Latent Differential Equation Modeling with Multivariate Multi-Occasion Indicators

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Abstract

A number of models for estimating the coefficients of dynamical systems have been proposed. One is the exact discrete model, another is the latent differences model or proportional change model, and a third is a continuous time manifest variable differential structural model. These models differ from standard growth curve modeling in that they intend to illuminate processes generating individual trajectories over time rather than just estimate an aggregate best trajectory. The current work proposes a novel approach to the modeling of multivariate change by first creating a lagged covariance matrix. Then rather than using factor loadings to estimate average growth characteristics as in other growth curve modeling related methods, confirmatory factor loadings are fixed across the time dimension and freed across the variables dimension, in such a way as to force the factor scores to estimate instantaneous derivatives. Then, the factor covariances are structured as a regression that allows the estimation of parameters of differential equation models of dynamical systems theories proposed to account for the data. Results of a simulation will be presented illustrating strengths and weaknesses of the latent differential equation model.

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Introduction

In the behavioral sciences, there is increasing interest in understanding and characterizing mechanisms of developmental and behavioral processes. Measurements of multiple indicators obtained on multiple occasions on a single individual may show some intraindividual change and intraindividual variability. Process–oriented theories may predict structural patterning in these ideographic measurements. Structural equations modeling techniques can be used to test such theories by fitting confirmatory models of the implied dynamical systems to repeated observations data. The current chapter explores one method for constructing and testing confirmatory latent variable structural models in which the latent constructs (a) evolve continuously over time and (b) have linear relationships between their derivatives. The method appears to generalize well and is expected to be able to be applied to systems well beyond the simple example presented here. The chapter will begin with a rationale for studying behavioral processes from a dynamical systems perspective, introduce latent differential equations confirmatory factor models, present the results of two simulations testing the viability of this model for estimating parameters of a simple linear system, and then discuss future substantive and methodological questions that this line of modeling may address.

Self–Regulating Systems

For the purposes of this chapter we will define a *psychological process* as the time–evolving evidence of some behavioral or developmental mechanism. A psychological process will be assumed to have associated with it a set of indicator variables that change over time in a way that is at least partially determined by the behavioral or developmental mechanism. One can consider this definition of a psychological process in terms of one or more latent variables whose values change in some, at least partially, deterministic way. The lawfulness of these changes is then considered to be evidence in support of a behavioral or developmental mechanism.

One form that psychological processes may take is that of a *self–regulating system*. Self–regulation involves the notion that changes in a system have orderly and lawful relations even in the absence of exogenous effects. Many psychological processes may fit within the framework of self–regulation. Some possible examples of self–regulating psychological processes include lifespan development of cognitive abilities (Donaldson & Horn, 1992; McArdle, Hamagami, Meredith, & Bradway, in press), adolescent substance abuse (Boker & Graham, 1998), self–reported mental health in recent widowhood (Bisconti, 2001), or anxiety levels of children (Cummings & Davies, 2002).

Self–regulation can be partitioned into two main categories: active and passive. A physical example of an active self–regulating system might be the heating and cooling system in a building. This temperature control system is self–regulating and has active elements: one or more temperature sensors, heat sources, cooling sources and perhaps fans for moving the air within the building. When temperature sensors indicate a measurement that differs from the desired equilibrium state of the system, active elements are engaged such that a change in temperature is effected in the building. This change is read by the sensor and some further activity is triggered. Active self–regulation generally implies some sort of sensor–effector feedback mechanism.

One physical example of a, passive self–regulating system is a pendulum with friction in the earth's gravitational field. If the pendulum is raised to one side and let go, the result is a regular oscillation until friction finally damps the velocity of the pendulum to its motionless equilibrium state along the axis between the pivot of the pendulum and the center of the earth. Although lawful relationships exist relating changes in the pendulum's motion to its current distance from equilibrium, there is no active sensor mechanism turning on and off an effector that pushes the pendulum first in one direction and then the other. The movement of the pendulum is a passive response to the unchanging gravitational field in which it embedded.

Consider the behavior of the system shown in Figure 1–a. The value of the variable (here labeled "displacement") starts as a positive number and then as time progresses, the value first becomes negative, then positive, then negative again; oscillating back and forth around an equilibrium point of zero displacement. Eventually, the oscillations are damped to nearly zero. The curve shown in Figure 1–a is called a *trajectory*; it describes the behavior of a single individual instance of a system. Note that when time is equal to zero, this trajectory has a value for its displacement. Also note that at time=0 there is a slope to the curve. These two values, the displacement and slope (or first derivative of displacement) are called the *initial values* for the trajectory (here $x = 10$, $\dot{x} = 0$). Every trajectory, that is every individual instance, of this system has a set of initial values — that is the state of the system at an arbitrarily assigned time of zero.

In Figure 1–b, the value of displacement (here labeled x) and its first derivative (here labeled $\dot{x}$) are plotted against one another for the same trajectory shown in Figure 1–a. The outer end of the spiral at $(x = 10, \dot{x} = 0)$ again represents the initial conditions for this trajectory. The regularity of the spiral demonstrates that there is a relationship between the displacement (x) and its first derivative ($\dot{x}$) with respect to time. However, this relationship alone does not determine the system, since for any value of x there is more than one possible value of $\dot{x}$.

In order to completely describe this system at some time t, one needs also to take into account the curvature (second derivative of x with respect to time) of the trajectory at time t. One way to visualize this is by the use of a *vector field* (Boker & McArdle, in press) as shown in Figure 1–c. Here we see an eleven by eleven grid of arrows. The tail of each arrow is located at one point in an eleven by eleven grid of initial conditions of x and $\dot{x}$. The head of the arrow points to where a trajectory would be a short interval τ later in time. Arrows that point straight up or straight down have not changed their value of $\dot{x}$. Since the second derivative of x (written as $\ddot{x}$) is the change in $\dot{x}$, these vertically oriented arrows represent initial conditions in which the trajectory had no curvature, i.e. initial conditions in which $\ddot{x} = 0$ during the interval of time τ.

Similarly, horizontal arrows in Figure 1–c represent initial conditions for which there was no change in x during the interval τ. Thus, these initial conditions had an average derivative, $\dot{x}$, of zero. It turns out that for this system, if we know the value of x and $\dot{x}$ at time t then we can exactly calculate the value for $\ddot{x}$ at time t. The way that these three quantities evolve over time will remain symmetric; that is, when one gets larger another gets proportionally smaller so that a weighted sum of x, $\dot{x}$, and $\ddot{x}$ will always be equal to zero.

It is important to note at this point that active and passive *mechanisms* for self–

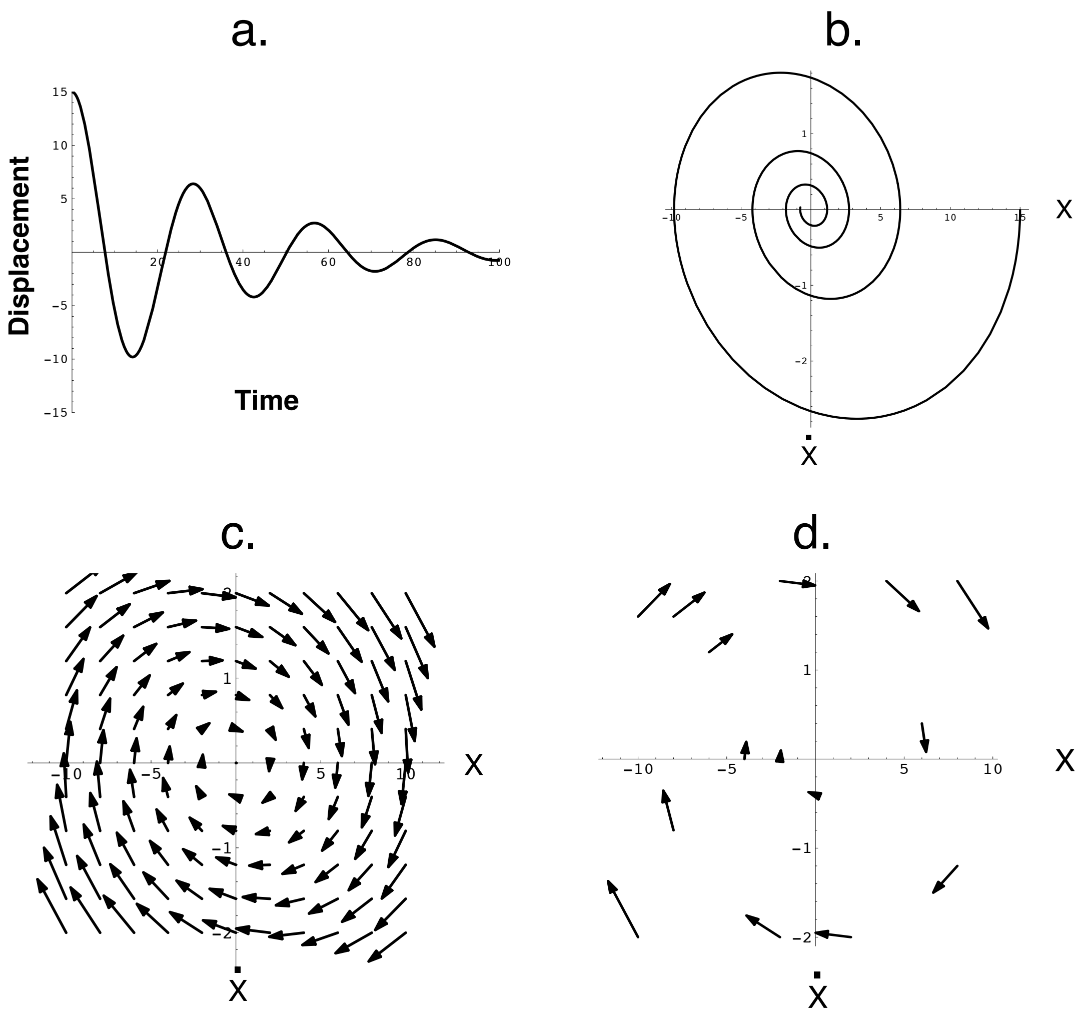

Figure 1. Four views of a damped linear oscillator. (a) A single trajectory: the evolving values over time of displacement from equilibrium for a single set of initial conditions. (b) A phase space: the evolving values over time of both displacement and the first derivative of displacement plotted against one another for a single set of initial conditions. (c) A vector field: the evolving values over one time step of an 11×11 grid of values of initial conditions of both displacement and the first derivative of displacement, and (d) A sample of initial conditions displayed as a vector field

regulation do not necessarily result in different self–regulating *processes*. For any observed process there might be many self–regulating mechanisms which could have generated the data. For instance, the same set of relationships between derivatives that produced the trajectories in the graphs in Figure 1 might have resulted from either an active or passive mechanism. The methods discussed in this chapter can be used to falsify hypotheses about processes. One must be careful to recall that in so doing, we may not necessarily falsify a corresponding hypothesis about mechanisms since the mapping from underlying mechanisms to observed processes can be many to one. The methods we discuss provide estimates of parameters of *intrinsic dynamics* of a hypothesized system, in other words parameters of a system that exhibits a self–regulating process.

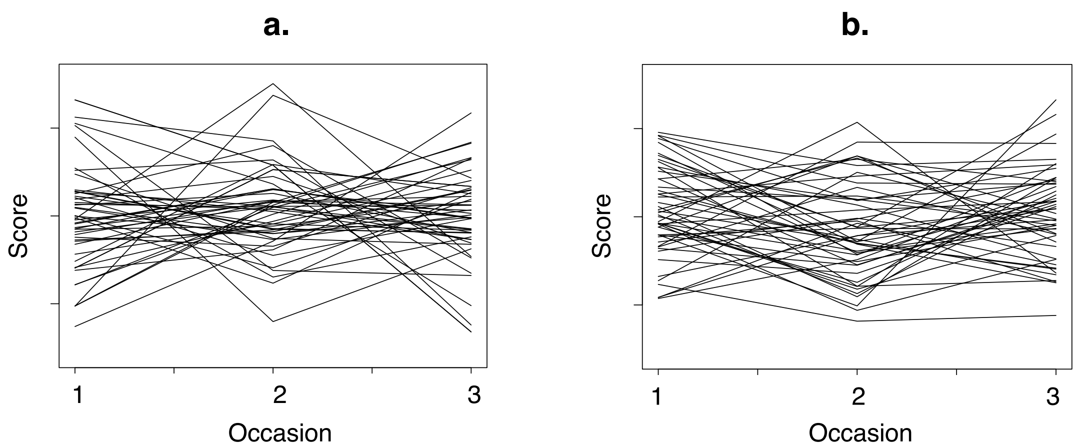

Figure 2. Measured values from three occasions from 100 instances of two different processes. (a) A random sample of initial conditions and three observations from a damped linear oscillator process. Each observation at occasions 2 and 3 is completely determined by the initial conditions at occasion 1. (b) A random sample from normally distributed random numbers. All observations at all occasions are independent of one another. In this case, a null hypothesis of no underlying process is true.

In Figure 1–d is displayed the trajectory evolution over a short interval of time τ of a random sample of initial conditions. Essentially, it is a random sample from the vector field displayed in Figure 1–c. This is the sort of data with which we are concerned: relatively few observations per individual and a random sample of individuals who may each have their own initial conditions. These initial conditions may be independent of the self–regulating psychological process which we wish to understand and for which we wish to quantify parameters. Such data might be represented by the graphs shown in Figure 2. In Figure 2–a are three observations drawn from 100 instances of the system shown Figure 1. In Figure 2–b are three observations drawn from 100 instances of normally distributed random numbers. All of the observations in Figure 2–b are independent: essentially measurement error. Any method that shows promise, must be able to reliably distinguish between these two cases. That is to say, if factor scores exhibit no deterministic change within individual, we must not mistake observed change for a self–regulating process.

Differential Equations Models

In the physical sciences, models of processes typically take the form of differential equations. Differential equations describe the relationships between the value of a variable and its derivatives with respect to time. Thus, if there were a proportional relationship between the value of a variable's displacement from equilibrium and its instantaneous slope, when displaced from equilibrium by some exogenous force, the variable would return to equilibrium with a trajectory that was exponential in shape. This is the differential equation form of a model also known as the *proportional change model* (see McArdle & Hamagami, this volume) and in a discrete time form is the autoregressive model with fixed coefficients over time.

One benefit to fitting differential equations models accrues in comparison with growth curve models (e.g. McArdle & Epstein, 1987). One way of thinking of growth curve models is that they estimate a single best aggregate trajectory for a differential equations model. Since each trajectory has its own set of initial conditions, this implies that a growth curve model is estimating a single best set of parameters as well as a single best set of initial conditions. A growth curve approach is useful if one is interested in finding this best trajectory (growth curve) and if the initial conditions for each individual are in relation to a reference time with a meaningful zero (such as date of birth) that can be meaningfully compared across individuals. However, when there is no reference time that can be used to equate individuals with respect to the dynamic of the system of interest, growth curves can confound individual differences in initial conditions with individual differences in the parameters for the curves (see Boker & Bisconti, in press, for examples). Fitting lagged state space models bypasses this problem since initial conditions need not be estimated. Examples of state space methods include the method proposed in this chapter, discrete time models (e.g. Jones, 1993), forms of dynamic factor analysis (e.g. Molenaar, 1985), or stochastic differential equations (e.g. Oud & Jansen, 2000)) In these models individual differences in initial conditions are not confounded with individual differences in the dynamics of the behavior since time is only treated as relative to other measurements. Thus state space models have a distinct advantage when the initial conditions may be due to unknown exogenous influences: a participant in a study may have an essentially random state when he or she begins an experimental protocol, but changes in behavior during the protocol may be reliable (see Boker & Nesselroade, 2002, for a more complete discussion of this so–called *phase problem*).

For the purposes of this chapter, we will consider one of the simplest differential equations: the damped linear oscillator. Many other examples of this differential equations models exist (see e.g. Hubbard & West, 1991; Thompson & Stewart, 1986, for introductions). Suppose there exists a latent variable F with a particular form of intrinsic dynamics such that at every time t

$$\ddot{F} = \zeta \dot{F} + \eta F + e_F \tag{1}$$

where the residual e_F is normally distributed with mean zero. Further suppose that the latent variable exhibits a factor structure such that

$$\begin{aligned} x_{ij} &= 1F_{ij} + u_{xij} \\ y_{ij} &= aF_{ij} + u_{yij} \end{aligned} \tag{2}$$

$$z_{ij} = bF_{ij} + u_{zij}$$

where x, y, and z are manifest indicators of F measured on individual i at occasion j, 1, a, and b are the factor loadings, and u_x, u_y, and u_z are the corresponding uniquenesses. The factor loading for x is constrained to be 1 in order to identify the scale of the latent variable F. In this way, we have defined a factor whose score changes over time such that it obeys the intrinsic dynamic characteristic of a damped linear oscillator. The two parameters η and ζ have useful meanings. The parameter η is proportional to the square of the frequency ω of oscillation such that $\eta = -(2\pi\omega)^2$. The parameter ζ is the damping parameter and when ζ is negative, it is similar to the "friction" of a swinging pendulum. When ζ is positive, it amplifies change in the system such that small perturbances at any given time tend to lead to larger changes later.

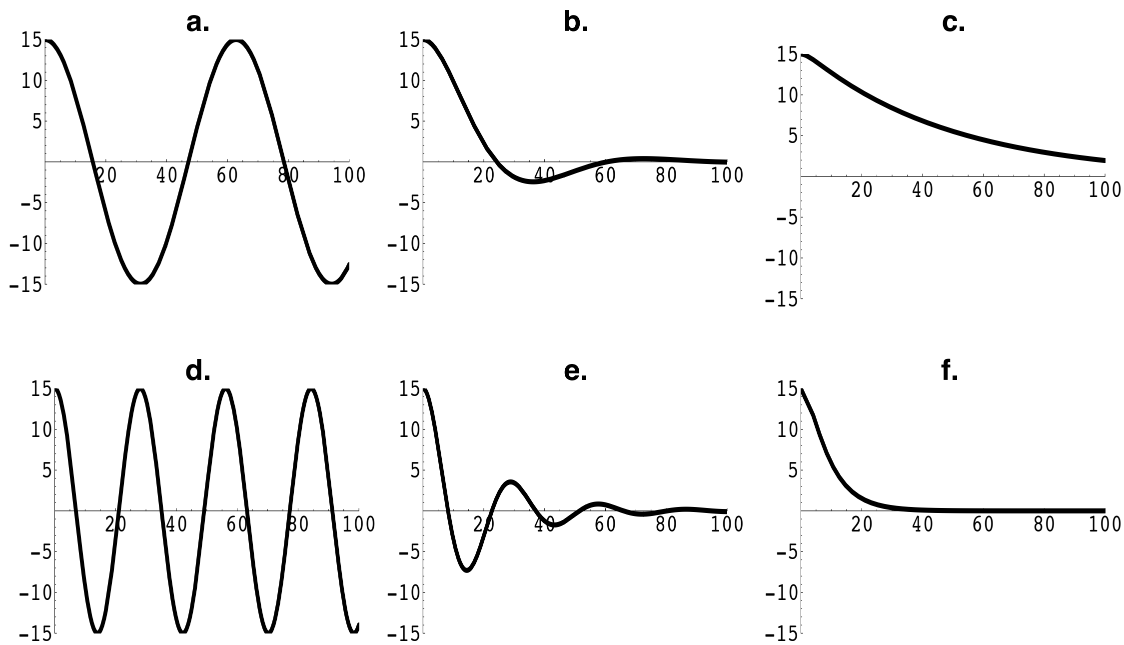

Figure 3. Six example trajectories for the latent variable F that conform to Equation 1. Trajectories (a) and (d) have slow and fast frequencies respectively, but have no damping, i.e. are "frictionless". Trajectories (b) and (e) have slow and fast frequencies with moderate damping. Trajectories (c) and (f) have slow and fast frequencies with high damping.

Figure 3 plots six possible trajectories that all conform to Equation 1, but which have differences in their values of η and ζ. The graphs in each row of Figure 3 have the same value of η but different values of ζ. The graphs in each column of Figure 3 have the same value of ζ but different values of η. The top row has a value of η that is closer to zero than the bottom row and thus the top row exhibits slower oscillations than the bottom row of graphs. In the leftmost column $\zeta = 0$, the value of ζ is a small negative number in the middle column, and a larger negative number in the rightmost column.

Of course factor scores are unobservable, so we are not able to estimate individual trajectories. We do not wish to estimate some optimum aggregate trajectory of these factor scores since that implies an estimation of the unobservable initial conditions of the trajectory. Instead, we wish to estimate the parameters of Equation 1, which are functions of the covariances between the factor and its derivatives. To do so, we will take advantage of the fact that covariances between latent variables can be estimated even when the latent scores themselves are unknown.

In the next section, we will place this method in context by first presenting a brief discussion of a two–step univariate manifest variable method called Local Linear Approximation (LLA). We will next extend that to the case of a Univariate Latent Differential Equation (ULDE). We will then present the Multivariate Latent Differential Equation (MLDE) model that can simultaneously estimate the parameters from Equations 1 and 2. Results of a simulation testing the viability of the MLDE model for estimation of parameters of a known system will be presented. A second simulation will test whether the MLDE model will give an answer that is incorrect when presented with factors that have no time deterministic structure (as in Figure 2–B). Finally, we will discuss potential applications of this method to more complex coupled systems and nonlinear models.

Local Linear Approximation

One approach to estimating the intrinsic dynamics of a psychological process is to first estimate the derivatives of the process for each occasion of measurement and then fit either a regression model (Boker & Nesselroade, 2002), a structural model (Boker, 2001), or multilevel model (Boker & Ghisletta, 2001) to those resulting variables. This approach has advantages and disadvantages. The two main advantages to estimating derivatives prior to estimating the dynamical parameters of a system are a great degree of flexibility in specifying the structure of the differential equation model and being able to use a wide variety of off–the–shelf estimation procedures. One method for estimating derivatives from manifest variable processes is Local Linear Approximation (LLA).

LLA assumes that the process can be approximated linearly over short intervals of time and that the derivatives at a time t can be estimated from measurements occuring within some small interval τ of the chosen time t. First the slopes between measurements at time $t-\tau$ and $t+\tau$ are calculated and then the estimates of the first and second derivatives at time t are given by the average of these two slopes and the change in these two slopes respectively. This simple–minded estimation of the derivatives can do remarkably well in estimating dynamical parameters.

While LLA has the advantage of using only three occasions of measurement to estimate the derivatives, it can prove to have biased estimates of the dynamical parameters when the interval τ is not optimal (Boker & Nesselroade, 2002). In addition, measurement error can masquerade as high frequency signal. While there are indications that there may be solutions to these technical problems, LLA is at the core a manifest variable method. If one is interested in the dynamics of a variable for which a score cannot be directly observed, then LLA is inappropriate. In this case we would wish to have a measurement model for such a latent construct.

Univariate Latent Differential Equation Model

There are two ways that measurement models are commonly constructed, either across variables as in a factor model or across time as in a latent growth curve model. We will start by building a measurement model across time, but with some differences from the standard growth curve approach. In most common forms of latent growth curve modeling, one allows one or more degrees of freedom in the loadings for each latent curve variable and also allows the latent variables to freely covary. In the latent differential equation approach, we allow no degrees of freedom in the loadings for the latent variables, constraining the loadings in such a way that the latent variables are estimates of the derivatives of the time series. This part of the approach is similar to Savitzky–Golay filtering (Savitzky & Golay, 1964). Then, we use the covariances between these latent derivatives to estimate regression parameters between them.

Suppose that we have measured a variable x at four equally spaced occasions separated by an interval of time τ on a sample of N subjects resulting in an $N \times 4$ data matrix $\mathbf{X}$. Now consider the three matrices $\mathbf{L}$, $\mathbf{A}$, and $\mathbf{S}$ defined in Equations 3, 5, and 6 below. A loading matrix $\mathbf{L}$ is constructed such that it will estimate the value of x, its first derivative, and second derivative at the time midway between the second and third occasions of measurement.

$$\mathbf{L} = \begin{bmatrix} 1 & -1.5\tau & (-1.5\tau)^2/2 \\ 1 & -0.5\tau & (-0.5\tau)^2/2 \\ 1 & 0.5\tau & (0.5\tau)^2/2 \\ 1 & 1.5\tau & (1.5\tau)^2/2 \end{bmatrix} \quad (3)$$

$$(4)$$

The matrix $\mathbf{L}$ is similar to a growth curve loading matrix in that the first column estimates an intercept. Thus the first column of $\mathbf{L}$ identifies a latent variable which takes on a value for each row vector of values $\{x_{i1}, x_{i2}, x_{i3}, x_{i4}\}$ where i is a row in the data matrix $\mathbf{X}$. We won't directly observe this latent variable, but will estimate its covariances with other latent variables.

The second column estimates a slope such that the value of the intercept occurs midway between the second and third occasions and the time scale of the slope is the interval of time τ between occasions. The value of the latent variable identified by the second column is then an estimate of the first derivative of each row of the data matrix $\mathbf{X}$ evaluated midway between the second and third columns.

The third column estimates a quadratic curvature in a latent variable that is scaled by τ and also scaled by 1/2. This latent variable takes on a value for each row in the data matrix $\mathbf{X}$ that is an estimate of the second derivative of that row at a time midway between the second and third occasions of measurement.

To understand why the loadings are constructed in this way, note that each column is the indefinite integral of the column to its left and centered around the middle time. Thus since $\int 1 d\tau = \tau$ and $\int \tau d\tau = tau^2/2$, we can construct an estimate of the first and second derivatives using these weights.

Then, the covariance structure between the latent variables is defined using McArdle and McDonald's RAM notation (McArdle & McDonald, 1984).

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \eta & \zeta & 0 \end{bmatrix} \tag{5}$$

$$\mathbf{S} = \begin{bmatrix} V_F & C_{FdF} & 0 \\ C_{FdF} & V_{dF} & 0 \\ 0 & 0 & V_{d2F} \end{bmatrix} \tag{6}$$

$$\mathbf{U} = \begin{bmatrix} V_{ux1} & 0 & 0 & 0 \\ 0 & V_{ux2} & 0 & 0 \\ 0 & 0 & V_{ux3} & 0 \\ 0 & 0 & 0 & V_{ux4} \end{bmatrix} \tag{7}$$

The error structure can then be defined in the matrix **U** as shown in Equation 7. In this case we are assuming independent error of measurement. Now, we can calculate the expected covariances $\hat{\mathbf{R}}$ between the observed variable x at the four occasions of measurement using the matrix expression shown in Equation 8.

$$\hat{\mathbf{R}} = \mathbf{L}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{S}(\mathbf{I} - \mathbf{A})^{-1'}\mathbf{L}' + \mathbf{U} \tag{8}$$

This model may then be fit using a structural modeling program such as Mx (Neale, Boker, Xie, & Maes, 1999). An Mx script for fitting this model as well as the multivariate case can be downloaded from the web at `http://www.nd.edu/~sboker`.

A path diagram of the example ULDE model using RAM diagrammatic conventions (McArdle & Boker, 1990; Boker, McArdle, & Neale, 2002) is presented in Figure 4. Note that with four occasions of measurement, this model is just identified, so the predicted covariance matrix can always exactly reproduce the observed covariance matrix. If one has five or more occasions of measurement, the ULDE model can provide a fit statistic estimating how well the dynamics of the process are fit by the model. However, note that at the latent variable level, the example damped linear oscillator differential model is saturated. Thus, there is no opportunity for misfit in this model at the latent variable level. Observed misfit in this example can only be at the measurement level. However, one might test whether either one or both of the parameters η and ζ are zero by fitting a model without them and testing the difference in fit between that and the latent variable saturated model.

If one has very many occasions of measurement on one variable and one individual, the ULDE method may still be used. The univariate time series may be embedded into a 4 or 5 dimensional space using the method of state space embedding (Sauer, Yorke, & Casdagli, 1991; Takens, 1985; Whitney, 1936) to create a lagged covariance matrix across a chosen interval τ. Furthermore, if one has many observations on many individuals, one might create an individual–identified state space embedding data matrix and fit a ULDE model using the raw scores so that individual differences in differential equations parameters might be estimated.

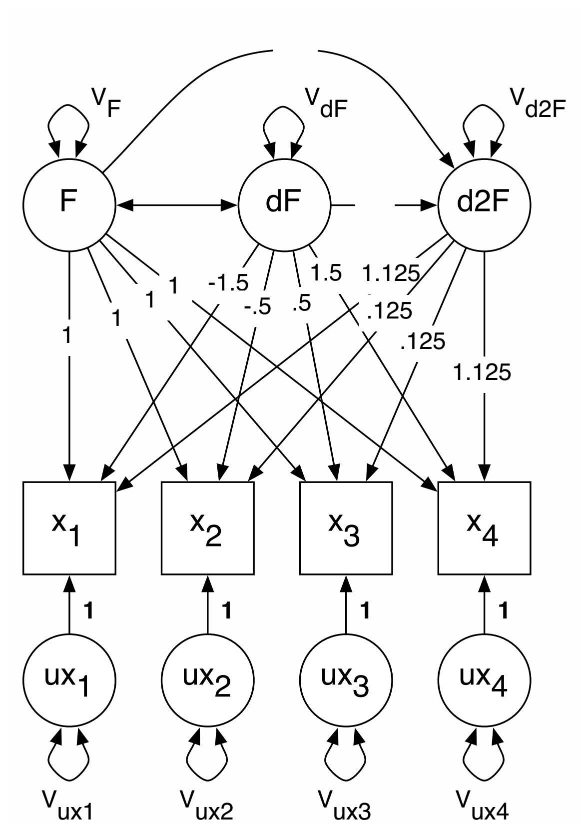

Figure 4. Path diagram of a Univariate Latent Differential Equation (ULDE) Model.

Multivariate Latent Differential Equation Model

We next consider the case where a measurement model for a latent variable is indicated both across manifest variables within time as well as within manifest variables across time. In the case of a single occasion of measurement, a measurement model for a latent variable is frequently constructed across variables as a confirmatory factor model. We present a model in which a confirmatory factor model holds within any single occasion of measurement and covariance between indicators across time is accounted for by the intrinsic dynamics of the latent variable: the differential equations model at the level of the latent structure.

Suppose we have observed three manifest variables at four occasions. This is the minimum number of variables and occasions that will allow the Multivariate Latent Differential Equation (MLDE) model to be identified both within occasion and across indicators as well as within indicator and across time. We now build a data matrix such that the first four columns are the four occasions of measurement for the first indicator, the next four columns are the four occasions of measurement for the second indicator and the last four columns are the four occasions of measurement for the third indicator. Thus one row of the data matrix would be

$$\{x_{i1}, x_{i2}, x_{i3}, x_{i4}, y_{i1}, y_{i2}, y_{i3}, y_{i4}, z_{i1}, z_{i2}, z_{i3}, z_{i4}\} \tag{9}$$

where x_{i1} is the first occasion of measurement for the first indicator for the ith row of the data matrix.

Now the predicted covariance matrix of these indicators can be calculated from the four matrices **L**, **A**, **S**, and **U**. The first four rows of the loading matrix **L** shown in Equation 10 are constructed as before with three columns using the fixed interval τ. The second set of four rows are the same, but are weighted by an estimated parameter a that is the factor loading for the variable y on the latent variable F. Similarly the third set of four rows are weighted by an estimated parameter b.

The structure of the covariance between the latent variable and its latent derivatives is defined using the matrices **A** and **S** shown in Equations 11 and 12. The example structure is again the second order linear differential equation defining a damped linear oscillator. This is by no means the only dynamical system that can be estimated using the MLDE approach. In fact, one of the principal advantages of this approach is that the model at the latent level is easily and flexibly specified and estimated for more than one factor.

$$\mathbf{L} = \begin{bmatrix} 1 & -1.5\tau & (-1.5\tau)^2/2 \\ 1 & -0.5\tau & (-0.5\tau)^2/2 \\ 1 & 0.5\tau & (0.5\tau)^2/2 \\ 1 & 1.5\tau & (1.5\tau)^2/2 \\ a & a(-1.5\tau) & a(-1.5\tau)^2/2 \\ a & a(-0.5\tau) & a(-0.5\tau)^2/2 \\ a & a(0.5\tau) & a(0.5\tau)^2/2 \\ a & a(1.5\tau) & a(1.5\tau)^2/2 \\ b & b(-1.5\tau) & b(-1.5\tau)^2/2 \\ b & b(-0.5\tau) & b(-0.5\tau)^2/2 \\ b & b(0.5\tau) & b(0.5\tau)^2/2 \\ b & b(1.5\tau) & b(1.5\tau)^2/2 \end{bmatrix} \tag{10}$$

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \eta & \zeta & 0 \end{bmatrix} \tag{11}$$

$$\mathbf{S} = \begin{bmatrix} V_F & C_{FdF} & 0 \\ C_{FdF} & V_{dF} & 0 \\ 0 & 0 & V_{d2F} \end{bmatrix} \tag{12}$$

We can now fit the model using a structural equations modeling package such as Mx. The predicted covariance of this model can be calculated in the same way as for the ULDE model as shown in Equation 13.

$$\hat{\mathbf{R}} = \mathbf{L}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{S}(\mathbf{I} - \mathbf{A})^{-1'}\mathbf{L}' + \mathbf{U} \tag{13}$$

In this example, the matrix of unique variances **U** is specified as a diagonal matrix of free parameters, thereby constraining all of the common variance between indicators within and across time to be accounted for by the differential equation relating the common factor and its derivatives. Note that while this is the minimum number of indicators required to identify a single factor within time across indicators and the minimum number of occasions to identify the model within indicator across time, there are many more degrees of freedom in the covariance matrix of indicators than there are estimated parameters. This is a strong test of the dynamics of a latent variable. But note that at the latent variable level, this example model is fully saturated and it is only in the measurement model that we have a potential for misfit to the data. Thus, if we observe substantial misfit, we might consider other more complicated relationships such as across–time factors unique to each indicator. Such a model would suggest that there was both a common dynamic to all of the indicators and a separate dynamic within each indicator.

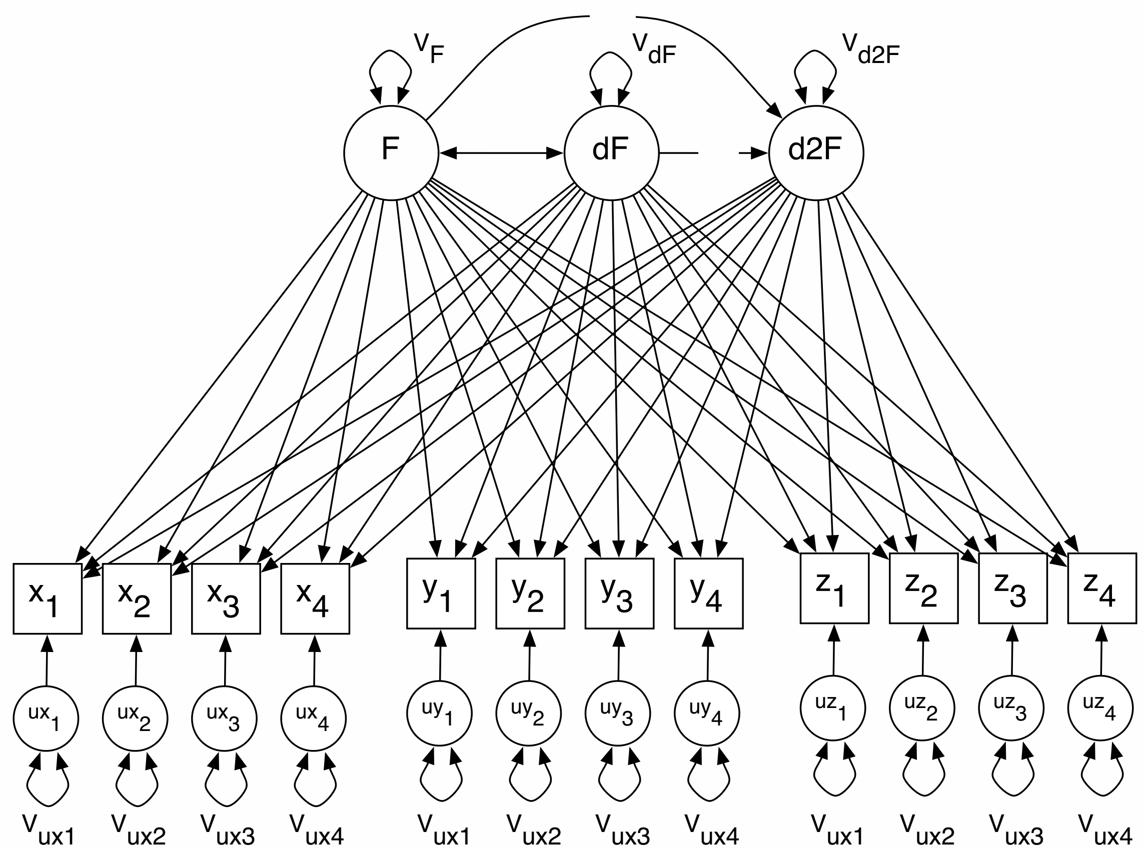

Figure 5. Path diagram of the example Multivariate Latent Differential Equation (MLDE) model with three indicators observed at four occasions and the latent differential structure modeled as a damped linear oscillator.

A path diagrammatic representation of this example MLDE model is presented in Figure 5. Again, we have used the RAM diagramming conventions for representing factor and unique variances. There are many ways in which this model might usefully be extended. For instance, we could use more indicators to gain a better estimate of the common factor. We might find that a single factor was insufficient to fit the measured variables. Two or more factors might have independent dynamics, or might be coupled over time. A second way this model might be extended is that we might have more occasions of measurement and find that higher order derivatives were required to fit the observed dynamics of the indicators.

This model may also be fit to data comprised of many occasions of measurement on a single individual using the state space embedding method for building a lagged data matrix as mentioned in the previous section. Or one might have multiple indicators and many occasions of measurement on many individuals. In this case a multiple group full information maximum likelihood approach could be used that would allow each individual to take on individual dynamical parameters while loading constraints force metric factor invariance of the measurement model across individuals.

Simulation of Multivariate Oscillators

In order to test the efficacy of the MLDE modeling procedure, two simulations were implemented. The first simulation tested the behavior of the MLDE model under a variety of parameter conditions and sampling intervals. The simulated data was calculated using Mathematica (Wolfram Research, 2002) using Runge–Kuttah fourth order numerical integration. We simulated data using the damped linear oscillator model from Equation 1. We created 90 instances of the damped linear oscillator each with one η parameter chosen from a set of 10 conditions,

$$\eta = \{-0.2, -0.6, -1.0, -1.4, -1.8, -2.2, -2.6, -3.0, -3.4, -3.8\} ,$$

one ζ parameter chosen from a set of 9 conditions,

$$\zeta = \{-0.04, -0.03, -0.02, -0.01, 0.00, 0.01, 0.02, 0.03, 0.04\} ,$$

and then numerically integrated the resulting differential equation to produce 10,000 observations of the oscillator. The integration step was chosen to be small (0.05) so that a wide range of simulated intervals between occasions of measurement could be tested.

Thus, for any chosen combination of η and ζ there was a vector of 10,000 "true scores" from a damped linear oscillator. A sampling interval, τ was chosen from the set of integers from 1 to 16. Then an instance of a 300 individuals by 24 observations simulated data matrix was constructed as follows. The ith row of the simulated data matrix was calculated from a sample "individual" set of 4 true scores $\{F_{it_i}, F_{i(t_i+\tau)}, F_{i(t_i+2\tau)}, F_{i(t_i+3\tau)}\}$ drawn from the selected damped linear oscillator vector where the index of the first occasion t_i was a pseudorandom number uniformly distributed on the interval $\{1 \ldots 1500\}$. Next, six indicator scores were generated for each true score F_{ik} where k is an element of the set $\{t_i, t_i + \tau, t_i + 2\tau, t_i + 3\tau\}$.

$$\begin{aligned}
x_{i1k} &= 1.0F_{ik} + 0.625u_{i1k} \\
x_{i2k} &= 0.5F_{ik} + 0.825u_{i2k} \\
x_{i3k} &= 0.4F_{ik} + 0.500u_{i3k} \\
x_{i4k} &= 0.7F_{ik} + 1.125u_{i4k} \\
x_{i5k} &= 0.6F_{ik} + 0.750u_{i5k} \\
x_{i6k} &= 0.3F_{ik} + 1.000u_{i6k}
\end{aligned} \tag{14}$$

where u_{ijk} is a pseudorandom number drawn from a normal distribution with zero mean and unit variance. The communalities of these observed scores depended on the variance of F, and thus on the sampling interval τ and on the selected combination of η and ζ from the true score vector.

In this way, 10 data matrices were generated for each combination of η, ζ and τ, resulting in a total of 14,400 data matrices. An MLDE model with 6 indicators, 4 occasions and a latent differential structure of a damped linear oscillator were fit to each of these data matrices using Mx. Results were aggregated over the 10 replications within each $\eta \times \zeta \times \tau$ condition cell.

The factor loadings from Equation 14 were recovered well when the model fit the simulated data reasonably well. There were some conditions of η and τ that violated the Nyquist limit (see e.g. Hamming, 1977, for an introduction) for our four occasion samples and thus models fit to those data matrices performed extremely poorly if they converged at all.

Figure 6 presents the results of fitting the MLDE model to all conditions of η and τ when $\zeta = 0$. This is the condition where there is no damping, i.e. similar to a frictionless pendulum. As can be seen in Figures 6–a and –b, there is a reasonably good correspondence between the true value of η and the mean estimated value of η except when large values of τ are combined with large negative values of η (seen as the "cliff" on the right side of the graph). In fact, when the value of τ is such that 4τ are greater than one half the period of the oscillation, the model does not fit. This is exactly the Nyquist limit which states that the sampling interval must be less than one half the period of the oscillation one wishes to estimate.

The mean bias in estimation of η is plotted in Figure 6–c. The bias is low except near the Nyquist limit and when the sampling interval is short. The median bias as a percentage of the true value of η over all cells that did not violate the Nyquist limit was 6.2%. This small positive bias was primarily due to cases approaching the Nyquist limit but which were not formal violations. When the sampling interval is short there is little change in the true score in comparison with the added measurement error. Thus, the communalities of the observed scores are quite low in this combination of conditions, resulting in highly variable estimates of η. Figure 6–d plots the mean likelihood ratio fit statistic (χ^2) over the 10 replications in each condition cell. Note that the fit statistic does a good job of flagging bias due to the Nyquist limit. Of course in real data, one does not know where this limit might be and thus having the χ^2 as a diagnostic is useful. Unfortunately, the χ^2 does not help in recognizing low communalities, but communalities can be estimated in other ways, so this is not problematic.

Figure 7 presents the results of the simulation for a chosen value of $\eta = -.06$, the slowest frequency shown in Figure 6. For values of $\tau > 8$, the estimated value of ζ is a reasonably good approximation of the true value of ζ, exhibiting low bias, although the variability of estimation is higher than for that of η. However, for values of $\tau < 8$, the estimated value of ζ shows very high variability. Again, for small values of τ, with a very small time step constant (0.05) in the numerical integration used for the simulation, there will be little variance in the derivatives in comparison with the added measurement error. Thus with low communalities, it is not unexpected that the standard error of estimation of ζ will be large when τ is small.

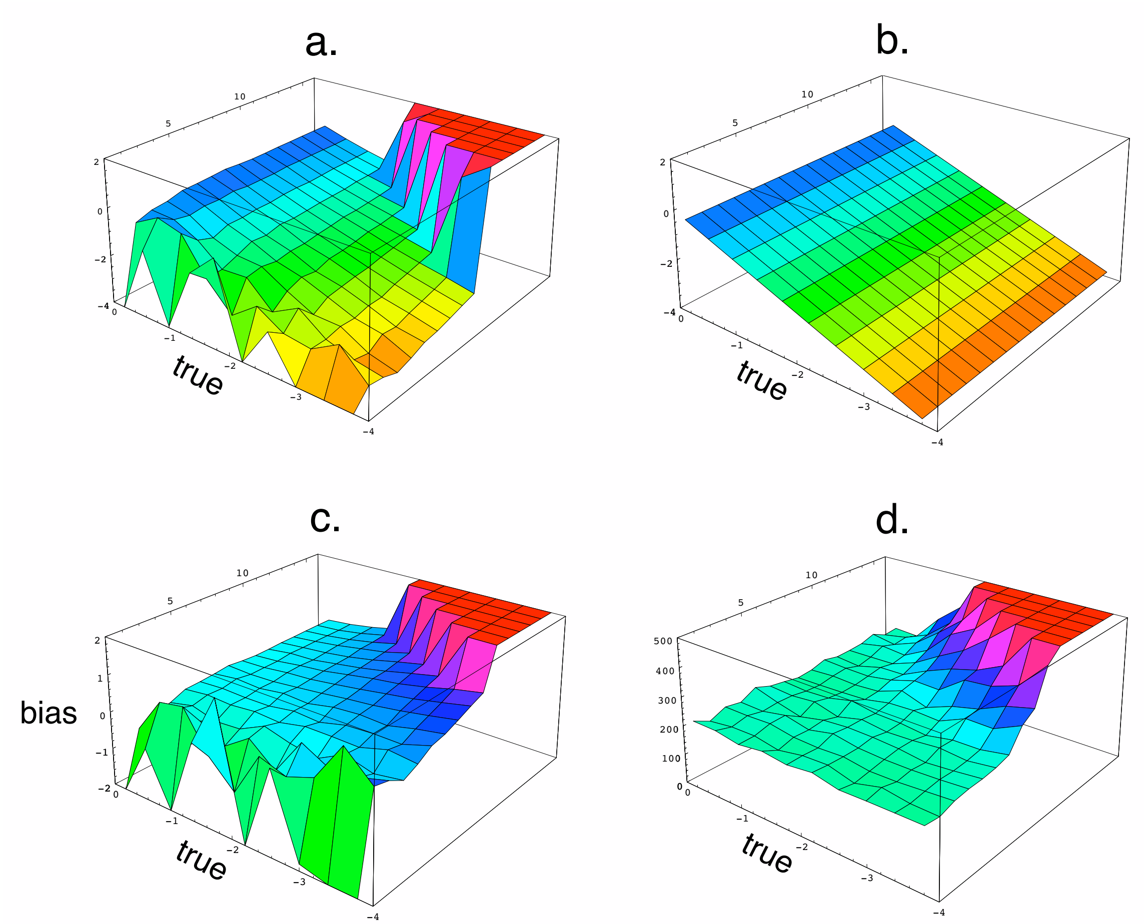

Figure 6. Results of fitting an MLDE model for $\zeta = 0$ over all conditions of η and τ. (a) The mean estimated value of η versus τ and the true value of η. (b) The true value of η versus τ and the true value of η. (c) Mean bias of estimation (Figure a minus Figure b). (d) The likelihood ratio fit function (χ^2).

Simulation with No Time Dependence

In discussing Figure 2 we suggested that a useful method would need to be able to distinguish random fluctuations in a score from fluctuations due to a self–regulatory process. The reason this can be problematic can be understood by considering Figure 2–b in which all observations are independent draws from a normal distribution. Suppose one drew an extreme observation at the second occasion. The expected value of the first and third observation given the extreme value are still zero. Thus, the more extreme the value of the second occasion, the greater the expected "bend" at the second occasion. Thus there is a built–in correlation between the second derivative at the second occasion and the value of the variable at that occasion. In fact, using Local Linear Approximation, there is a calculated correlation of -0.8 between the value of the variable and its estimated second derivative. This is why it is difficult to distinguish between the cases in Figures 2–a and

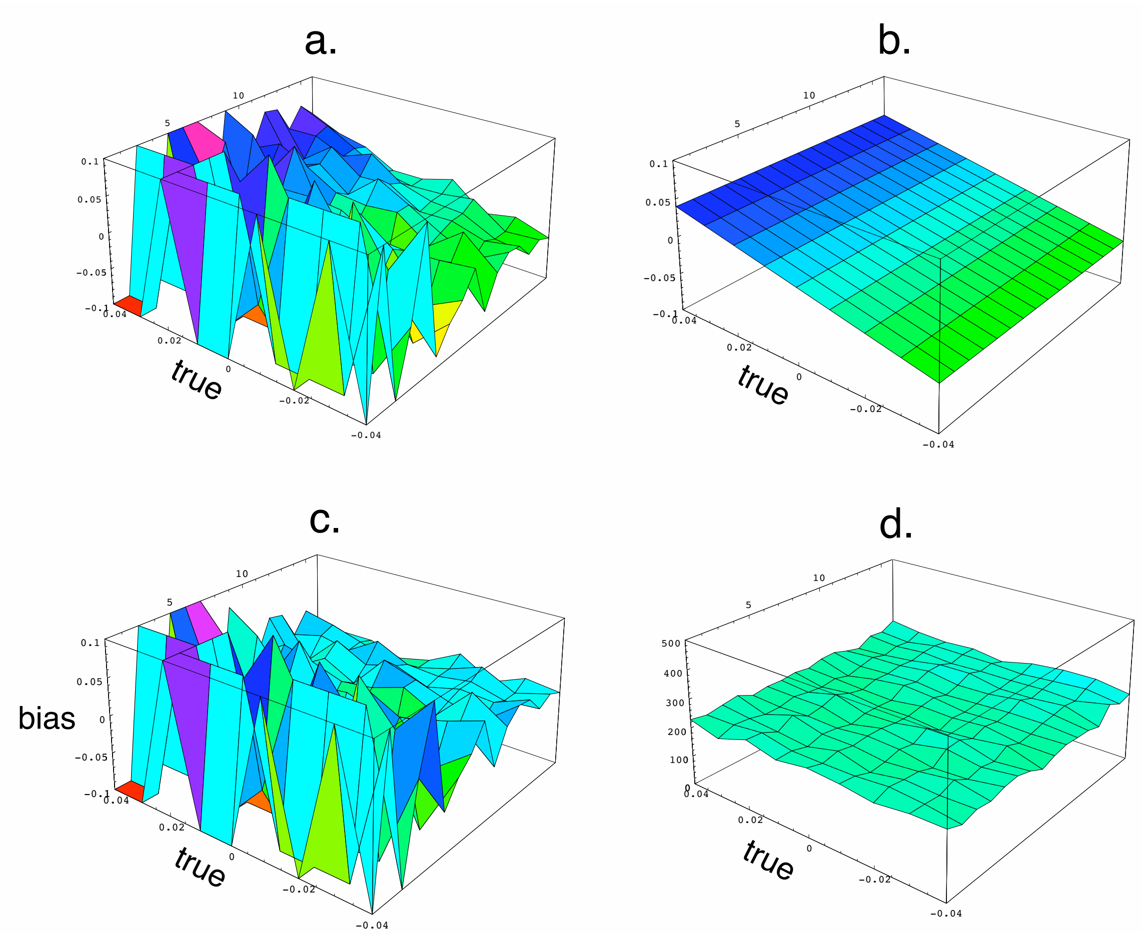

Figure 7. Results of fitting an MLDE model for $\eta = -0.6$ over all conditions of ζ and τ. (a) The mean estimated value of ζ versus τ and the true value of ζ. (b) The true value of ζ versus τ and the true value of ζ. (c) Mean bias of estimation (Figure a minus Figure b). (d) The likelihood ratio fit function (χ^2).

2–b.

We simulated a vector of factor scores as independent draws from a normal distribution and repeated the simulation experiment described above. There was an immediately obvious difference between the results of this simulation and the simulation with a true linear oscillator generating the factor scores. The values of the χ^2 fit function for the case with no time dependence in the factors were on average approximately 50 times larger than the fit function values of for the simulation with true linear oscillation.

In the first simulation, maximum χ^2 fit function value for the true linear oscillator across all conditions was 335 when τ was small enough that the 4 occasions were within the Nyquist limit. Even when Nyquist limit violations are included, the maximum χ^2 value was 1699 for the true linear oscillator data.

By contrast, the minimum value of χ^2 in the case in which the factor scores were independent across time was 10,294 (160 simulated data sets). In every one of the simulated data sets with no time dependence, the linear oscillator was clearly rejected by the value of the fit function. It should be noted that the within occasion factor loadings were, in almost every case, correctly calculated for the time independent data. Thus it was not simply that the models did not converge correctly for the time independent data.

Discussion

Data sets were simulated that mimicked an experimental design in which 300 independent individuals were measured on six indicator variables on four occasions separated by equal intervals of time. All individuals in each simulated data set had a single factor that had an intrinsic dynamic in accord with a damped linear oscillator differential equation model with fixed parameters. Independent identically distributed measurement error was added to each observation. The MLDE model was able to simultaneously recover low bias estimates of the factor loadings and differential equations parameters if the total interval between the first and last observation was(a) smaller than the Nyquist limit of one half the period of the true oscillation and (b) large enough that the communalities of the indicators was greater than 0.5. The MLDE method appears to be much less sensitive to measurement interval than other methods for direct estimation of differential equations parameters from derivatives explored by the authors (Boker & Nesselroade, 2002; Boker, 2001). This means that the MLDE method does not require more than a gross estimate of the period of any hypothesized cyclicity in the process under analysis.

In addition, the inclusion of a measurement model opens up a variety of possibilities for extensions to the model. For instance, many longitudinal designs are not equal interval. If all subjects are measured on the same schedule, the time interval τ used in the matrix $\mathbf{L}$ can take on appropriate values for each row so that estimates of the covariance between latent derivatives can still be obtained and thus the covariance between their derivatives can still be obtained. This applies even when some indicators are measured on a different schedule than others as long as there is a centering time around which all observations can be synchronized. This could be very useful when attempting to estimate the latent dynamic structure of a variable measured, for instance, with pencil and paper as well as physiological instruments. Physiological measures are likely to be observed much more frequently than questionnaire or psychometric measures. Being able to correct for these time scale differences is critical to estimating coupling between psychological and physiological measures.

A further extension of the model could use latent indicators for missing observations (as in e.g. McArdle & Hamagami, 1992). When many observations are available on each individual (or pre–defined group), it is possible to build a multigroup model where each individual's (or group's) dynamic parameters could be estimated while constraints on factor invariance were maintained.

Weaknesses

There are several weaknesses of the LDE methods. First, the data requirements are substantial. One must have measured several variables on many occasions on many individuals in order to both estimate within and between individual parameters. The model as presented here also requires that the process be stationary, that is, the estimated parameters may not change over time. A windowed extension to this method (perhaps along the lines of Boker, Xu, Rotondo, & King, 2002) may be able to relax the stationarity requirement.

The chosen interval between occasions of measurement must be short enough so that at least 8 observations can occur within a single period of oscillation when the latent structure includes a second derivative. This means that a process must be measured relatively often in comparison with its period of fluctuation.

Finally, when the rows of the lagged data matrix are not independent observations, that is when single individuals may contribute more than one row to the lagged data matrix, the standard errors for the dynamic parameters calculated by maximum likelihood will be smaller than the true variability in these parameters. Resampling by blocks may be one solution, but as far as is known to the authors, this is still an open problem.

Future Directions

While adding a multivariate measurement model to direct differential equations estimation has benefits in and of itself, the main benefit foreseen by the authors is extension to dynamical systems with multiple factors and coupling between factors. As a first step in this direction, consider the model shown in the path diagram in Figure 8.

Here, two latent variables each have a separate dynamic structure and each of them influences the dynamic of the other. At the latent level, this is a system of two second order differential equations. Each latent variable has its own set of indicators and these indicators need not be measured at the same intervals as long as there is a synchronizing time t that is the same at the center of each group of observations. This type of model could easily be extended to systems of three or more (possibly nonlinear) differential equations.

Finally, we see promise for the MLDE method to be applied to behavioral genetics data. A reasonable hypothesis might be that a dynamical process has both additive genetic as well as environmental influences. The MLDE method seems likely to be able to be adapted to estimate these influences. Sibling interaction may possibly be constructively modeled using coupled systems similar to the coupled oscillator shown in Figure 8.

If one is attempting to design experiments that can take advantage of methods in dynamical systems modeling, we have the following recommendations. It goes without saying that you should measure as often as you can afford, obtain as many occasions per individual as you can afford, and measure as many individuals as you can afford. When budgets are limited, trade–offs must be made. The absolute minimum number of occasions per individual is four in order to use an ULDE or MLDE model. But if at all possible try to obtain ten so that you will have access to more options and better parameter stability. In this case you will still be making an assumption that all individuals' dynamic parameters are equal. If you wish to relax that assumption you will need a minimum of around 30 observations per individual and will have much better power with 100 observations per individual. In order to get stable estimates of the factor loadings, you will need at least 300 quadruples of measurements. This sounds forbidding, but remember that this need not be 300 individuals if you have many quadruples of observations from each individual. Finally, it is extremely important to remember that if you expect cyclicity in your data you must measure often enough that the interval between the first and last observation in a quadruple of occasions is less than one half the period of the cycle.

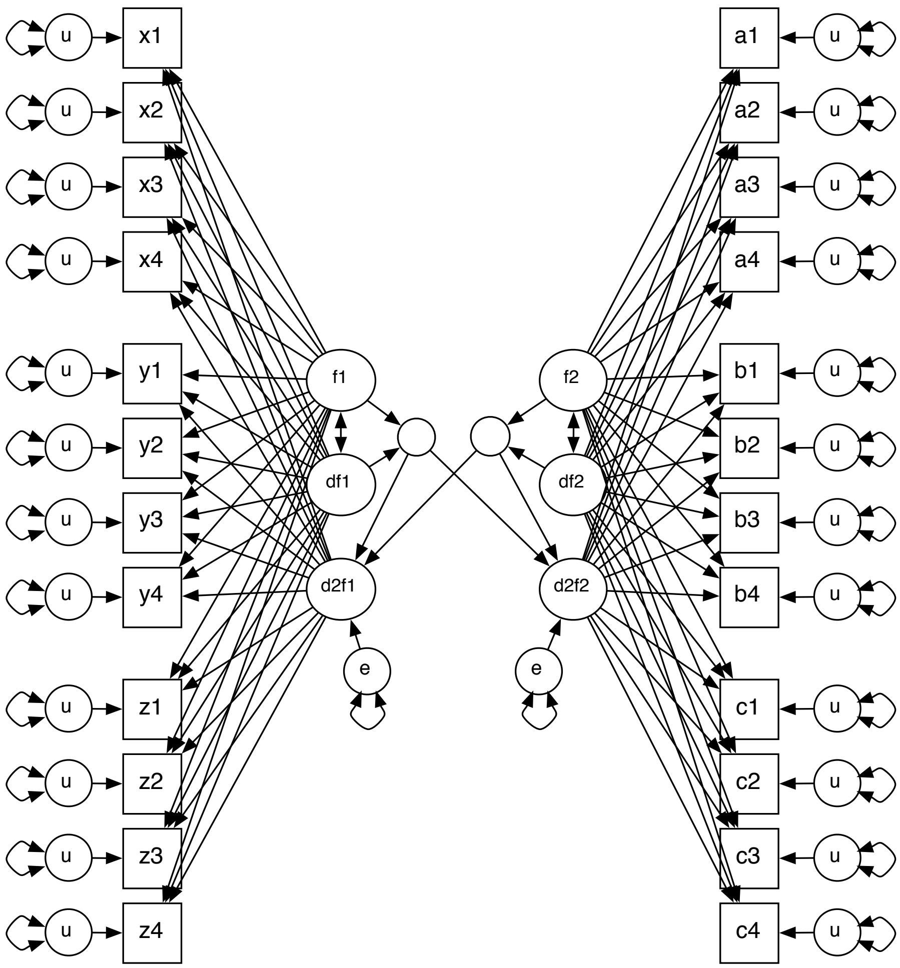

Figure 8. Path diagram of a multivariate latent differential equations model with two coupled latent variables.

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