efects model increases, so does the computational demands. Given the relative complexity of a mixed-efects location scale model to a mixed-efects model, researchers might consider this

<span id="page-12-0"></span><sup>5</sup> The data were provided by Scott Chaiken of the Armstrong Laboratory, Brooks Air Force Base.

#### **Table 2** (continued)

across trial blocks, homogeneity of the autocorrelation between subjects, and heterogeneity of variance between subjects



<span id="page-13-0"></span>**Fig. 3** Response latencies on a quantitative skill acquisition task for a selection of 16 participants

strategy to help improve the computational demands of ftting these models.

To begin, we applied three nonlinear mixed-efects models based on diferent growth functions to the performance scores. Among them, the exponential function<sup>[6](#page-13-1)</sup> in  $(2)$  $(2)$ , with each random coefficient specified as a function of QWM, provided the best ft:

$$
\beta_{0i} = \gamma_{00} + \gamma_{01} QWM_i + u_{0i}, \qquad (11a)
$$

$$
\beta_{1i} = \gamma_{10} + \gamma_{11} QWM_i + u_{1i}, \qquad (11b)
$$

$$
\beta_{2i} = \gamma_{20} + \gamma_{21} QWM_i + u_{2i}, \qquad (11c)
$$

<span id="page-13-3"></span>where  $\gamma_{00}$ ,  $\gamma_{10}$ , and  $\gamma_{20}$  are the performance levels at the first trial, potential level, and rate parameter, respectively, for a subject with QWM equal to the sample mean and whose random effects  $u_{0i}$ ,  $u_{1i}$ , and  $u_{2i}$  are equal to 0. The coefficients  $\gamma_{01}$ ,  $\gamma_{11}$ , and  $\gamma_{21}$ are the effects of QWM on the three learning coefficients. The residuals of  $(11a)$  $(11a)$ – $(11c)$ ,  $u_{0i}$ ,  $u_{1i}$ , and  $u_{2i}$ , are the subject-specific efects after accounting for the efects of QWM. This model, Model 5a, assumed that the trial-level residuals were i.i.d. normal and independent with constant variance across trials and subjects:  $\Theta_{\varepsilon} = \sigma_{\varepsilon}^2 \mathbf{I}_{11}$ , where  $\sigma_{\varepsilon}^2$  is the common variance.

<span id="page-13-2"></span>Next, we fitted Model 5b that assumed a fixed rate parameter to test whether a random rate parameter was needed. A deviance test between these models suggested that the rate parameter varied between subjects ( $\chi^2(3 \text{ df}) = 39, p < .001$ ). To then explore the idea of using an AR(1) structure to reduce the

<span id="page-13-1"></span><sup>6</sup> Based on AIC index values, the exponential function in Eq. ([2](#page-4-1)) yielded better ft to the data overall relative to a logistic function (Eq. [7\)](#page-6-2) and a Gompertz function:  $y_{ij} = \beta_{1i} exp\{ln(\frac{\beta_{2i}}{\beta_{1i}})exp\{-t\beta_{3i}\}\} + \epsilon_{ij}$ 

number of random effects, a third model, Model 5c, was fit that assumed an AR(1) structure at level 1 and a fxed nonlinear rate parameter. We then compared the ft of Model 5a that assumed all three growth coefficients were random and that the level-1 residuals were independent between trials to the ft of Model 5c that assumed two random growth coefficients (intercept and asymptote), a fixed rate parameter, and an  $AR(1)$  structure at the trial level. According to the AIC and BIC, model ft was relatively better under Model 5c, suggesting that an AR(1) structure might be used to reduce the number of random coefficients in a growth model, and consequently the total number of model parameters and computational demands, while achieving better overall model ft. The mean and covariance structures of Models 5a–5c are summarized in Supplemental Table S4. Estimates and ft indices for Models 5a–5c are in Table [3](#page-15-0).

Next, we followed a similar strategy in ftting models in the context of a mixed-efects location scale model. The frst model, Model 6a, was a mixed-efects location scale model in which the three growth coefficients were random, as in Model 5a; the level-1 residuals were assumed to be independent with constant variance across trials, but the variance could vary by subject according to QWM and unmeasured sources:  $\mathbf{\Theta}_{\varepsilon_{ij}} = \sigma_{\varepsilon_i}^2 \mathbf{I}_{11}$ , where

$$
\sigma_{\varepsilon_i}^2 = exp(\tau_0 + \tau_1 QWM_i + v_i),
$$

where  $\tau_0$ , when exponentiated, is the residual variance for a subject whose QWM score is equal to the sample mean and random scale effect  $v_i$  is equal to 0;  $\tau_1$  is the effect of QWM on the exponent. The random scale effect  $v_i$  is the residual after accounting for QWM and is assumed to be lognormally and independently distributed between subjects. Adding a random scale efect, the level 2 covariance matrix included the variance of the random scale and its covariances with the conditional random effects of the growth model, like [\(7](#page-6-2)).

A second model, Model 6b, assumed a fxed rate parameter so that we could test whether a random rate parameter was needed under this mixed-efects location scale model. A deviance test between Models 6a and 6b suggested that the rate parameter varied by subject  $(\chi^2(3 \text{ df}) = 30, p < .001)$ . We then reduced the complexity of the growth model by fxing the rate parameter and adding an AR(1) structure to create a third model, Model 6c, where it was assumed that the autocorrelation coefficient was fixed and the residual variance was random. We then compared the ft of Model 6a that assumed all three growth coefficients were random and the level-1 residuals were independent between trials to the ft of Model 6c that assumed two random growth coefficients (intercept and asymptote), a fixed rate parameter and an AR(1) structure. According to the AIC and BIC values, model ft was better under Model 6c, suggesting that an AR(1) structure could be used to reduce the number of random coefficients in a mixed-effects location scale model while improving model fit. Estimates, 95% confidence intervals,

and indices of model ft for Models 6a–6c are in Table [4](#page-16-0). The mean and covariance structures of Models 6a–6d are summarized in Supplemental Table S4.

## **Discussion**

The collection of repeated measures and longitudinal data is central for investigations that seek to understand change, development, or growth in measured behaviors. Mixed-efects models, a popular choice in statistical methodology, have evolved considerably since they were introduced in Laird and Ware [\(1982\)](#page-18-31). The advantages of this major statistical framework that unify models for the population-level response and that of the individual are now numerous, including, but not limited to, the specifcation of linear and nonlinear models and a wide range of response distributions, handling of missing data, and data observed at diferent times for diferent subjects.

In applying a mixed-efects model to data, it is important to consider the structures necessary to address sources of heterogeneity of variance, both within and between subjects. This may be done to improve statistical inference or model ft (Blozis & Harring, [2021;](#page-18-3) Chi & Reinsel, [1989;](#page-18-4) Ferron et al., [2002;](#page-18-5) Funatogawa & Funatogawa, [2018;](#page-18-17) Harring & Blozis, [2014;](#page-18-6) Sivo et al., [2005\)](#page-19-0). For instance, Chi and Reinsel show that neglecting serial correlation between level-1 residuals can result in overestimation of the variances of the random efects at the second level of a linear mixed-efects model, and Blozis and Harring showed how assumptions about the residual covariance structure (including serial correlations and heterogeneity of variance) can impact the estimated variances of the random efects at the subject level of a nonlinear mixed-efects model. Recommendations relating to statistical inference about the random-effects covariance structure at the subject level are that researchers consider alternative residual covariance structures at the frst level. This is especially relevant given recent developments in mixed-efects location scale models that specifcally aim to model heterogeneity of variance at both levels (Blozis et al., [2020](#page-18-23); Hedeker & Nordgren, [2013;](#page-18-22) Williams et al., [2019\)](#page-19-1).

Considering computational burden, we also considered a point of discussion in Chi and Reinsel [\(1989\)](#page-18-4) that concerned the application of linear mixed-efects models to repeated measures data. Specifcally, they discuss the use of an AR(1) structure for the level-1 residuals as a potential means to reduce the number of random effects needed to characterize a response. We explored this when fitting the nonlinear models here, including the nonlinear mixed-effects location scale models, as reducing the number of random coefficients could be helpful in reducing computational demands when ftting such complex models. Although this strategy was useful in the examples presented here, it is important to note that because one model provides a better ft than another, this is not to suggest that the best ftting model is the one that generated the data. It is simply that one might consider an alternative way

	Model 5a	Model 5b	Model 5c $AR(1)$ with $\sigma_a^2$	
Within-subject covariance structure	$\sigma_e^2 \mathbf{I}_{11}$	$\sigma_e^2 \mathbf{I}_{11}$		
Fixed effects	MLE [95% CI]	MLE [95% CI]	MLE [95% CI]	
Initial level, $\gamma_{10}$	2.46 [2.44, 2.48]	2.45 [2.42, 2.48]	2.47 [2.45, 2.50]	
QWM, $\gamma_{11}$	$-0.30$ [ $-0.39$ , $-0.21$ ]	$-0.30$ [ $-0.46$ , $-0.14$ ]	$-0.34$ [ $-0.46$ , $-0.21$ ]	
Asymptote, $\gamma_{20}$	2.00 [1.98, 2.03]	2.05 [2.02, 2.08]	2.06 [2.03, 2.09]	
QWM, $\gamma_{21}$	$-0.24$ [ $-0.31$ , $-0.17$ ]	$-0.30$ [ $-0.40$ , $-0.20$ ]	$-0.28$ [ $-0.40$ , $-0.16$ ]	
Rate, $\gamma_{30}$	$0.26$ [0.23, 0.30]	$0.24$ [0.22, 0.27]	$0.25$ [0.22, 0.28]	
QWM, $\gamma_{31}$	$-0.07$ [ $-0.13$ , $-0.01$ ]	$-0.19$ [ $-0.30, -0.08$ ]	$-0.17$ [ $-0.30$ , $-0.05$ ]	
Within-subject covariance parameters				
$\tau_0$	$-5.0$ [ $-5.0$ , $-4.9$ ]	$-4.9$ [ $-5.0, -4.8$ ]	$-4.8$ [ $-4.9$ , $-4.7$ ]	
$\rho$			.22	
Between-subject covariance parameters				
Intercept, $\alpha_{10}$	$-2.5$ [ $-2.6$ , $-2.3$ ]	$-2.5$ [ $-2.6$ , $-2.3$ ]	$-2.4$ [ $-2.6$ , $-2.2$ ]	
Asymptote, $\alpha_{20}$	$-3.1$ [ $-3.3$ , $-3.0$ ]	$-2.9$ [ $-3.1, -2.7$ ]	$-2.9$ [ $-3.1, -2.7$ ]	
Rate, $\alpha_{30}$	$-4.1$ [ $-4.4$ , $-3.8$ ]			
Corr $(u_2, u_1)$ , $\phi_{u_2u_1}$	.65	.72	.76	
Corr $(u_3, u_1)$ , $\phi_{u_3u_1}$	$-.16$			
Corr $(u_3, u_2)$ , $\phi_{u_3u_2}$	.09			
Additional variance estimates				
Residual, $\sigma_{e_0}^2$	0.007	0.007	0.008	
Initial, $\phi^2_{u_1}$	0.085	0.097	0.090	
Asymptote, $\phi_{u_2}^2$	0.044	0.058	0.054	
Rate, $\phi^2_{u_2}$	0.017			
$-2lnL$	$-3421$	$-3382$	$-3430$	
$\rm AIC$	$-3395$	$-3362$	$-3408$	
<b>BIC</b>	$-3352$	$-3329$	$-3372$	

<span id="page-15-0"></span>**Table 3** ML estimates of a mixed-effects model for quantitative skill acquisition scores (n = 204)

 $QWM = Q$ uantitative working-memory capacity (centered to the sample mean). The within-subject covariance structures are as follows:  $\sigma_e^2 \mathbf{I}_{11}$ denotes independence between trials and homogeneity of variance across trial blocks and subjects;  $AR(1)$  with  $\sigma_e^2$  denotes a first-order autocorrelation with constant variance across trial blocks and subjects;  $\sigma_{e_i}^2 \mathbf{I}_{11}$  denotes independence between trials, homogeneity of variance across trial blocks and heterogeneity of variance between subjects;  $AR(1)$  with  $\sigma_{e_i}^2$  denotes a first-order autocorrelation with constant variance across trial blocks, homogeneity of the autocorrelation between subjects, and heterogeneity of variance between subjects

of accounting for dependencies in the data. In the end, it is the individual researcher who makes the decision about how a model is to be specifed to test particular questions about a behavior. The models presented here offer alternative methods for specifying models to test or account for heterogeneity of responses.

Estimation of mixed-efects models can be carried out using ML and Bayesian approaches. Although the current paper relies on ML, there are advantages to considering a Bayesian approach (Lin et al., [2018\)](#page-18-8). For example, in one form of the model considered here, an AR(1) structure was applied to repeated measures data that permitted between-subject heterogeneity of the residual variance and the autocorrelation coefficient (see Example 2). The residual variance was modeled using an exponential function, and tests of covariate effects were carried out assuming that the efects were lognormal. Thus, this did not require special attention to the distributional assumptions made about the

coefficients of the variance model. Estimation of this model using PROC NLMIXED, however, assumed that the random effect corresponding to the autocorrelation coefficient was approximated by a truncated normal distribution (with lower and upper bounds to limit the distribution between -1 and 1). Using a Bayesian approach, such as by using the SAS PROC MCMC statistical software program (Chen, [2009](#page-18-32)) would increase fexibility in the assumptions made about random effects.

## **Appendix**

/\* SAS PROC NLMIXED is a procedure that can be used to estimate nonlinear mixed-efects models. For a two-level model, the default specifcation for the residual covariance

<span id="page-16-0"></span>**Table 4** ML estimates of a mixed-effects location scale model for quantitative skill acquisition scores (n = 204)

	Model 6a	Model 6b	Model 6c	
Within-subject covariance structure	$\sigma_e^2 \mathbf{I}_{11}$	$\sigma_e^2 \mathbf{I}_{11}$	$AR(1)$ with $\sigma_{e_i}^2$	
Fixed effects	MLE [95% CI]	MLE [95% CI]	MLE [95% CI]	
Initial level, $\gamma_{10}$	2.46 [2.43, 2.49]	2.48 [2.46, 2.49]	2.48 [2.46, 2.51]	
QWM, $\gamma_{11}$	$-0.29$ [ $-0.38$ , $-0.20$ ]	$-0.30[-0.39, -0.21]$	$-0.29$ [ $-0.42, -0.16$ ]	
Asymptote, $\gamma_{20}$	2.02 [1.99, 2.05]	2.08 [2.06, 2.10]	2.08 [2.05, 2.10]	
QWM, $\gamma_{21}$	$-0.35$ [ $-0.43$ , $-0.28$ ]	$-0.24$ [ $-0.31$ , $-0.17$ ]	$-0.24$ [ $-0.34$ , $-0.13$ ]	
Rate, $\gamma_{30}$	$0.26$ [0.22, 0.29]	$0.26$ [0.24, 0.29]	$0.27$ [0.24, 0.30]	
QWM, $\gamma_{31}$	$-0.20$ [ $-0.31, -0.10$ ]	$-0.14$ [ $-0.24$ , $-0.05$ ]	$-0.16$ [ $-0.27, -0.04$ ]	
Within-subject covariance parameters				
$\tau_0$	$-5.1$ [ $-5.3$ , $-5.0$ ]	$-5.1$ [ $-5.2$ , $-5.0$ ]	$-5.0$ [ $-5.1$ , $-4.9$ ]	
QWM, $\tau_1$	$-0.48$ [ $-1.0, 0.06$ ]	$-0.34$ [ $-0.84$ , 0.16]	$-0.38$ [ $-0.89$ , 0.14]	
			.22	
Between-subject covariance parameters				
Intercept, $\alpha_{10}$	$-2.7[-2.9, -2.6]$	$-2.7[-2.7, -2.6]$	$-2.6[-2.8, -2.5]$	
QWM, $\alpha_{11}$	$-0.67$ [ $-1.1, -0.24$ ]	$-0.78$ [ $-1.2, -0.37$ ]	$-0.64$ [ $-1.2, -0.04$ ]	
Asymptote, $\alpha_{20}$	$-3.4[-3.7, -3.2]$	$-3.0[-3.1, -2.9]$	$-3.0[-3.1, -2.9]$	
QWM, $\alpha_{21}$	$-0.02$ [ $-0.68$ , 0.63]	$-0.18$ [ $-0.61$ , 0.25]	$-0.17[-0.83, 0.48]$	
Rate, $\alpha_{30}$	$-4.4[-4.7, -4.2]$			
QWM, $\alpha_{31}$	$0.71$ [-0.50, 1.9]			
Scale, $\alpha$ <sub>v</sub>	$-0.47$ [ $-0.63$ , $-0.33$ ]	$-0.49$ [ $-0.66$ , $-0.35$ ]	$-0.48$ [ $-0.64$ , $-0.33$ ]	
Corr $(u_2, u_1)$ , $\phi_{u_2u_1}$	.64	.67	.69	
Corr $(u_3, u_1)$ , $\phi_{u_3u_1}$	$-.23$			
Corr $(u_3, u_2), \phi_{u_3u_2}$	.02			
Corr(v, $u_1$ ), $\phi_{vu_1}$	.36	.42	.43	
Corr(v, $u_2$ ), $\phi_{vu_2}$	.45	.56	.58	
Corr(v, $u_3$ ), $\phi_{vu_3}$	$-.35$			
Additional variance estimates				
Residual, $\sigma_{e_0}^2$	0.006	0.006	0.007	
Initial, $\phi_{u_1}^2$	0.064	0.070	0.071	
Asymptote, $\phi^2_{u_0}$	0.032	0.051	0.049	
Rate, $\phi_{\mu}^2$	0.012			
Scale, $\phi^2$	0.39	0.37	0.39	
$-2lnL$	$-3613$	$-3583$	$-3637$	
$\rm AIC$	$-3571$	$-3551$	$-3603$	
BIC	$-3501$	$-3498$	$-3546$	

 $QWM =$  Quantitative working-memory capacity (centered to the sample mean). The within-subject covariance structures are as follows:  $\sigma_e^2 \mathbf{I}_{11}$ denotes independence between trials and homogeneity of variance across trial blocks and subjects;  $AR(1)$  with  $\sigma_e^2$  denotes a first-order autocorrelation with constant variance across trial blocks and subjects;  $\sigma_{e_i}^$ blocks and heterogeneity of variance between subjects;  $A_{R(1)}$  with  $\sigma_{e_i}^2$  denotes a first-order autocorrelation with constant variance across trial blocks and heterogeneity of variance between subjects;  $A_{R(1)}$  wit blocks, homogeneity of the autocorrelation between subjects, and heterogeneity of variance between subjects

structure at the frst level is that the residuals are independent within and between level-2 units. The GENERAL model statement is used to specify alternative residual covariance structures.

Below is syntax for ftting a logistic growth model to a set of performance scores from the fight simulation task (the second example presented in the paper). The data set includes 9 repeated measures for each of 140 subjects. Two individual diference covariates, Mathematics Knowledge (MK) and Coding Speed (CS), are included in the models; each is centered about their respective sample mean. The within-subject residuals are assumed to be normally distributed.

Each script corresponds to the models reported in the manuscript for the second example. \*/

```
alp00 4.1658
alp01 -0.09845
alp02 0.004995
rho10 0.6007
alp10 3.8947
alp11 0.01609
alp12 0.02062
rho20 -0.3513
rho21 -0.4187
alp20 -2.5532
alp21 -0.1446
alp22 0.007881
rhov0 -0.1769
rhov1 0.02015
rhov2 0.05191<br>alpv -0.892
     -0.892tau0 2.3015
tau1 -0.0297
tau2 0.004737
rho 0.3143;
covariates and a random scale effect vi;
s2e=exp(tau0 + tau1*gm MK + tau2*gm CS + vi);
sdv=sqrt(exp(alpv));
sd0=sqrt(exp(alp00 + alp01*gmMK + alp02*gmCS));sd1=sqrt(exp(a1p10 + alpha11*qmMK + alpha12*qmCS));
sd2=sqrt(exp(alp20 + alp21*gmMK + alp22*gmCS));ni=9; ln2pi = 1.8378770664; 
rho2 =rho * rho;
ka = 1 / (1 - rho2);kb = -ka * rho;kc = ka * (1 + rho2);f0 = b00 + b01*gm MK + b02*gm_CS + u0;
f1 = b10 + b11*gmMK + b12*gmCS + u1;f2 = b20 + b21*gmMK + b22*gmCS + u2;yh = (f0*f1)/(f0+\sqrt{(f1-f0)*exp(-f2*(x[1])))};e[1] = y[1] - yh;w2=0; w3=0;
do j = 2 to ni;
f0 = b00 + b01*gm MK + b02*gm CS + u0;
f1 = b10 + b11*qm MK + b12*qm CS + u1;
f2 = b20 + b21*gm_MK + b22*gm_CS + u2;yh = (f0*f1)/(f0+\sqrt{(f1-f0)*exp(-f2*(x[j])))};e[j] = y[j] - yh;w2 = w2 + e[j] * e[j-1];w3 = w3 + e[j]*e[j];end;
w1 = e[1] * e[1] + e[ni] * e[ni];w3 = w3 - e[ni]*e[ni];quad = (ka * w1 + 2 * kb * w2 + kc * w3) / s2e;lndet = ni * log(s2e) + (ni-1) * log(1-rho2);*loglikelihood;
Li = -0.5 * (ni * ln2pi + lndet + quad);
dm=1;model dm ~ general(Li);
random u0 u1 u2 vi ~ normal([0, 0, 0, 0],
[sd0*sd0,
 rho10*sd0*sd1,sd1*sd1,
  rho20*sd0*sd2,rho21*sd1*sd2,sd2*sd2,
 rhov0*sd0*sdv,rhov1*sd1*sdv,rhov2*sd2*sdv,sdv*sdv])subject=subj;
bounds -1 \le rho10 rho20 rhov0 rhov1 rhov2 rho21 \le=1;
```
 $b22 -0.00202$ 

**Supplementary Information** The online version contains supplementary material available at<https://doi.org/10.3758/s13428-023-02133-1>.

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