

# Dynamic Structural Equation Modeling with Cycles

Bengt Muthén & Tihomir Asparouhov \*  
Mplus

Loes Keijsers  
Erasmus University Rotterdam

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## Abstract

Cyclical phenomena are commonly observed in many areas of repeated measurements, especially with intensive longitudinal data. A typical example is circadian (24-hour) rhythm of physical measures such as blood pressure, heart rate, glucose level, and alertness. This paper focuses on positive affect which is a common measure in psychological studies and for which circadian rhythm has been observed but not analyzed by modern statistical methods. The paper demonstrates that a large new analysis arsenal is available for analysis of cyclical features in intensive longitudinal data. This can help researchers extract more information from their data to get more valid estimates of coupled processes and to get new theoretical insights into circadian rhythms of mood. To assist in this effort, the analyses are based on general models with a rich set of features while still being accessible without an unduly steep learning curve. Scripts for the Mplus software are available for all the analyses presented.

Keywords: intensive longitudinal data, Experience Sampling Methods, individual differences, cosinor model, amplitude, phase, two-level modeling, cross-classified modeling, RDSEM

# 1 Introduction

Cyclical phenomena are commonly observed in many areas of repeated measurements, especially with intensive longitudinal data, which consist of many repeated measurements obtained from the same cases, such as individuals, households, companies, or countries. A typical example is circadian (24-hour) rhythm of physical measures such as blood pressure, heart rate, glucose level, and alertness. Cycles of varying length are also observed in areas as diverse as electricity consumption, menstruation, and weekly drinking patterns. This paper focuses on modeling of cycles exemplified by a common measure in psychology, positive affect (PA). PA is of theoretical importance due to it being a marker of healthy functioning, for example, as a predictor of motivation and task performance (Brose et al., 2014), as a predictor of internalizing problems in childhood (Brieant et al., 2018), and as a resilience factor among remitted depressed patients (Hoorelbeke et al., 2019). Evidence of circadian rhythm for PA was described in for instance Watson et al. (1999) where a midday peak was observed in several different samples. In contrast, negative affect showed no such cycles.

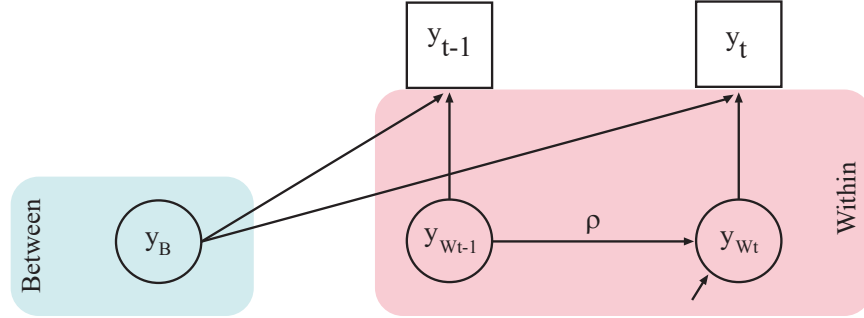
The modeling with cycles is important both because of new information that can be uncovered in the data and because of the biases that can be avoided. The timing and fluctuations of cyclical patterns can be determined. Person-specific variation in the cycles can be explored and related to background characteristics of the person. Taking cycles into account may provide more valid estimates of bivariate associations, because confounding time effects can be controlled for, while ignoring cycles can lead to biased estimates of within-person relationships (see, e.g., Liu & West, 2015).

This paper shows how to model cyclic variation across the hours of the day and also across the days of the week in order to estimate population characteristics as well as person variation around these. In addition to studying an overall measure of PA, the cyclic variation is examined for different dimensions of PA, showing different cycles for factors measured by different types of PA items. The variation across time in PA and the different variation across time for different dimensions of PA raise questions of how an individual’s PA is best represented.

To model cycles, and trends more generally, this paper considers two types of models for intensive longitudinal data, two-level dynamic structural equation models (DSEM) and cross-classified DSEM. Statistical theory for modeling and estimation was presented in Asparouhov, Hamaker and Muthén (2018) and Asparouhov and Muthén (2020) with applications discussed in e.g. Hamaker, Asparouhov and Muthén (2023). Two-level analysis allows variation in parameters across individuals while cross-classified analysis also allows variation across time. Cross-classified analysis may for example allow variation across time in  $x$  predicting  $y$ . The flexibility of across-time variation of cross-classified DSEM is shown to offer a convenient way to detect cycles. The cycles can then be modeled using sine-cosine curves in line with Ram et al. (2005), Shumway and Stoffer (2011, pp. 175-177), Madden et al. (2018), and Zong et al. (2023). This can also be combined with dummy covariates representing deviations from the cycles, e.g. for specific days of the week.

Section 2 gives an introduction to two-level and cross-classified DSEM as implemented in the Mplus software (Muthén & Muthén, 2018). Section 3 describes sine-cosine modeling of cycles and presents a simulation study using cycles modeling with two-level and cross-classified DSEM. Section 4 presents an example of using cycles modeling with data from an intensive longitudinal study of positive affect (PA). Section 5

Figure 1: Two-level DSEM



extends this example to item-level factor analysis and covariates. Section 6 discusses extensions to analysis of random coefficients for factor cycles including amplitude and phase. Section 7 concludes. Throughout the paper, the models are presented in figures that correspond to Mplus input. Mplus scripts used in the analyses are given in the Supplementary material.

## 2 Two-level and cross-classified DSEM

To model cycles, this paper considers four major types of models for intensive longitudinal data observed for a sample of individuals, two-level dynamic structural equation model (DSEM), residual DSEM (RDSEM), cross-classified DSEM, and residual cross-classified DSEM. These models were proposed for the analysis of intensive longitudinal data in Asparouhov, Hamaker and Muthén (2018) and Asparouhov and Muthén (2020) using the Mplus software (Muthén & Muthén, 2018). To allow for flexible models with many random effects, Bayesian estimation is carried out. For applications, see, e.g., Hamaker, Asparouhov and Muthén (2023). Following is a brief introduction to basic forms of these models.

### 2.1 Two-level DSEM

Consider a continuous variable  $y$  measured in a long time series for a sample of individuals as is common in intensive longitudinal data settings. For example, 200 individuals are sampled 6 times per day for 14 days (84 measurements per person). At each assessment, they report on their positive affect (here  $y$ ). Figure 1 shows the  $y$  measurement (squares) at two consecutive timepoints  $t$  and  $t - 1$ . The figure shows that the observed  $y$  is decomposed into two latent parts denoted by circles, a between part (blue) that varies over individuals ( $y_B$ ) and a within part (red) that represents within-person variation over time ( $y_W$ ). The arrows from between and within to the observed  $y$  can be understood in terms of regression with coefficients 1 and no residual, reflecting the decomposition  $y = y_B + y_W$  as in random effects anova. The two-level model in the

figure is specified as follows for individual  $i$  at time  $t$ ,

$$\text{Level 1 : } y_{it} = y_{Bi} + \rho(y_{it-1} - y_{Bi}) + \epsilon_{it}, \quad (1)$$

$$\text{Level 2 : } y_{Bi} = \mu + \delta_i. \quad (2)$$

Here,  $\rho$  is the auto-regressive coefficient of lag 1 seen in Figure 1. Note that this two-level model has a random intercept  $y_{Bi}$  which is also used to center the  $y_{it-1}$  predictor. The latent variable centering is essential to avoiding biases (Nickell, 1981; Asparouhov & Muthén, 2019). Equation (1) can be expressed as:

$$\underbrace{y_{it} - y_{Bi}}_{y_{Wit}} = \rho \underbrace{(y_{it-1} - y_{Bi})}_{y_{Wit-1}} + \epsilon_{it}, \quad (3)$$

emphasizing that there is a within- and between-level model part in line with Figure 1,

$$\text{Within : } y_{Wit} = \rho y_{Wit-1} + \epsilon_{it}, \quad (4)$$

$$\text{Between : } y_{Bi} = \mu + \delta_i. \quad (5)$$

The specification of the within and between parts of the model translates into the specification in the Mplus software (Muthén & Muthén, 2018).

A more general two-level DSEM version is shown in Figure 2. It is a bivariate cross-lagged Vector Auto-Regressive (VAR) model including a contemporaneous effect. Such models can for instance be used to assess whether dynamic processes are coupled, e.g., does the level of tobacco use affect a persons positive affect? Parameters in the within part of the model that show filled circles are random effects, that is, parameters varying across persons. These random effects are shown in the between part of the model, influenced by a time-invariant covariate.

## 2.2 Cross-classified DSEM

Another modeling option offered by Mplus is cross-classified DSEM. While two-level DSEM decomposes the observed variable into two latent variables,

$$y_{it} = \underbrace{y_{Bi}}_{\text{Between person}} + \underbrace{y_{Wit}}_{\text{Within person}}, \quad (6)$$

cross-classified DSEM decomposes the observed variable into three latent variables,

$$y_{it} = \underbrace{y_{Bi}}_{\text{Between person}} + \underbrace{y_{Wit}}_{\text{Within person}} + \underbrace{y_{Tt}}_{\text{Between time}}. \quad (7)$$

Here,  $y_{Bi}$  refers to variation between persons that is constant over time, while  $y_{Tt}$  refers to variation between timepoints that is constant over persons. The latent variables  $y_{Bi}$ ,  $y_{Wit}$ ,  $y_{Tt}$  are specified as normally distributed where  $y_{Wit}$  and  $y_{Tt}$  have zero means.

Figure 3 shows an example of the three parts of the model, Between ID (person), Within, and Between Time. The within part of the model has a lag 1 auto regression while the between time part contributes time-specific influence that is not related over time,

$$y_{Bi} = \mu + \delta_i, \quad (8)$$

$$y_{Wit} = \rho y_{Wit-1} + \epsilon_{it}, \quad (9)$$

$$y_{Tt} = \xi_t. \quad (10)$$

Figure 2: Two-level DSEM with cross-lagged, contemporaneous, and random effects

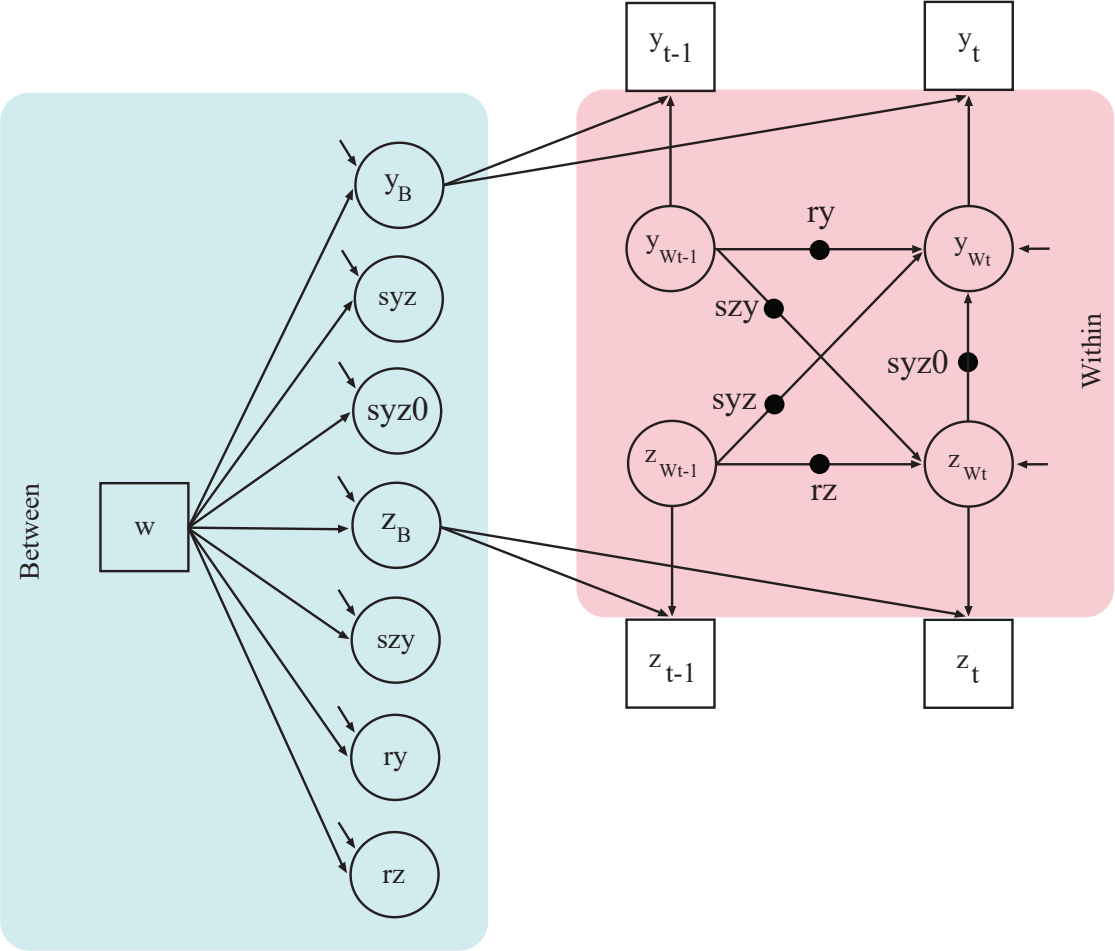
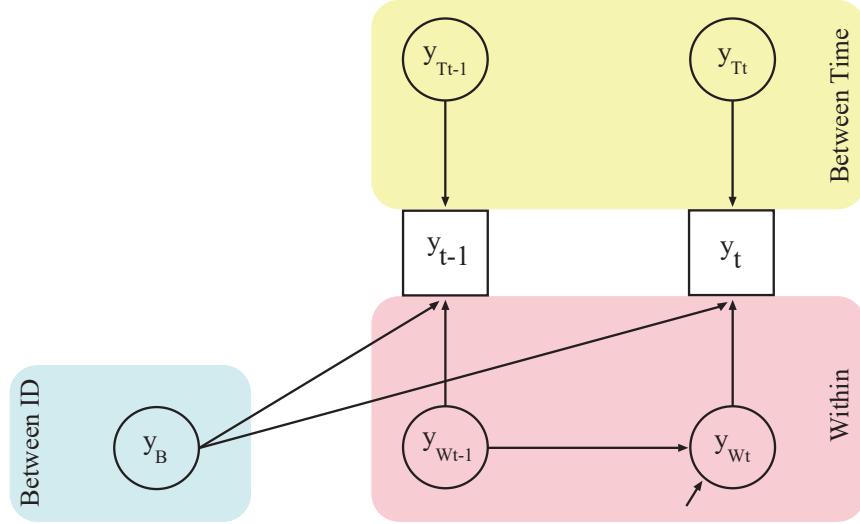


Figure 3: Cross-classified DSEM



A more elaborate model on the within level is possible in line with the within part of Figure 2.

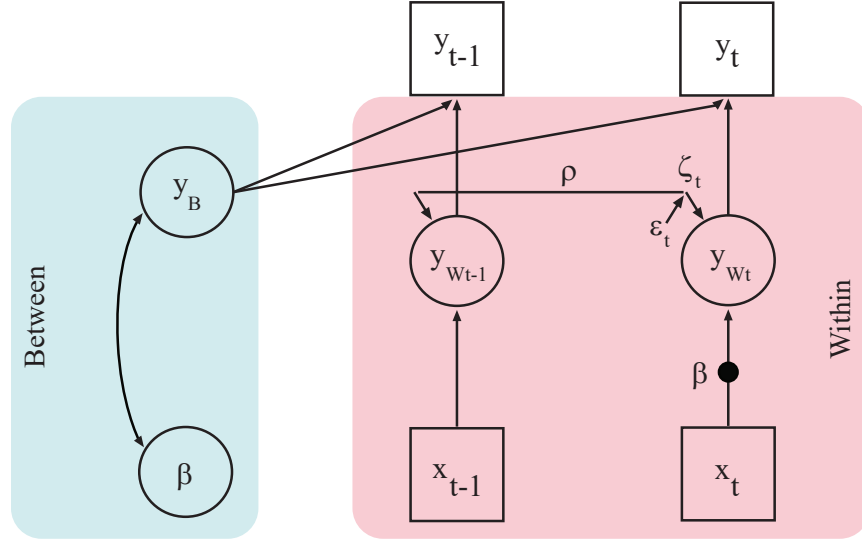
The advantage of cross-classified DSEM is that the  $y_T$  term can discover trends over time such as cycles. The model is therefore an essential tool of cycles analysis. The model can be estimated without imposing a specific cycles function. The  $T$   $y_{Tt}$  estimates can be plotted against time to generate ideas for cycles modeling. The cycles modeling can then be carried out in either cross-classified or twolevel DSEM as discussed in Section 3. In time series analysis, decisions on cycles and their durations are made using spectral analysis (see, e.g., Shumway & Stouffer, 2011). In the current  $N > 1$  setting, spectral analysis is typically applied to the time series of averages over individuals (see, e.g., Larsen & Kasimatis, 1990) or for one individual at a time (see, e.g., Ram et al., 2005). The multilevel modeling of cross-classified DSEM is a more advanced way to decide on cycles and their duration because it works with the raw data for all individuals and allows individual differences and auto-regressions.

It should be noted that the Asparouhov et al. (2018) modeling framework is quite general in that the latent variables in (6) and (7) can be multivariate and follow a structural equation model. For example, with multiple indicators of factors, a CFA model can be specified for each of the three levels of the cross-classified DSEM. This will be utilized when analyzing item-level data for positive affect in the application section.

### 2.3 Two-level and cross-classified residual DSEM (RDSEM)

When adding time-varying covariates to DSEM, a residual DSEM (RDSEM) model can be specified. RDSEM is useful for modeling cycles. Consider a simple example with only one covariate  $x$ . For the two-level DSEM model, adding  $x$  to the lag 1 model

Figure 4: Two-level RDSEM with a random slope for a time-varying covariate



in (4) can be expressed as

$$y_{Wit} = \rho y_{Wit-1} + \beta_i x_{it} + \epsilon_{it}, \quad (11)$$

so that the auto-regression refers to  $y_W$ . In contrast, the two-level RDSEM model specifies the auto regression for the residual  $\zeta$  in the  $y_W$  regression on  $x$ ,

$$y_{Wit} = \beta_i x_{it} + \zeta_{it}, \quad (12)$$

$$\zeta_{it} = \rho \zeta_{it-1} + \epsilon_{it}. \quad (13)$$

This two-level RDSEM model is shown in Figure 4. With  $x_{it} = t$  in (12), the contemporaneous effect of RDSEM corresponds to that of a linear growth model with random intercept ( $y_B$ ) and random slope ( $\beta_i$ ) growth factors just like in a regular (non-DSEM) two-level framework for growth modeling.

As pointed out in Asparouhov and Muthén (2020), the DSEM and RDSEM models are substantially different. DSEM lets the covariate at  $t - 1$  influence  $y_{it}$  indirectly via  $y_{it-1}$  whereas there is no such indirect effect in RDSEM but the effect of the covariate on  $y$  is instead only contemporaneous. In many cases when the covariate is a function of time, DSEM and RDSEM are equivalent models representing different parameterizations but RDSEM has a simpler and more intuitive interpretation (Asparouhov et al., pp. 374 -376).

An RDSEM version of the cross-classified model is also available in line with the two-level RDSEM model and is discussed in connection with Figure 9 in the next section.



### 3 Sine-cosine curves

This paper analyzes cycles using sine-cosine curves. Consider the cyclical curve  $F(t)$  as a function of time  $t$ ,

$$F(t) = A \cos(2\pi\omega (t - \phi)) \quad (14)$$

$$= A \sin(2\pi\omega\phi) \sin(2\pi\omega t) + A \cos(2\pi\omega\phi) \cos(2\pi\omega t) \quad (15)$$

$$= \beta_1 x_{1t} + \beta_2 x_{2t}, \quad (16)$$

where

$$\beta_1 = A \sin(2\pi\omega\phi), \quad (17)$$

$$\beta_2 = A \cos(2\pi\omega\phi), \quad (18)$$

$$x_{1t} = \sin(2\pi\omega t), \quad (19)$$

$$x_{2t} = \cos(2\pi\omega t), \quad (20)$$

and where  $A$  is the amplitude defined as half the difference between the highest and lowest values,  $\phi$  is a phase shift, and  $\omega$  is a frequency index where the inverse of  $\omega$  is the duration of one cycle. The aim is to fit a regression for an outcome  $y(t)$  using the two covariates  $x_{1t}$  and  $x_{2t}$ ,

$$y(t) = \beta_0 + \beta_1 x_{1t} + \beta_2 x_{2t} + \zeta_t, \quad (21)$$

where the cycles coefficients  $\beta_1$  and  $\beta_2$  carry information about the amplitude and phase. The amplitude and phase can be expressed in terms of  $\beta_1$  and  $\beta_2$  as

$$A = \sqrt{\beta_1^2 + \beta_2^2}, \quad (22)$$

$$\phi = \tan^{-1}(\beta_1/\beta_2). \quad (23)$$

Special attention is, however, required for the expression of phase  $\phi$  and its interpretation. Typically,  $F(t)$  in (14) is presented somewhat differently with respect to  $\phi$  (see, e.g., Shumway and Stoffer; 2011, pp. 175-177; Madden et al., 2018),

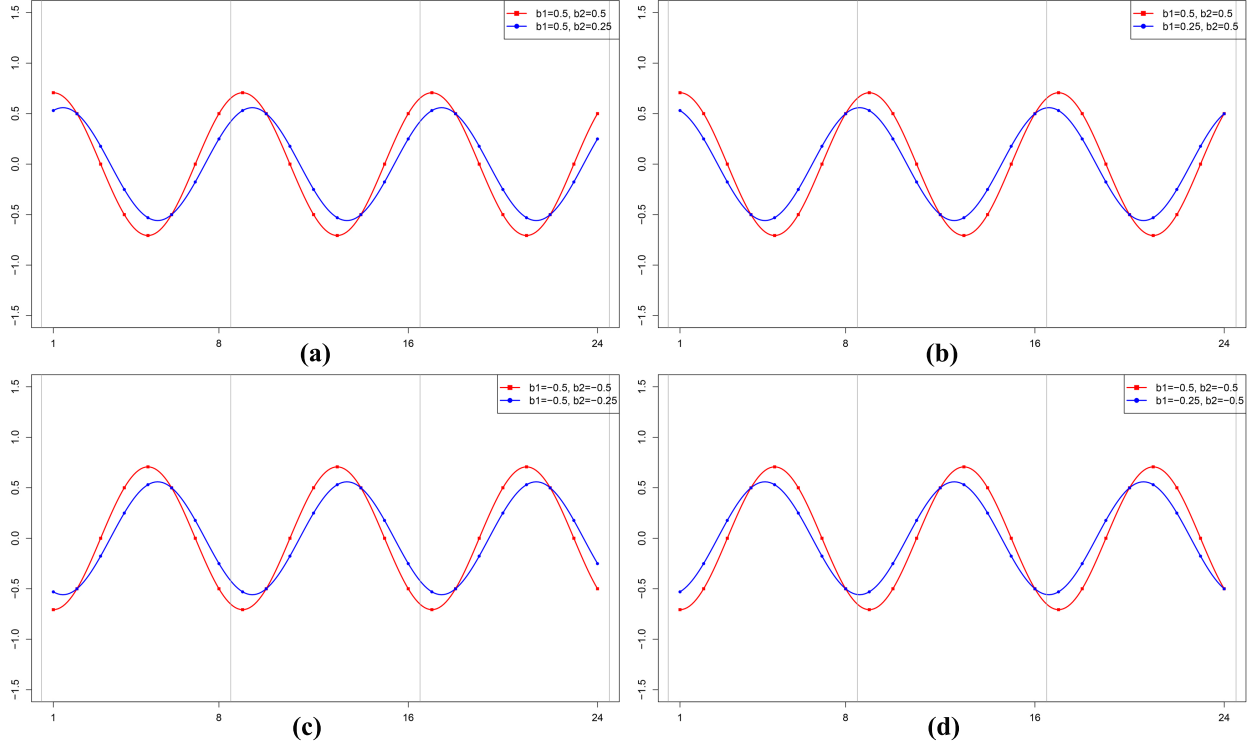
$$F(t) = A \cos (2\pi \omega t + \phi). \quad (24)$$

The alternative of using (14) ensures that  $\phi$  can be interpreted on the scale of  $t$  and as the first peak of the curve after  $t = 0$ . It is then possible to connect  $\phi$  directly to the time series plots of the variable. This definition of  $\phi$  is described in detail in the Supplementary material and is especially important for analyses allowing individually-varying phase using Bayesian estimation.

The frequency index  $\omega$  is chosen by the analyst and can be understood by the following examples. In a 24-hour cycle,  $\omega = 1/24$  with cycles duration is 24. The variable  $t$  can also be used to represent the  $t^{\text{th}}$  measurement. For example, with measurements every third hour, the 24-hour cycle is represented by eight measurements so that  $\omega = 1/8$  with cycles duration 8. With a 24-hour cycle represented by three measurements,  $\omega = 1/3$  with cycles duration 3.

Figure 5 shows the sine-cosine function in (14) for 24-hour cycles over three days using  $\omega = 1/8$  corresponding to eight measures per day. For panel (a), the red curve

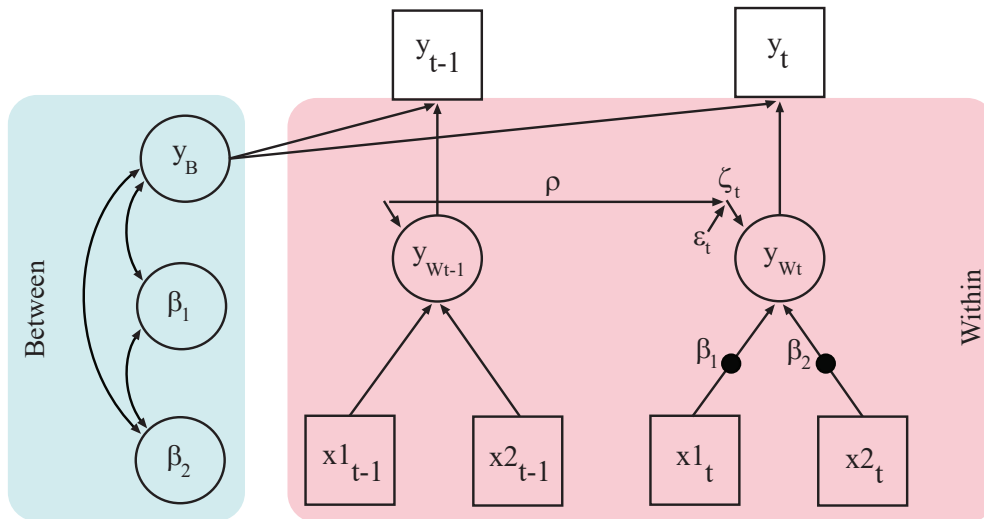
Figure 5: Sine-cosine curves for daily cycles over 3 days



marked by dots has  $\beta_1 = \beta_2 = 0.5$  and the blue curve marked by squares has  $\beta_1 = 0.5$ ,  $\beta_2 = 0.25$ . Compared to the red curve, the blue curve has a lower amplitude due to a smaller  $\beta_2$  value (red amplitude = 0.71, blue amplitude = 0.56). Because the  $\beta_1/\beta_2$  ratio for the blue curve is not 1 as for the red curve, the phase is also different for the red and blue curves (red phase = 1, blue phase = 1.4). For both curves, the peaks occur right after midnight. The blue curve emphasizes the sine part more than the cosine part and has its peaks later than the red curve. The red curve is the same for panels (a) and (b) but the blue curve in (b) reverses the sine-cosine emphasis, using  $\beta_1 = 0.25$ ,  $\beta_2 = 0.5$  and showing that the peaks occur late at night instead of right after midnight as for the red curve (for curve (b), red phase = 1, blue phase = 0.6). The curves of panels (a) and (b) may be representative of cycles for tiredness, a variable that will be studied in the examples section. The bottom panels (c) and (d) reverse the signs of  $\beta_1$ ,  $\beta_2$  as compared to panels (a) and (b). The sign change does not affect the amplitudes so they are the same as for (a) and (b). The reverse sign makes the peaks appear midday instead of in the evening/at night (red curve phase = 5 for both (c) and (d), blue curve phase for (c) = 5.4, and blue curve phase for (d) = 4.6). The red curve is the same for (c) and (d). Comparing (c) to (d) for the blue curve shows that the larger emphasis on the cosine component in (d) makes the peaks appear earlier in the day. Panels (c) or (d) are possible candidates for the PA cycles.

The function in (14) and (24) has been used in a regression setting referred to as the cosinor model (see, e.g., Portaluppi et al., 1988). Allowing for random effects, Madden

Figure 6: Two-level RDSEM with random slopes for cycles



et al. (2018) considered the cosinor model for individual  $i$  and timepoint  $t$ ,

$$y_{it} = \beta_{0i} + \beta_{1i}x_{1t} + \beta_{2i}x_{2t} + \zeta_{it}, \quad (25)$$

where  $\beta_{0i}$ ,  $\beta_{1i}$ , and  $\beta_{2i}$  are random coefficients varying over individuals and  $\zeta_{it}$  has an auto-regressive structure to take into account that measurements across time are likely to be correlated not only due to their random effects but also due to being close in time. The Madden et al. (2018) application to blood pressure cycles also explored multi-component cosinor modeling obtained by using a sum of cosinor functions having cycles of different duration.

The cosinor model fits into the twolevel RDSEM framework shown in Figure 6. The filled circles  $\beta_1$  and  $\beta_2$  in the within part of the figure represent the random slopes for  $x_1$  and  $x_2$ . Their variation is shown in the between part of the model together with the random intercept  $y_B$ . Using the decomposition  $y_{it} = y_{Bi} + y_{Wit}$ , this is expressed in line with (12), (13) as a two-level RDSEM with a within and between part,

$$y_{Wit} = \beta_{1i}x_{1,t} + \beta_{2i}x_{2,t} + \zeta_{it}, \quad (26)$$

$$\zeta_{it} = \rho \zeta_{it-1} + \epsilon_{it}, \quad (27)$$

$$y_{Bi} = \mu + \delta_{0i}, \quad (28)$$

$$\beta_{1i} = \beta_1 + \delta_{1i}, \quad (29)$$

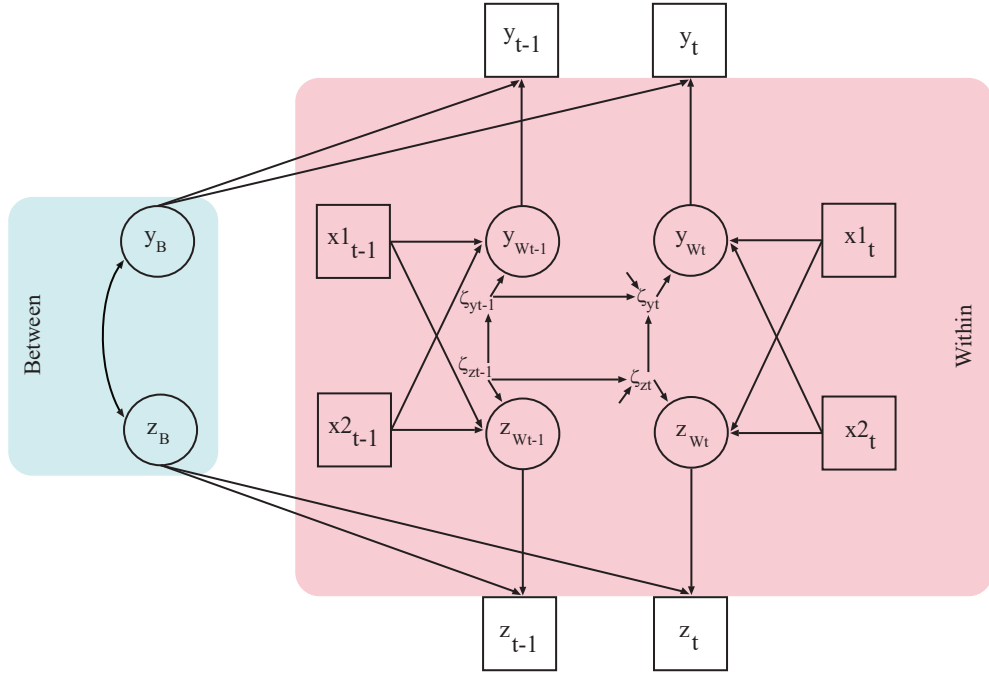
$$\beta_{2i} = \beta_2 + \delta_{2i}. \quad (30)$$

Relating this to the cosinor model (25),  $\rho$  represents the auto-regressive coefficient for  $\zeta$ ,  $y_{Bi}$  represents the random intercept  $\beta_{0i}$ , and  $\beta_{1i}$ ,  $\beta_{2i}$  are the random slopes.

Figure 7 shows a generalization of the cosinor model with cycles for two outcomes. This bivariate version also fits into the framework of the two-level RDSEM model as implemented in Mplus. The two variables  $y$  and  $z$  both follow cycles models but have different  $\beta$  slopes.<sup>1</sup> This model is of interest when the focus is on whether there is

<sup>1</sup>Compared to Figure 6, the  $x_1$ ,  $x_2$  variables are moved to the side to make the figure more clear.

Figure 7: Bivariate two-level RDSEM with cycles



a residual relationship between the two variables after accounting for the cycles, for instance, if a researcher wants to know whether tiredness is related to PA above and beyond circadian rhythms. This relationship is expressed in the within part of the model as a regression of  $\zeta_y$  on  $\zeta_z$ . This regression may have a random slope.

A cross-classified DSEM model is shown in Figure 8. This uses the three model parts, Between ID, Within, and Between Time based on the 3-way latent variable decomposition in (7),  $y_{it} = y_{Bi} + y_{Wit} + y_{Tt}$ , where

$$y_{Bi} = \mu + \delta_i, \quad (31)$$

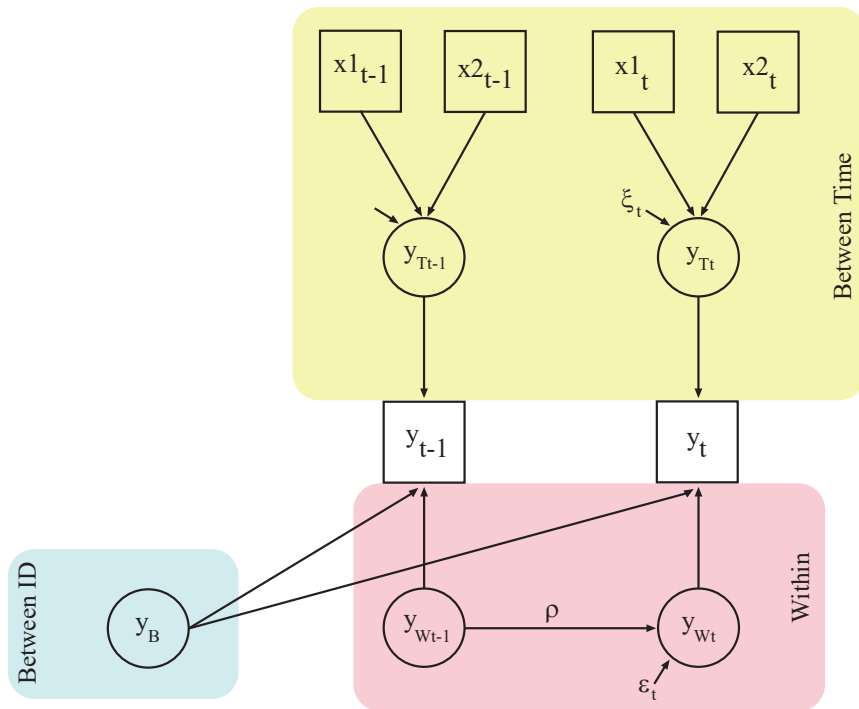
$$y_{Wit} = \rho y_{Wit-1} + \epsilon_{it}, \quad (32)$$

$$y_{Tt} = \beta_1 x_{1,t} + \beta_2 x_{2,t} + \xi_t. \quad (33)$$

Here, (33) does not have random cycles coefficients  $\beta$  as for the two-level RDSEM in (26). The extension to random coefficients will be discussed next in conjunction with cross-classified RDSEM in Figure 9. A more elaborate model on the within level is possible in line with the within part of Figure 2.

The cross-classified model of Figure 8 can also be expressed as in Figure 9. In line with two-level RDSEM of Figure 6, Figure 9 specifies the cycles on the within level instead of on the between time level. The between time level consists of only the time-specific components without a structure, just like in Figure 3. Instead of (31) - (33),

Figure 8: Cross-classified DSEM with cycles



the Figure 9 model is written as

$$y_{Bi} = \mu + \delta_i, \quad (34)$$

$$y_{Wit} = \beta_1 x_{1,t} + \beta_2 x_{2,t} + \zeta_{it}, \quad (35)$$

$$\zeta_{it} = \rho \zeta_{it-1} + \epsilon_{it}, \quad (36)$$

$$y_{Tt} = \xi_t. \quad (37)$$

This is referred to as cross-classified RDSEM instead of cross-classified DSEM because the within level relationship over time is specified as auto-regression for the residuals  $\zeta$ . The models of Figure 8 and Figure 9 are, however, equivalent. This can be seen by the implied observed  $y_{it} = y_{Bi} + y_{Wit} + y_{Tt}$  which can be re-written as

$$\text{Figure 8 : } y_{it} = \mu + \delta_i + \beta_1 x_{1,t} + \beta_2 x_{2,t} + \xi_t + y_{Wit}, \quad (38)$$

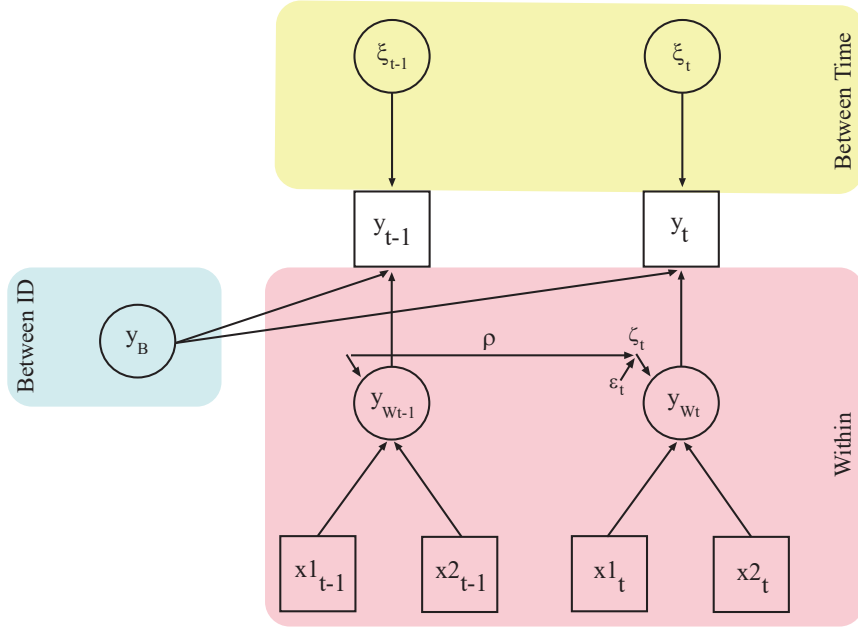
$$\text{Figure 9 : } y_{it} = \mu + \delta_i + \beta_1 x_{1,t} + \beta_2 x_{2,t} + \xi_t + \zeta_{it}, \quad (39)$$

where all terms are the same with  $\zeta_{it}$  of Figure 9 playing the role of  $y_{Wit}$  in Figure 8. The cycles coefficients  $\beta_1, \beta_2$  are the same in (33) and (35), the within-level regression slope  $\rho$  is the same, and the residual  $\xi_t$  is the same. The residual refers to the across-time variation that the cycles don't explain. In the model of Figure 9, these residuals can be estimated and plotted which makes this model version useful in the search for deviations from cycles as will be seen in the example section.<sup>2 3</sup>

<sup>2</sup>This model was introduced in Mplus version 8.11.

<sup>3</sup>Unlike the  $y_{Tt}$  components of Figure 8, however, the estimated  $y_{Tt}$  components of Figure 9 have the

Figure 9: Cross-classified RDSEM with cycles on within



The cross-classified DSEM model of Figure 9 has the advantage over the Figure 8 model in that it can be extended to allow random cycles coefficients for the within level just like in the two-level RDSEM of Figure 6. The random coefficient version of the Figure 9 model is more general than the two-level RDSEM model of Figure 6 because of the Between Time part that allows time-specific, person-invariant deviations from the cycles. This version of Figure 9 is yet another extension of the cosinor model. The random coefficients are added to the Between ID part of the model together with  $y_B$ . In contrast, random cycles coefficients cannot be used in the Between Time part of the model in Figure 8 or Figure 9 because the components of the Between Time part of the model cannot vary across persons, only across time.

### 3.1 Summary of analysis steps and models

Table 1 gives a summary of the different categories of cycles models presented so far and a look ahead to the analyses in the example section. The different categories are shown in the form of five recommended analysis steps that will be used in the example section. The model names and the corresponding figures are listed together with a comments column that will be elaborated on in the example section. Step 1 is to find indications of cycles and their duration. The models in 1a and 1b are referred to as unrestricted cross-classified models because they do not impose any structure on the development over time. The step 1a model was discussed in connection with Figure 3. The factor analysis alternative 1b will be discussed in the examples section. Step 2 is fitting cycles

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disadvantage that they don't contain the cycles so a time series plot of the cycles cannot be directly obtained by Mplus from that model.

models based on the step 1 findings. Models with fixed as opposed to random cycles coefficient is a recommended start for simplicity. Here, there are several cross-classified and two-level model alternatives depending on analysis findings. The step 2a model alternative discussed in connection with Figure 8 is the recommended first approach. The factor analysis alternative 2b will be discussed in the examples section as will the bivariate model of 2d. Step 3 aims to find important deviations from the cycles model, also using the fixed coefficients approach for simplicity. Different approaches for this step are discussed in the examples section. Step 4 is using random cycles coefficients to explore if there is important variation across persons in the cycles. Here, there are also several modeling approaches depending on the analysis findings and the aims of the study. The recommended first alternative 4a is the cosinor model of (25). Step 5 is relating the variation in the cycles coefficients to time-invariant, person-specific background variables. These models are discussed in the examples section.

### 3.2 Monte Carlo simulations with cycles using twolevel and cross-classified RDSEM

Before turning to the examples section, a small simulation study examines the twolevel and cross-classified models used to fit the circadian cycles of analysis steps 2 and 4 in Table 1. Based on the models of Figure 6, Figure 7, and Figure 8, the simulations explore how well the cycle parameters can be recovered under different measurement designs. The first design matches that of the PA example discussed in the next section with eight measures per day for seven days for a total of 56 timepoints ( $T = 56$ ). Often times, in ILD, compliance is not 100% and there may be limitations to the feasibility of collecting more than 50 assessments. Therefore, scenarios of having fewer assessments per person is of interest. The question is if fewer measures per day over fewer days can give good results, here represented by three measures per day for five days ( $T = 15$ ). The population parameter values are based on the analyses in the example section. A sample size of 200 is used and the Monte Carlo runs are carried out with 500 replications.<sup>4</sup> Sample sizes of 50 and 800 are also briefly considered.

Table 2 presents results for the two-level RDSEM model with random cycles coefficients shown in (26) - (30) and Figure 6. This is the cosinor model of (25) and corresponds to the step 4a model in terms of Table 1. The first column shows the parameters. Here,  $\hat{Y}_1$  refers to the auto-regression coefficient  $\rho$  among the residuals. The key estimates of the means of the random  $\beta_1, \beta_2$  are found in the Between Level rows labeled SX1, SX2. The second and third columns show the parameter values generating the data which can be compared to the average estimates over the replications to check for bias in the estimates. The fourth column shows the standard deviation over the replications which is used to check agreement with the fifth column of estimated standard error averages over the replications. The 6th and 7th columns show the mean squared error (M.S.E.) of the estimate and the 95% credibility interval coverage. The last 2 columns show the power to reject a zero parameter value as judged by the proportion of replications for which the credibility interval does not include zero.

The top part of the table shows the results for  $T = 56$  with 8 measures per day for 7 days. The parameter values are well recovered, the standard error averages (S.E. Average column) agree well with the empirical variation (Std. Dev. column), and the

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<sup>4</sup>Mplus scripts are given in the Supplementary material.

Table 1: Summary of analysis steps

Steps	Models and Figures	Comments
<b>1. Finding cycles and their duration</b>		
1a	Cross-classified DSEM, Figure 3	Unrestricted model, time series plot of $y_{Tt}$ estimates
1b	Cross-classified DSEM, Figure 14	Unrestricted model, factor analysis
<b>2. Fitting cycles, fixed cycles coefficients</b>		
2a	Cross-classified DSEM, Figure 8	Cycles duration based on step 1
2b	Cross-classified DSEM, Figure 15	Factor analysis
2c	Two-level RDSEM Figure 6, simplified to fixed coefficients	If small residual variance on Between Time level of 2a
2d	Two-level RDSEM, Figure 7	Bivariate model and small 2a residual variance
<b>3. Finding deviations from cycles</b>		
3a	Cross-classified DSEM, Figure 8	Adding dummy variables (approach 1) or BSEM (approach 2)
3b	Cross-classified RDSEM, Figure 9, Figure 15	Testing significance of Between Time estimates (approach 3)
<b>4. Fitting cycles, random cycles coefficients</b>		
4a	Two-level RDSEM, Figure 6, cosinor model (25)	If small residual variance on Between Time level of 2a
4b	Two-level RDSEM, Figure 7, extended to random coefficients	Bivariate model and small 2a residual variance
4c	Cross-classified RDSEM, Figure 9, extended to random coefficients	More time consuming than two-level analysis
<b>5. Explaining random cycles coefficients by covariates</b>		
5a	Two-level RDSEM, Figure 17	Factor analysis
5b	Analysis of amplitude and phase	Multiple imputation plus single-level analysis



95% coverage is good. The power to reject zero  $\beta$  coefficients is 1.000 for SX1 but only 0.130 due to the lower population value of SX2 (% Sig Coeff column). The bottom part of the table shows results for  $T = 15$  with 3 measures per day for 5 days. The results are still good but estimates have somewhat higher variability as expected. This shows that for these cycle parameter values, the parameters are well recovered so that a data collection design of only 3 measures per day for 5 days is sufficient to capture the cycles. Note, however, that this conclusion is based on generating data with the parameter values found in the current example and cannot be counted on to generalize to other studies.

Table 3 presents results for the bivariate two-level RDSEM model shown in Figure 7, using both the  $T = 56$  and the  $T = 15$  data collection designs. This is the step 2d model in terms of Table 1. The simulation results are good also for this bivariate cycle model. Once again, the power to reject zero  $\beta$  coefficients for the cycles varies strongly as a function of the size of the population value. The key residual relationship between the two outcomes, accounting for their cycles, is reported on the within level row labeled  $\hat{Y} \text{ ON } \hat{Z}$ . This parameter is well estimated also with the  $T = 15$  design with power 1.000. The variability of the estimate is, however, approximately twice as large for the  $T = 15$  design as for the  $T = 56$  design so that the  $T = 56$  design gives a much more precise estimate.

Table 4 presents results for the cross-classified DSEM model of (31) - (33) and Figure 8. This is the step 2a model in terms of Table 1. The key estimates of  $\beta_1$ ,  $\beta_2$  are found in the Between TIME Level rows labeled Y ON X1 X2. The top part of the table shows the results for the  $T = 56$  case. The parameter values are well recovered, the standard error averages agree well with the empirical variation, and the 95% coverage is good. The power to reject zero  $\beta$  coefficients is high with estimated values of 0.996 and 0.834, respectively. The high power for the  $\beta_2$  coefficient may be due to its higher population value than in Table 2 and Table 3. The bottom panel of Table 4 shows the results for the  $T = 15$  case. The estimation is still satisfactory but variability of the estimates is larger. For instance, the variation in the  $\beta_1$  coefficient for X1 with  $T = 56$  is only 61% of that with  $T = 15$  (see the St. Dev. column). The power estimates for the two cycles coefficients have now dropped to 0.616 and 0.306, respectively. This model has an extra parameter relative to the cosinor model with fixed cycles coefficients, namely the Between Time level residual variance. This parameter is well estimated for the  $T = 56$  design but not for the  $T = 15$  design.

Changing the sample size affects the cycles slope estimates differently for the different models. Increasing the sample size by a factor of 4 from  $N = 200$  to  $N = 800$  for the two-level random RDSEM in Table 2 cuts the variability of the mean  $\beta_1$  estimate in half. Decreasing the sample size by a factor of 4 from  $N = 200$  to  $N = 50$  doubles the variability of the mean  $\beta_1$  estimate. This is as expected for parameters on the between level where sample size has a direct impact. The simulation results are still satisfactory for  $N = 50$ .

Changing the sample size has less effect on the results for the cross-classified model in Table 4 where the cycles slopes are not random and are therefore not between-level parameters. For  $T = 15$ , the variability of the  $\beta_1$  estimate when quadrupling the sample size to  $N = 800$  is reduced by only 8%. The power is also affected very little, changing from 0.616 to 0.696. Decreasing the sample size to  $N = 50$ , however, increases the variability of the  $\beta_1$  estimate by 35% and decreases the power to 0.360.

Table 2: Monte Carlo simulations using two-level random RDSEM cycles analysis with N = 200

T=56: 8 measures per day, 7 days							
	ESTIMATES			S.E.	M.S.E.	95% Cover	% Sig Coeff
	Population	Average	Std. Dev.	Average			
Within Level							
Y^ ON							
Y^1	0.372	0.3735	0.0090	0.0093	0.0001	0.956	1.000
Residual Variances							
Y	0.511	0.5116	0.0069	0.0072	0.0000	0.948	1.000
Between Level							
Y WITH							
SX1	-0.005	-0.0063	0.0130	0.0139	0.0002	0.964	0.062
SX2	-0.013	-0.0150	0.0116	0.0125	0.0001	0.964	0.240
SX1 WITH							
SX2	-0.001	-0.0006	0.0029	0.0026	0.0000	0.902	0.118
Means							
Y	5.673	5.6719	0.0599	0.0650	0.0036	0.974	1.000
SX1	-0.089	-0.0890	0.0150	0.0147	0.0002	0.950	1.000
SX2	-0.007	-0.0077	0.0142	0.0129	0.0002	0.918	0.130
Variances							
Y	0.748	0.7790	0.0760	0.0831	0.0067	0.954	1.000
SX1	0.015	0.0162	0.0049	0.0046	0.0000	0.936	1.000
SX2	0.008	0.0086	0.0034	0.0032	0.0000	0.942	1.000
T=15: 3 measures per day, 5 days							
	ESTIMATES			S.E.	M.S.E.	95% Cover	% Sig Coeff
	Population	Average	Std. Dev.	Average			
Within Level							
Y^ ON							
Y^1	0.372	0.3839	0.0226	0.0223	0.0006	0.896	1.000
Residual Variances							
Y	0.511	0.5148	0.0153	0.0150	0.0002	0.942	1.000
Between Level							
Y WITH							
SX1	-0.005	-0.0065	0.0165	0.0165	0.0003	0.944	0.076
SX2	-0.013	-0.0139	0.0152	0.0157	0.0002	0.956	0.152
SX1 WITH							
SX2	-0.001	-0.0015	0.0037	0.0035	0.0000	0.922	0.086
Means							
Y	5.673	5.6681	0.0649	0.0671	0.0042	0.966	1.000
SX1	-0.089	-0.0890	0.0172	0.0168	0.0003	0.952	0.998
SX2	-0.007	-0.0057	0.0170	0.0158	0.0003	0.928	0.086
Variances							
Y	0.748	0.7655	0.0863	0.0881	0.0077	0.958	1.000
SX1	0.015	0.0169	0.0064	0.0062	0.0000	0.942	1.000
SX2	0.008	0.0107	0.0047	0.0046	0.0000	0.916	1.000

Table 3: Monte Carlo simulations using bivariate two-level RDSEM cycles analysis with N = 200

T=56: 8 measures per day, 7 days							
	ESTIMATES			S.E.	M.S.E.	95%	% Sig
	Population	Average	Std. Dev.	Average		Cover	Coeff
Within Level							
Y ON							
X1	-0.093	-0.0925	0.0122	0.0123	0.0001	0.934	1.000
X2	-0.015	-0.0158	0.0128	0.0118	0.0002	0.918	0.310
Y^ ON							
Y^1	0.353	0.3529	0.0089	0.0088	0.0001	0.946	1.000
Z^	-0.124	-0.1245	0.0051	0.0053	0.0000	0.944	1.000
Z ON							
X1	-0.037	-0.0357	0.0208	0.0197	0.0004	0.936	0.450
X2	0.526	0.5266	0.0200	0.0198	0.0004	0.942	1.000
Z^ ON							
Z^1	0.387	0.3875	0.0091	0.0089	0.0001	0.946	1.000
Residual Variances							
Y	0.492	0.4916	0.0067	0.0067	0.0000	0.946	1.000
Z	1.411	1.4113	0.0197	0.0191	0.0004	0.944	1.000
Between Level							
Y WITH							
Z	-0.534	-0.5494	0.0874	0.0901	0.0079	0.950	1.000
Means							
Y	5.667	5.6680	0.0623	0.0615	0.0039	0.940	1.000
Z	3.556	3.5551	0.0883	0.0881	0.0078	0.946	1.000
Variances							
Y	0.746	0.7621	0.0746	0.0835	0.0058	0.972	1.000
Z	1.440	1.4777	0.1573	0.1623	0.0261	0.944	1.000
T=15: 3 measures per day, 5 days							
	ESTIMATES			S.E.	M.S.E.	95%	% Sig
	Population	Average	Std. Dev.	Average		Cover	Coeff
Within Level							
Y ON							
X1	-0.093	-0.0923	0.0145	0.0151	0.0002	0.948	1.000
X2	-0.015	-0.0153	0.0163	0.0151	0.0003	0.912	0.202
Y^ ON							
Y^1	0.353	0.3608	0.0206	0.0199	0.0005	0.914	1.000
Z^	-0.124	-0.1272	0.0108	0.0108	0.0001	0.932	1.000
Z ON							
X1	-0.037	-0.0374	0.0238	0.0238	0.0006	0.952	0.344
X2	0.526	0.5261	0.0260	0.0250	0.0007	0.940	1.000
Z^ ON							
Z^1	0.387	0.3978	0.0221	0.0206	0.0006	0.888	1.000
Residual Variances							
Y	0.492	0.4950	0.0131	0.0138	0.0002	0.940	1.000
Z	1.411	1.4274	0.0401	0.0395	0.0019	0.930	1.000
Between Level							
Y WITH							
Z	-0.534	-0.5305	0.0963	0.0963	0.0093	0.950	1.000
Means							
Y	5.667	5.6672	0.0644	0.0636	0.0041	0.940	1.000
Z	3.556	3.5530	0.0893	0.0929	0.0080	0.964	1.000
Variances							
Y	0.746	0.7540	0.0825	0.0895	0.0069	0.964	1.000
Z	1.440	1.4363	0.1734	0.1765	0.0300	0.950	1.000

Table 4: Monte Carlo simulations using cross-classified DSEM cycles analysis with N = 200

T = 56: 8 measures per day, 7 days							
	ESTIMATES			S. E.	M. S. E.	95% Cover	% Sig Coeff
	Population	Average	Std. Dev.	Average			
Within Level							
Y ON							
Y&1	0.371	0.3723	0.0092	0.0091	0.0001	0.958	1.000
Residual Variances							
Y	0.513	0.5131	0.0069	0.0069	0.0000	0.946	1.000
Between TIME Level							
Y ON							
X1	-0.088	-0.0897	0.0196	0.0197	0.0004	0.938	0.996
X2	-0.060	-0.0587	0.0193	0.0199	0.0004	0.964	0.834
Residual Variances							
Y	0.006	0.0063	0.0018	0.0019	0.0000	0.950	1.000
Between ID Level							
Means							
Y	5.676	5.6753	0.0654	0.0641	0.0043	0.952	1.000
Variances							
Y	0.740	0.7444	0.0806	0.0833	0.0065	0.940	1.000
T = 15: 3 measures per day, 5 days							
	ESTIMATES			S. E.	M. S. E.	95% Cover	% Sig Coeff
	Population	Average	Std. Dev.	Average			
Within Level							
Y ON							
Y&1	0.371	0.3782	0.0202	0.0215	0.0005	0.958	1.000
Residual Variances							
Y	0.513	0.5161	0.0130	0.0142	0.0002	0.960	1.000
Between TIME Level							
Y ON							
X1	-0.088	-0.0906	0.0319	0.0392	0.0010	0.968	0.616
X2	-0.060	-0.0597	0.0332	0.0399	0.0011	0.966	0.306
Residual Variances							
Y	0.006	0.0083	0.0044	0.0070	0.0000	0.958	1.000
Between ID Level							
Means							
Y	5.676	5.6740	0.0674	0.0669	0.0045	0.956	1.000
Variances							
Y	0.740	0.7422	0.0822	0.0822	0.0067	0.946	1.000

The simulation results are still satisfactory for  $N = 50$ . It should be emphasized that these simulation results are strongly dependent on the parameter values chosen for data generation. Although they are derived from the analyses of the example, other studies may have quite different parameter values. Using the Mplus scripts in the Supplementary material as templates, researchers can use parameter values relevant for their studies to plan measurement designs using further Monte Carlo simulations.

The simulation study just presented focuses on the situation where the cyclicity is known, in this case 24-hour cycles. As mentioned earlier, to explore if there is cyclical behavior and what the cycle length is, it is useful to as a first step do a cross-classified DSEM analysis without a cyclical model imposed, obtaining the  $T y_{Tt}$  estimates of (7). In Table 1, such an analysis was referred to as an unrestricted cross-classified DSEM. In principle, it is of interest to do a study where data are generated from a cross-classified DSEM with a specific cyclical model and analyzed with an unrestricted cross-classified DSEM. The  $T y_{Tt}$  estimates can then be plotted to see how clearly the known cycles patterns can be discerned. In such a study, the data collection design choice of number of measurements per day, number of days, and sample size may be more critical. For example, the  $T = 15$  design with only 3 measurement per day may not give a clear pattern. Such a study is, however, beyond the scope of this paper.

## 4 Example

The cycles illustration uses data from a study designed to detect at-risk mood profiles related to depression in adolescents (see, e.g., de Haan-Rietdijk et al., 2017 and Dittvorst et al., 2021). Experience Sampling Method (ESM) questionnaires measuring positive and negative affect were administered to 240 Dutch adolescents ages 12 to 16 with 63% girls. Several measures per day were collected for seven days, Tuesday - Monday. Positive affect (PA) was measured as the average of six 7-category items, relaxed, satisfied, confident, happy, energetic, and excited. The PA analyses will focus both on the average and the items it consists of. Fluctuations in PA will be related to a measure of tiredness. Covariates gender, age, SDQ (measure of childhood emotional problems) were collected at baseline and will be used to predict PA fluctuations.

Participants filled out ESM questionnaires throughout the day, including during school hours with questionnaires delivered on the adolescents' own smartphones. The intention was to obtain eight measurements per day taken randomly in three blocks of time between 8 am and 10pm: A morning measurement between 8 am and 10 am, six measurements between 10 am and 8 pm, and an evening measurement between 8 pm and 10 pm. The individually-varying random time points are handled as described in Hamaker et al. (2023) and Muthén and Asparouhov (2023), synchronizing time by inserting missing data for individuals when times are not observed. A choice is made to represent the 24 hours by eight 3-hour intervals with zero and 24 representing midnight: 0-3, 3-6, 6-9, 9-12, 12-15, 15-18, 18-21, 21-24.<sup>5</sup>

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<sup>5</sup>This uses the TINTERVAL option in Mplus with TINTERVAL = 3.

## 4.1 Understanding the longitudinal data features

A first concern is to get a picture of the data in a reasonably summarized form as a basis for further analysis. The individual data points are too sparse and varied to give good clues of the development over time. Figure 10 shows three efforts to characterize the PA values for the 56 timepoints of the seven days of Tuesday through Monday. In order of the legend, curve number 1 (red curve marked with dots) shows the observed means over individuals at each time point. The y-axis range is about one PA standard deviation computed over all persons and time points. The different time points are represented by quite different number of individuals and the means therefore have different precision. For instance, the lowest values early Saturday and Monday are observed by only 10 and 9 individuals, respectively. In contrast, the two highest values on Friday evening are observed by 128 and 29 individuals, respectively. The curve may also suffer from non-MCAR missingness in that the means are computed using only the available data at a certain time point as opposed to all time points jointly.

Curve number 2 (green curve marked with triangles) shows the means estimated by maximum-likelihood<sup>6</sup> in a single-level, 56-variable wide format so that MAR missingness is allowed for by drawing on information from all time points. The model chosen for this uses a random intercept factor influencing all time points with loadings 1 and uses equal auto-regressions with lag 1 for the residuals in line with the twolevel DSEM model of (1), (2), except allowing fixed-effects means that are different across time. Note that this is different from a two-level analysis which would hold both the means and the residual variances equal over time providing no information on mean changes over time. It is seen that curve 1 is higher than curve 2 at several time points. Although most differences may be insignificant, this suggests a possible selection phenomenon where at lower PA values, individuals are more likely to have missing data. A partial support for this notion is a small positive correlation of 0.123 (.067) between the PA mean at a certain time point and the number of individuals at this time point.

Curve number 3 (blue curve marked with squares) is obtained by the Figure 3 cross-classified DSEM model of (8) - (10). This is the step 1a model in the summary of Table 1. As for curve 2, cross-classified DSEM allows MAR missingness due to each  $PA_{Tt}$  estimate drawing on information from all time points jointly. The plot shows the 56  $PA_{Tt}$  estimates, adding the 5.690 estimate of the  $\mu$  mean of  $PA_{Bi}$  to place the random effects on the same scale as the other two curves. As opposed to the curve 2 means, the curve 3  $PA_{Tt}$  values are random effects specified to have a normal distribution. The normality serves as a prior that avoids more extreme values based on few observations. In this way, the curve exhibits the usual multilevel shrinking towards the mean. Curve 3 is also the preferred approach when the number of timepoints make the wide approach of curve 2 infeasible.

All three curves show a daily cyclical pattern with lower PA values in the morning, increasing to a peak around midday and staying high into the late afternoon and evening. A similar pattern was also observed in Watson et al. (1999). The pattern is more clearly seen in curves 2 and 3 which substantially reduce the volatility of the observed means of curve 1, with curve 3 being the least volatile.

The cross-classified DSEM analysis informs about the relative contribution to the PA variance from the three components,  $PA_B$ ,  $PA_W$ , and  $PA_T$ . The variances are

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<sup>6</sup>Bayes estimation gives very similar results.

Figure 10: PA means for Tuesday - Monday estimated by three methods (the x-axis corresponds to the 56 timepoints)

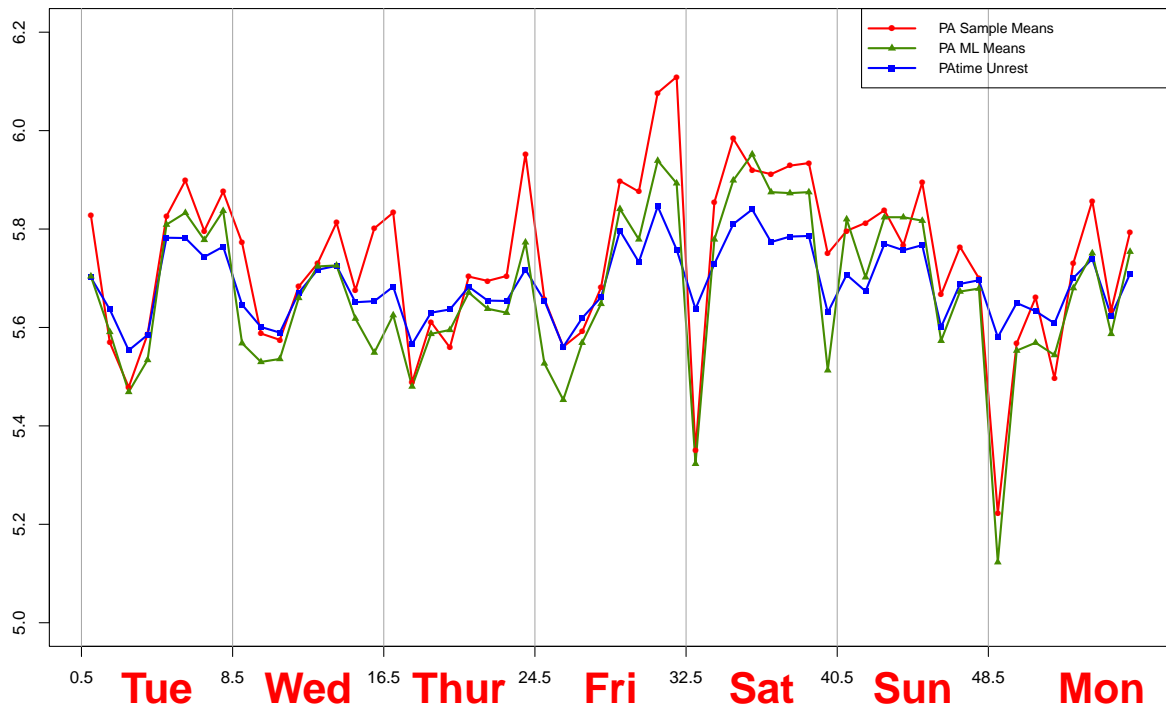


Table 5: Estimated cyclical cross-classified DSEM

	Estimate	Posterior S.D.	95% C.I.		Significance
			Lower 2.5%	Upper 2.5%	
Within Level					
PA ON					
PA&1	0.371	0.015	0.342	0.401	*
Residual Variances					
PA	0.513	0.010	0.493	0.532	*
Between TIME Level					
PA ON					
X1	-0.088	0.024	-0.137	-0.039	*
X2	-0.009	0.025	-0.057	0.039	
Residual Variances					
PA	0.006	0.003	0.002	0.014	*
Between ID Level					
Means					
PA	5.676	0.061	5.557	5.797	*
Variances					
PA	0.740	0.078	0.612	0.914	*

0.743, 0.593, and 0.010, adding up to a total PA variance of 1.346. Although this means that  $PA_T$  contributes less than 1% to the total variance, the spread in PA due to this component is 0.4 when considering  $\pm 2$  standard deviations, so that cycles can be clearly discerned.

## 4.2 Modeling the cycles and finding deviations from cycles

The next analysis step is to apply cyclical cross-classified DSEM modeling using (31) - (33) and Figure 8. This is the model of step 2a in the summary Table 1. The x values in (33) are computed as in (19) and (20),

$$x_{1t} = \sin(6.2831853 \times 1/8 \times t), \quad (40)$$

$$x_{2t} = \cos(6.2831853 \times 1/8 \times t), \quad (41)$$

where  $t$  ranges from 1 to 56. The estimates are given in Table 5. The auto-regression  $\rho$  is estimated as 0.371. The estimated  $\beta$  coefficients and their 95% credibility intervals are  $\hat{\beta}_1 = -0.088$  [-0.137 -0.039],  $\hat{\beta}_2 = -0.009$  [-0.157 0.039] so that the PA cycles curve is dominated by the sine component.

The use of  $R^2$  is helpful to describe model quality but needs a bit of elaboration.  $R^2$  values presented in Mplus refer to variance explained on each level separately. The



cycles account for a sizeable portion of the  $PA_T$  variance with an  $R^2$  of 0.409 but this needs to be viewed in the context of the total variance of PA which can be expressed as

$$V_{Total} = V_1(Between_{ID}) + V_2(cycles) + V_3(Between\ Time\ residual) \quad (42)$$

$$+ V_4(Within\ lag) + V_5(Within\ residual), \quad (43)$$

where the estimated  $R^2$  of 0.409 is computed using  $V_2/(V_2 + V_3)$ .<sup>7</sup> If the analysis instead places the cycles on the within level as in Figure 9, the within-level  $R^2$  is  $(V_2 + V_4)/(V_2 + V_4 + V_5)$  with an estimate of 0.149. From the estimates in Table 5, the estimated variances and percentages of total variance are<sup>8</sup>

$$1.344 = 0.740 + 0.004 + 0.006 + 0.082 + 0.513, \quad (44)$$

$$100 = 55.1 + 0.3 + 0.5 + 6.1 + 38.2. \quad (45)$$

Although the  $R^2$  percentage due to the  $V_2$  cycles is less than one percent, Figure 11 shows that the cycles can be clearly discerned. The figure displays the estimated cycles with the added constant of the estimated PA mean of 5.676 to put the cycles on the PA scale. As a comparison, the curve for the estimates from the previous unrestricted analysis of curve 3 in Figure 10 is also included.<sup>9</sup> It is clear that the cycles capture much of the daily variation, but there are also interesting deviations from the cycles. For instance, the fact that the PA on Saturday is higher than what the cycles predict seems reasonable in that school-aged adolescents may be waking up excited about being off school and thinking about the weekend. Deviations are also seen for Thursday and Sunday.

While Figure 11 shows curves from two different analyses that contrast the fitted cycles model with the unrestricted model, another way to study deviations from cycles is to plot the cycles together with the  $PA_T$  values from the Between Time part of the model from the same analysis so that the  $PA_T$  values are obtained from the model with the cycles imposed. This is shown in Figure 12. The deviations are now less pronounced and are mainly seen for Saturday.

The cross-classified DSEM model with cycles fits the means of the 56 timepoints using only two parameters in addition to the overall mean. An interesting question is how one can determine which days or timepoints have deviations from cycles that are of significant magnitude. It is of interest to find substantive explanations for large deviations. Three strategies for finding significant deviations from the cycles are used here. Once deviations have been found, the model can then be adjusted by adding dummy covariates to capture those deviations and thereby increase  $R^2$ .

A first, simple strategy to detect deviations from the cycles in the cross-classified DSEM is to add a dummy covariate for a certain day or timepoint and see if the regression coefficient is significant. This is analysis step 3a of the summary Table 1.

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<sup>7</sup>Given that  $x_1$  and  $x_2$  are uncorrelated, the  $V_2$  cycles variance is computed as the sum of the squared coefficients times their 0.5 variances.

<sup>8</sup>Due to variance stationarity,  $V(PA_t) = V(PA_{t-1})$ , the  $V_4$  variance due to the lag is computed using  $V(PA) = \rho^2 V(PA) + \theta$ , i.e.,  $V(PA) = \theta/(1 - \rho^2)$ , where  $\theta$  is the within residual variance. This gives  $V_4 = \rho^2 V(PA) = \rho^2 \theta/(1 - \rho^2)$ .

<sup>9</sup>To more clearly show difference between the two curves, the y-axis range is now about half of a PA standard deviation.

Figure 11: PA cross-classified DSEM estimates using cycles versus unrestricted (curves obtained from two separate analyses)

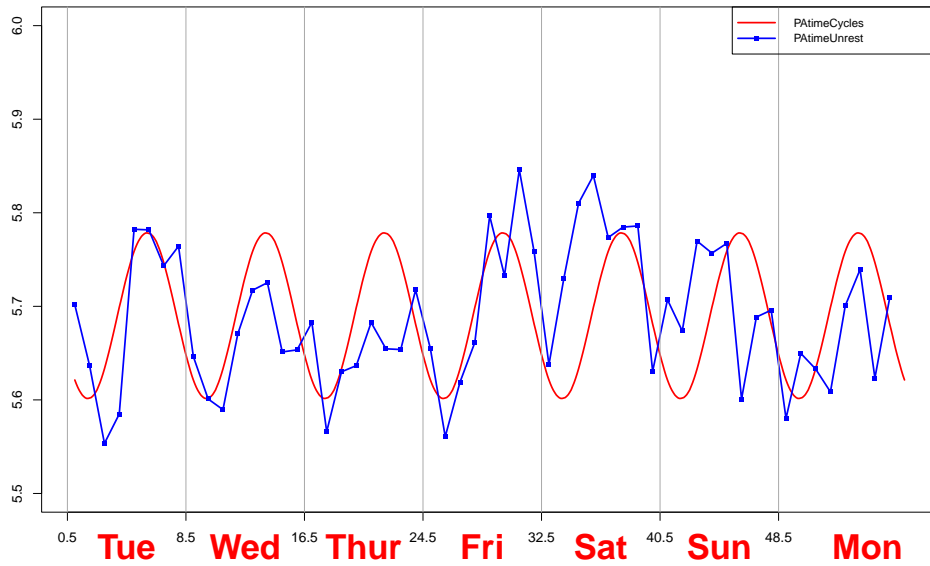
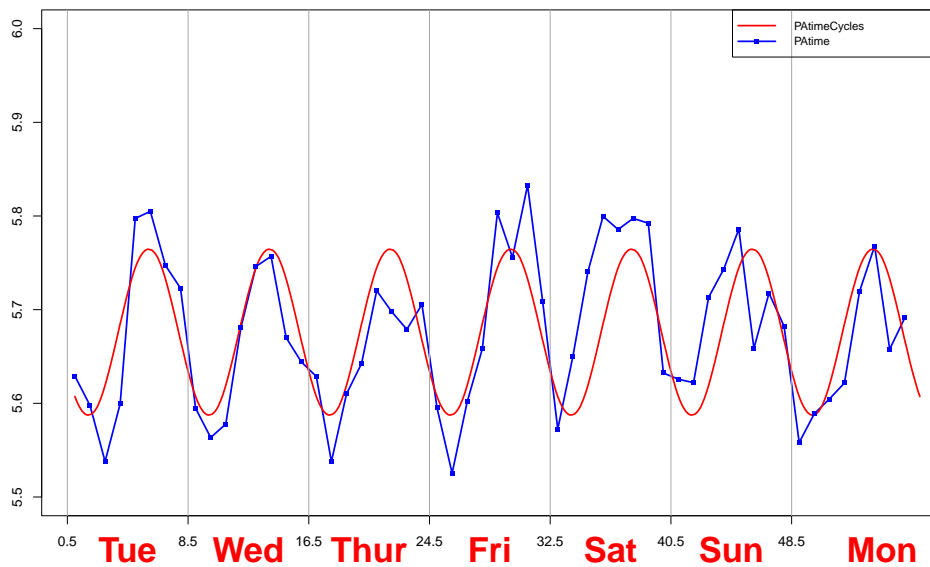


Figure 12: PA cross-classified DSEM estimates using cycles versus restricted (curves obtained from one analysis)



The day by day approach showed a significant effect only for Saturday with the  $R^2$  increasing from 0.409 with cycles only to 0.713. The effect is positive as expected based on Figure 11 and Figure 12.

A second strategy to detect deviations from the cycles is to use the BSEM approach of Muthén and Asparouhov (2012) where otherwise nonidentified parameters can be included in the model when applying small-variance priors. By this approach, it is possible to add a dummy covariate for each timepoint in addition to the cycles of the cross-classified DSEM, which would be cumbersome to do using the approach of adding a covariate for each timepoint at a time. The variance of the priors is chosen so that the data can overpower the priors and thereby inform on which timepoints need dummy covariates. Here, the prior  $N(0, 0.01)$  is used in line with Muthén and Asparouhov (2012). Using dummies for each of the 56 timepoints says that an added dummy covariate is needed only for timepoint 35 which represents the time slot of 6am - 9am on Saturday. Adding this dummy covariate increases the  $R^2$  from 0.409 to 0.881. The estimate for the covariate coefficient is significant positive as expected. An alternative BSEM approach is to instead explore dummy covariates for each weekday. This results in a significant positive effect for Saturday with an  $R^2$  of 0.737. The weekday dummy modeling can, however, also be done without BSEM priors, letting all dummy covariates have free coefficients while fixing the overall PA mean at zero. In comparison to the average weekday effect, this points to a significantly larger Saturday effect while also showing a significantly smaller effect for Thursday. The  $R^2$  is 0.790. Both effects agree with the differences between curves that the plots show in Figure 11 and Figure 12.

A third strategy to detect deviations from the cycles is to use the cross-classified RDSEM model of Figure 9 with cycles on the within level. This is analysis step 3b of the summary Table 1. Here, the significance of the between time random effects in (37) for the 56 timepoints suggests which timepoints show important deviations from the cycles. This is accomplished in Mplus by saving the Bayes posterior mean scores and their posterior standard deviations and checking which ratios exceed 1.96. Three timepoints show significant deviations, 31 (Friday 6pm - 9pm), 35 (6am - 9am Saturday), and 36 (9am - 12noon Saturday). Adding those three effects results in an  $R^2$  of 0.690.

The three strategies for finding deviations from the cycles give similar results in that they all point to a Saturday deviation and none of them finds a significant Sunday deviation despite the visual appearance of such a discrepancy. The second approach adds a Thursday deviation and the third approach adds a Friday deviation. In further analyses that investigate individual variation in the cycles and relate them to background characteristics, determinants of individual variation in these added effects can also be explored.

### 4.3 Random cycles coefficients

As mentioned in connection with the cross-classified RDSEM model with cycles on within shown in Figure 9, it is possible to let the coefficients of the cycles covariates vary across individuals. This is the model of step 4c in the summary Table 1. The cross-classified RDSEM estimates of the mean of the random cycles coefficients are almost the same as in the fixed case of cross-classified DSEM, -0.089, CI = [-0.138, -0.038] and -0.007, CI = [-0.057, 0.038]. The variances are not large relative to their

standard deviations, 0.015 (SD = 0.007) with CI = [0.004, 0.030] and 0.007 (SD = 0.005) with CI = [0.001, 0.020].<sup>10</sup> To get an appreciation for the magnitude of the estimated variation in the cycles coefficients, it is useful to relate it to the amplitude of (22). For example, how does the amplitude compare for individuals at the mean versus one standard below the mean of each cycle coefficient? Based on the means of the two coefficients, the amplitude is computed using (22) as  $\sqrt{-0.089^2 - 0.007^2} = 0.09$ . Subtracting one standard deviation (square root of the estimated variance) to each mean, the amplitude is 0.23. The estimated amplitude values can be related to the vertical range of the observed data means as estimated by the maximum-likelihood curve 2 in Figure 10. For Monday, that range is approximately 0.3. Because amplitude is defined as half of the maximum minus minimum of a cycle, this would suggest an amplitude of the magnitude 0.15. Individuals one standard below the mean of each cycle coefficient therefore have an amplitude that is approximately 50% higher. Amplitude will be studied in a more straightforward fashion in the section on random cycles coefficients for factors related to time-invariant covariates.

#### 4.4 Bivariate analysis of PA and tiredness

Figure 13 shows that the reported PA score at the top and the reported tiredness at the bottom have clear 24-hour cycles that are negatively related. When tiredness dips during the day, PA peaks. A question arises: How much more than not being tired does PA measure? Once the cycles of both PA and tiredness have been accounted for, is there a residual relationship? These questions can be addressed by the bivariate cycles model of Figure 7. Similar issues were raised in Liu and West (2015) who analyzed weekly cycles in alcohol consumption related to stress using dummy covariates representing week days. They employed a multistep analysis where the residuals from the stress time series were first computed and then used as predictors of consumption together with the consumption dummies. Using the bivariate two-level RDSEM cycles model of Figure 7, the Bayesian approach estimates the model in a single step.

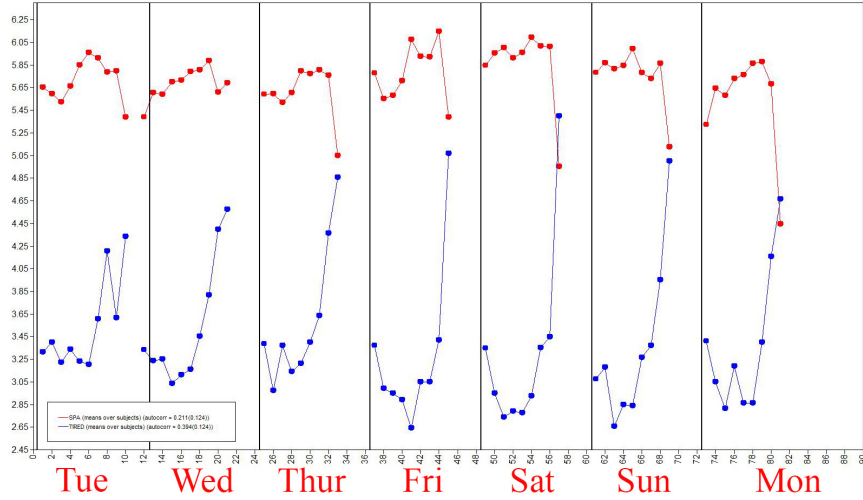
The current application uses a random slope version of the bivariate two-level RDSEM cycles model in Figure 7 that allows individual variation in the key parameter of the within-level regression of the residual  $\zeta_{PA_t}$  on  $\zeta_{Tired_t}$ . This is a random slope version of the model referred to as step 2d in the summary Table 1. The cycles do not have random coefficients but such a model is also possible. It is also possible to relate the variation in the random slope to time-invariant background variables.

The analysis finds that the mean of the  $\zeta_{PA_t}$  on  $\zeta_{Tired_t}$  regression slope is significant and negative. The within-level standardized estimate averaged over individuals shows a medium effect of -0.199. The conclusion is that even accounting for daily cycles in both variables, tiredness has a substantial influence on PA. The variance of the coefficient has an estimate of 0.014, a standard deviation of 0.003, and a CI = [0.009, 0.020]. The cycles for the tiredness variable give a tiredness  $R^2$  averaged over individuals of 0.208. The PA  $R^2$  averaged over individuals, which accounts for both cycles and tiredness influence, is 0.210. While tiredness has a significant influence on PA even when accounting for their cycles, considerable PA variation remains unexplained.

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<sup>10</sup>Mplus practice is to require a ratio of the estimate to the SD of at least 3 for a well determined variance estimate.

Figure 13: PA and tiredness



## 5 Cycles for factors

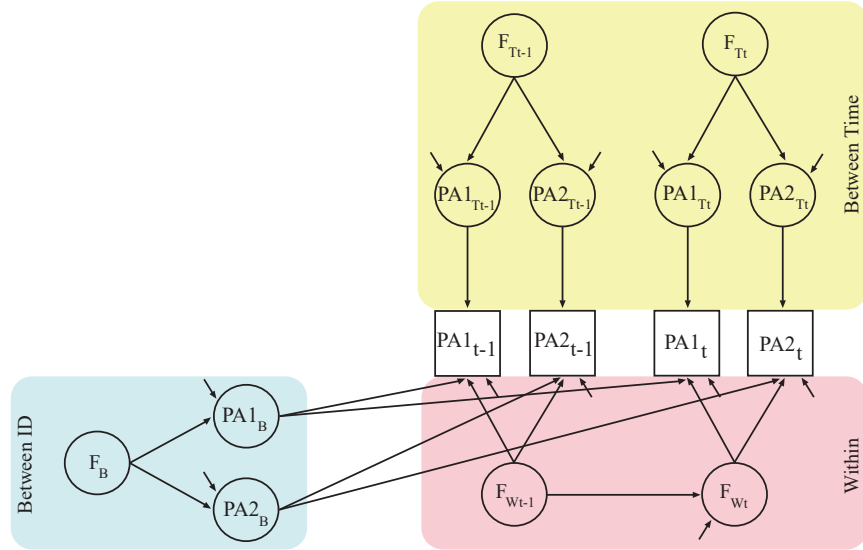
This section illustrates the use of cycles modeling with factors that are measured by multiple indicators. A cross-classified DSEM factor analysis model is shown in Figure 14 for a simple case with one factor measured by two items. The Within level shows a factor auto-regression.<sup>11</sup> On the Between ID level there is one latent variable for each of the two indicators and one factor behind these two latent variables. On the Between Time level there is a factor behind the two indicator-specific latent variables.

Factor analysis is relevant for PA in the example because the items that the score is based on may measure several dimensions of affect (c.f. factor analyses of the PANAS-X in Watson & Clark, 1999). The different dimensions may follow different cycle patterns which may be confounded in the cycles for the average PA score. The factor modeling can be carried out in a two-level DSEM or a cross-classified DSEM format.

A first step is to carry out an analysis without cycles to determine the factor structure. Table 6 shows the six 7-category items which are averaged to create the PA score previously analyzed. The first three items were characterized by the investigators as low arousal PA and the next three as high arousal PA. A two-level exploratory factor analysis indicates that the items measure two separate factors corresponding to the low-high arousal distinction with the high-arousal Happy item loading about equally on both factors. Table 6 shows the confirmatory factor analysis solution suggested by this exploratory analysis. The estimates are obtained by cross-classified DSEM factor analysis without imposing cycles in line with Figure 14. This is analysis step 1b of the summary Table 1. The Between ID level loadings are larger than on the other levels, reflecting the different meanings of the factors. The Within and Between Time factors refer to residual variation after the individual-specific Between ID factors have been extracted. Within and Between Time factor loadings are held equal to reflect that

<sup>11</sup>For simplicity in showing the factor model, the indicator-specific latent variables on Within are not drawn.

Figure 14: Cross-classified DSEM factor analysis (one factor measured by two items)



these levels are concerned with the same residual factors. The correlations between the two factors for the three levels are: Between ID = 0.85, Within = 0.66, Between Time = 0.15.

To validate the two factors, the cross-classified DSEM factor analysis model is expanded to include tiredness as a predictor of the factors on all three levels. It is found that tiredness has a significant negative effect on the two factors on the within level. The effect on the low-arousal factor is, however, very small while the effect on the high-arousal factor is substantial. On the face of it, it makes sense that items referring to feeling Relaxed and Satisfied have less to do with tiredness than feeling Energetic and Excited.

Cross-classified RDSEM with cycles for the factors is carried out in line with Figure 8 with the cycles covariates influencing the factors on the between time level as shown in Figure 15 for the one-factor case. This is the model of step 2b in the summary Table 1. For each of the two factors, Figure 16 shows the resulting curve of the  $F_{T_t}$  estimates in blue in together with the estimated cycles in red. It is clear that the variation is much larger for the low- than the high-arousal factor. The  $F_{T_t}$  variance is estimated as 0.046 for the low-arousal factor and as 0.020 for the high-arousal factor.

The cycles model shows that the cycles pattern is different for the two factors. It estimates the cycles coefficients for the low-arousal factor as -0.165 [-0.244, -0.079] and 0.125 [0.045, 0.212] so that the sine and cosine parts are both significant but have opposite signs.  $R^2 = 0.479$  which is of similar magnitude as the earlier PA analysis. For the high-arousal factor the estimates are -0.061 [-0.126, 0.003] and -0.142 [-0.212, -0.066] so that only the cosine part is significant and is of opposite sign of the low-arousal factor.  $R^2 = 0.594$ . Using the formula (22), the amplitude is 0.21 for the low-arousal factor and 0.15 for the high-arousal factor. The low-arousal factor peaks a little later in the day than the high-arousal factor.

The deviations between the cycles curve and between time factor scores are also

Table 6: Factor analysis of the six PA items

	<u>Between ID</u>		<u>Within = Between Time</u>	
	PA Low	PA High	PA Low	PA High
Relaxed	0.94	0	0.76	0
Satisfied	1.00	0	0.86	0
Confident	0.80	0	0.73	0
Happy	0.52	0.49	0.44	0.45
Energetic	0	0.96	0	0.82
Excited	0	1.00	0	0.91

Figure 15: Cross-classified RDSEM factor analysis with cycles (one factor measured by two items)

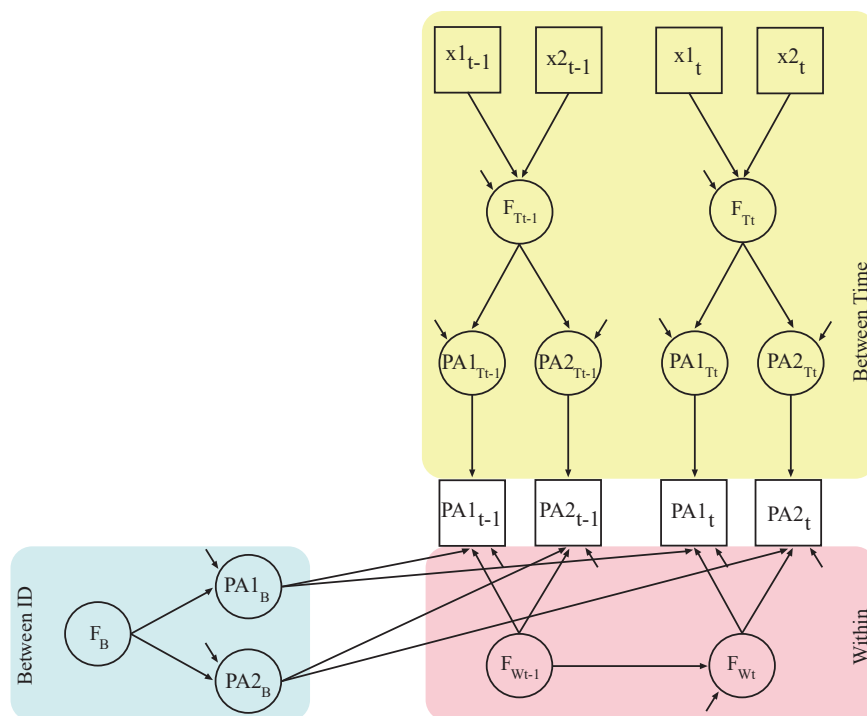
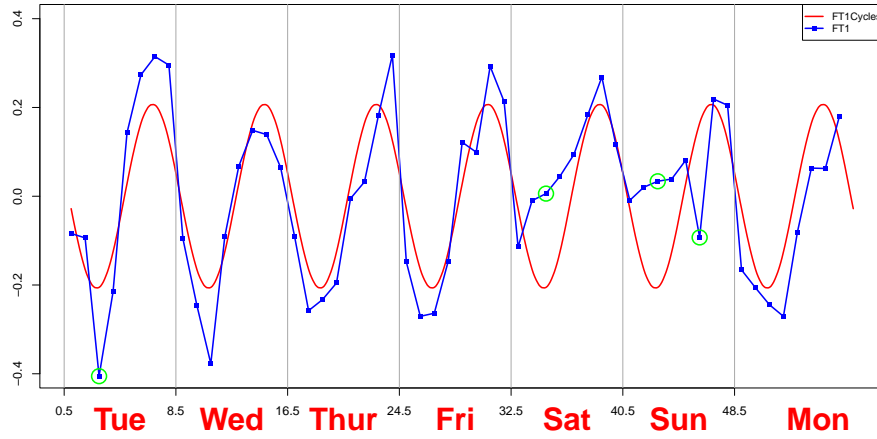
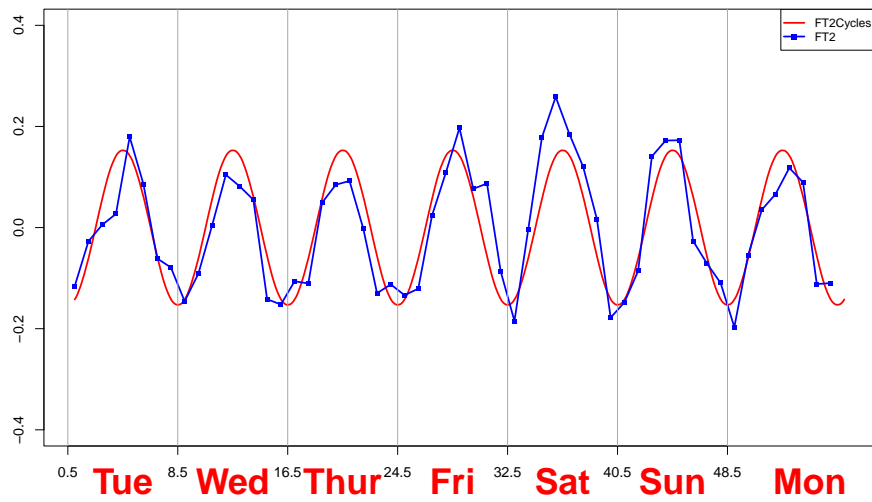


Figure 16: Estimated between time factor scores and cycles from cross-classified RDSEM



(a) Low arousal PA factor



(b) High arousal PA factor



different for the two factors. The significance of the deviations were checked with the third approach used with PA, that is, having the cycles on the within level so that the between time level effects reflect deviations from the cycles. This showed no significant deviations for the high-arousal factor and deviations at 4 timepoints for the low-arousal factor marked by circles in Figure 16 (a) for Tuesday (3am-6am), Saturday (6am-9am), and Sunday (6am-9am and 3pm-6pm).

Cosinor modeling can be applied to cycles of more than one duration (Madden et al. (2018)). A model with both a daily cycle and a 7-day cycle was explored. The 7-day cycle is in line with the findings of mood in Larsen and Kasimatis (1990); see also Stone et al. (1985). The 7-day cycle was found to have a significant negative sine coefficient for both factors and resulted in an increase towards the end of the week. This model is not pursued further here, however, due to space limitations and also because the current dataset has observations for only one week.

## 6 Random cycles coefficients for factors related to time-invariant covariates

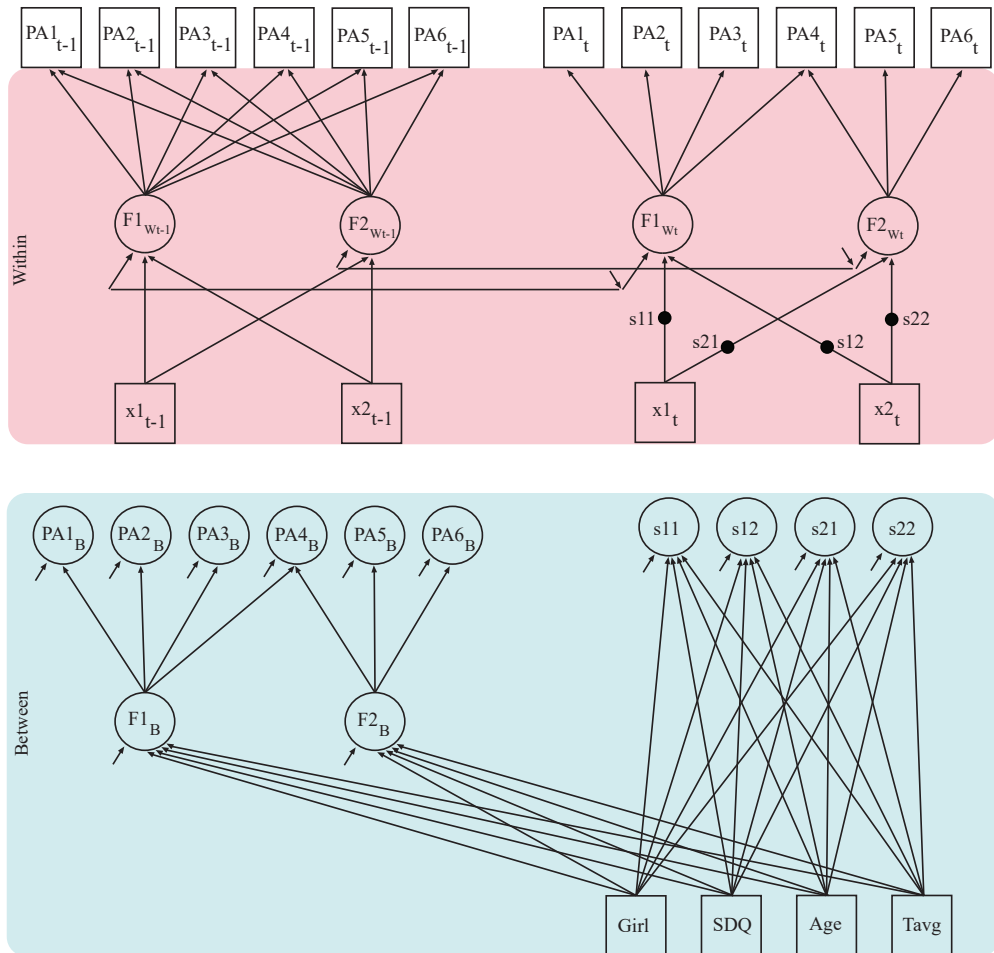
Random coefficients for the cycles of the two factors can be explored further by relating them to covariates. This can be done using either two-level RDSEM or cross-classified RDSEM. The two-level approach is chosen here for simplicity. This model is referred to as step 5a in the summary Table 1. The analysis shows that the means of the random cycles coefficients for the two factors are very close to those of the fixed coefficients of cross-classified RDSEM. Compared to the PA random cycles results, the random coefficient variances for the factors are now larger, especially for the high-arousal factor. It is therefore of interest to relate these random coefficients to background characteristics of the individuals. Four such time-invariant covariates are used, gender, age, the SDQ measure of childhood emotional problems, and across-time average of tiredness. This model is presented in Figure 17 where the measurement of the two factors by the six PA items is displayed.<sup>12</sup> The time-invariant covariates have two types of effects, effects on the overall level across time captured by the between-level factors labeled  $F1_B$  (low-arousal),  $F2_B$  (high-arousal) and effects on the random cycles coefficients captured by the between-level latent variables  $S11 - S22$ .

SDQ and average tiredness are found to have significant negative effects on both of the  $F1_B$ ,  $F2_B$  factors. This means that if adolescents had more emotional problems or more overall tiredness, compared to others, they also reported lower levels of PA (both low and high arousal). Age has a significant negative effect on the high-arousal factor  $F2_B$ , suggesting that with increasing age, high arousal PA is lower as is well-known in adolescent literature. There are no significant effects of gender. For the random coefficients of the cycles, significant effects were found for the sine component of the low-arousal factor for age (positive effect) and average tiredness (negative effect). Significant effects were also found for the cosine component of the high-arousal factor for SDQ (positive effect) and average tiredness (negative effect). The meaning of these cosine effects will be discussed in the following.

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<sup>12</sup>For simplicity, arrows from the six between-level  $PA_B$  variables to the six observed PA items are not drawn.

Figure 17: Two-level RDSEM with random cycles coefficients for factors related to time-invariant covariates



While the interpretation of the effects of the time-invariant covariates is straightforward for the overall factor level represented by  $F1_B$ ,  $F2_B$ , interpreting the effects on the random cycles coefficients for the sine and cosine components is more involved. As an example of the latter, consider the amplitude effects of Age where Age was significant for the sine component of the low-arousal factor. The mean of the sine coefficient is negative and the Age effect is positive thereby reducing the absolute value of the sine coefficient. The mean of the cosine coefficient is positive, and the Age effect is negative, albeit not significant, also reducing the absolute value of the cosine coefficient. Because amplitude is essentially a function of the sum of the two absolute values, this implies that the amplitude of the low-arousal factor decreases with increasing age. This indirect relationship of the cycles coefficients to e.g. amplitude illustrates the fact that substantively, the cycles coefficients may not be the most meaningful characterizations of the cycles. A more interpretable alternative to studying the cycles coefficients is to instead focus on the amplitude and phase of the cycles. This is considered next.

## 6.1 Amplitude and phase regression

Instead of the sine-cosine coefficients  $\beta_1$  and  $\beta_2$ , the variation in the cycles can be studied in more easily interpretable terms using the amplitude and phase of the cycles. A complicating factor is that the amplitude and phase are non-linear functions of the coefficients as shown in (22) and (23), but this complication can be circumvented by the following two analysis steps. Using the just presented step 5a two-level RDSEM random cycles analysis of Figure 17, “plausible values” of the between-level factor scores and random cycle coefficients are obtained in the same analysis by multiple imputation (Asparouhov & Muthén, 2010). Each person obtains for instance 200 plausible values to account for the uncertainty of the scores. These 200 data sets of plausible values can then be analyzed in a subsequent step using a single-level regression analysis.<sup>13</sup> This is step 5b in the summary Table 1. In this second step, amplitude and phase are computed from the cycles coefficients, followed by regressing these amplitude and phase variables, together with the two between-level factors, on the time-invariant covariates. The step 5a covariates are the same as the step 5b covariates as recommended in Mislevy et al. (1992a, b) and Asparouhov and Muthén (2010, Section 4). To account for possibly non-symmetric credibility intervals, Bayesian analysis is used but maximum-likelihood analysis is also possible. The results of the Bayesian analyses of the different data sets are summarized as described in Asparouhov and Muthén (2021). As discussed in the Supplementary material, the two-step Bayesian analysis is preferable to a single-step Bayesian analysis when phase is allowed to vary across individuals.

Table 7 shows the estimated regression coefficients of the second step in a standardized metric. The suffixes 1 and 2 for AMP (amplitude) and PHASE refer to the cycles of the low-arousal factor 1 and the high-arousal factor 2. Significant regression coefficients are found for:

- Low-arousal factor F1B regressed on SDQ (negative) and average tiredness (negative)
- High-arousal factor F2B regressed on SDQ (negative) and average tiredness (negative and larger than for F1B)

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<sup>13</sup>The Mplus TYPE = IMPUTATION option of the DATA command is used.

Table 7: Standardized regression of between-level factors, amplitude, and phase on time-invariant covariates using Bayesian analysis (1 refers to low-arousal and 2 refers to high-arousal factors, amplitude and phase)

	Estimate	Posterior S.D.	95% C.I.		Significance
			Lower 2.5%	Upper 2.5%	
F1B ON					
AGE	-0.043	0.061	-0.161	0.076	
SDQ	-0.293	0.063	-0.411	-0.166	*
GIRL	0.040	0.064	-0.086	0.163	
TIREDAVG	-0.342	0.059	-0.452	-0.219	*
F2B ON					
AGE	-0.106	0.056	-0.214	0.005	
SDQ	-0.240	0.058	-0.352	-0.124	*
GIRL	0.104	0.056	-0.007	0.213	
TIREDAVG	-0.518	0.051	-0.611	-0.414	*
AMP1 ON					
AGE	-0.472	0.112	-0.701	-0.254	*
SDQ	-0.136	0.100	-0.322	0.083	
GIRL	-0.001	0.108	-0.238	0.207	
TIREDAVG	0.437	0.109	0.237	0.638	*
AMP2 ON					
AGE	-0.097	0.144	-0.423	0.134	
SDQ	-0.151	0.138	-0.402	0.132	
GIRL	0.079	0.119	-0.140	0.330	
TIREDAVG	0.324	0.119	0.091	0.554	*
PHASE1 ON					
AGE	-0.274	0.150	-0.449	0.090	
SDQ	-0.098	0.102	-0.289	0.106	
GIRL	-0.044	0.109	-0.281	0.146	
TIREDAVG	0.176	0.087	0.001	0.342	*
PHASE2 ON					
AGE	-0.130	0.110	-0.335	0.091	
SDQ	0.033	0.138	-0.202	0.337	
GIRL	-0.075	0.108	-0.299	0.127	
TIREDAVG	0.134	0.106	-0.093	0.324	

- Amplitude for low-arousal factor regressed on age (negative) and average tiredness (positive)
- Amplitude for high-arousal factor regressed on average tiredness (positive)
- Phase for low-arousal factor regressed on tiredness (positive)

The negative effects of SDQ and average tiredness on the between-level values of the two factors were found also in the earlier Figure 17 analysis. The positive effect of average tiredness on the amplitudes of the two factors is a new finding made possible by the imputation analysis. It is interesting that individuals with higher average values of tiredness tend to have lower overall factor level for both low- and high-arousal PA across time but greater peaks and valleys of the cycles for the factors. Another new finding is that the amplitude for the cycles of the low-arousal factor is lower for older individuals. Yet another new finding relates to the phase of the cycles for the low-arousal factor which is significantly higher for individuals with higher average tiredness. This means that individuals with higher average tiredness peak later in the day for the low-arousal factor. Regarding the average phase (not shown in the table), the low-arousal factor is found to peak later in the day than the high-arousal factor, a finding in agreement with Figure 16.

## 7 Conclusions

Many psychological phenomena are dynamic. They vary over time. Even though intensive longitudinal data are suited to assess such fluctuations, time dynamics are often not modeled in statistical analyses. In this paper we demonstrate a large new analysis arsenal that is available for analysis of cyclical features in ILD. This can help researchers extract more information from their data. To assist in this effort, the analyses are based on general models with a rich set of features while still being accessible without an unduly steep learning curve. Mplus scripts are available as Supplementary information for all the analyses presented.

These novel techniques help to better understand how theoretically and clinically relevant phenomena, such as an individual’s mood, may be a function of time. This may for instance help to understand when people are most motivated to engage in a challenging task, when they are at highest risk of alcohol use, or when to leave an adolescent alone (because they are not in the mood for talking). Understanding the time dynamics of psychological phenomena also helps to inform scholars how to best design their future ESM studies, allowing sufficient measurement points to adequately assess the speed of the underlying process (Hamaker & Wichers, 2017; Kuppens et al, 2022). Applying these analytical methods to a pilot study may improve the study design and/or reduce unnecessary burden on participants. Finally, taking cycles into account may provide more precise and valid estimates of bivariate associations because confounding time effects can be controlled for. For instance, in this paper, it was found that tiredness is related to PA independent of the time cycles in both variables.

The DSEM cycles analyses uncovered several new findings. The observed PA score is actually a combination of two different factor dimensions corresponding to low- and high-arousal items. The high-arousal factor has a stronger negative within-level relationship with the time-varying covariate of tiredness than the low-arousal factor. Both

factors show cyclical behavior over each day, but the cyclical behavior has more amplitude for the low-arousal factor. In terms of between-level variation across individuals, time-invariant covariates have effects on both the factors, which represent overall level across time, and on the cycles coefficients representing fluctuations across time. The means of the two factors are both negatively influenced by childhood emotional problems as well as tiredness. Furthermore, the amplitude of the low-arousal factor is lower for older individuals. The phase for the low-arousal factor is higher for individuals with higher tiredness, that is, the cycles peak later in the day. No gender effect is found.

The analysis results for the PA example raise the question of how PA - and measurements with cyclical features more generally - should be best represented. It is clear that PA varies depending on the dimensions captured by the items, varies by the day, and varies over the hours of the day. What is the most meaningful representation of an individual's PA? A similar dilemma is well-known in terms of measuring blood pressure. As discussed in Madden et al. (2018), the long-term average is important but so is the morning surge in blood pressure, that is, a change measure. The RDSEM analyses provide estimates of long-term behavior in terms of the between-level factor scores for different dimensions. RDSEM also provides between-level random effect estimates of amplitude and phase which are important measures in the change category. Individual scores for weekday effects may also be of substantive interest. These are latent variable alternatives to a single observed PA score.

The Monte Carlo studies showed that time-relevant parameters of the DSEM model can be well recovered for data collection designs with time series as short as 3 measures per day for 5 days, allowing applications in pilot projects. To seriously consider a latent variable representation of PA, however, a follow-on question is how well latent variable scores can be recovered under different designs. In this connection, one may consider a latent variable measurement instrument for an individual that draws on parameter estimates from a large study from a similar population. This enables an  $N = 1$  analysis with known, fixed parameter values where only the factor scores and random effects are estimated for the individual.

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