Web-based Supplementary Materials for:

"Modeling Mood Variation Associated with Smoking: An Application of a Heterogeneous Mixed-Effects Model for Analysis of Ecological Momentary Assessment (EMA) Data"

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Below is a sample of syntax necessary to run Model II (albeit, to simplify the presentation we have omitted the day-of-week indicators in the specification of the mean model below). Expressions with all uppercase letters are used for SAS-specific syntax, while expressions including lowercase letters are used for user-defined entities. In this example, `NegAff` denotes the negative affect outcome, `SmkEvent` represents the dummy code for whether an occasion is a random prompt (=0) or a smoking event (=1), `SmkMean` denotes the subject-level mean of the variable `SmkEvent`, and `id` is a subject-level identifier. The code below is illustrated for the covariate `Nmr`, a subject's level of negative mood regulation. In terms of the random subject effects, `u0` is for the random prompts and `u1` for the difference between smoking events and random prompts (here, we use the Latin letter "u" to denote the Greek letter upsilon that was used in our equations).

The model for the mean response is summarized by `z`, with the regression coefficients named `b0`, `bSmkEvent`, `bSmkMean`, `bNmr`, and `bNmrSmk` (*i.e.*, these would correspond to the parameters $\beta_0, \beta_1, \ldots, \beta_4$ in our equations). The model for the random prompt variance is given by `varu0`, with `alpha00` indicating the reference variance (*i.e.*, the variance when the covariate equals 0), in natural log units, and `alpha01` representing how this variance varies with the covariate `Nmr`. Similarly, for the model of the slope variance (*i.e.*, the variance in mood changes associated with smoking events, relative to random prompts), `varu1` is modeled in terms of a reference variance `alpha10`, in natural log units, with `alpha11` specified for the influence of `Nmr` on this slope variance. Note that the distinguishing feature

of Model II is the inclusion of covariates in the specifications of varu0 and varu1. Finally, c01 is the covariance between the two random subject effects, and vare is the error variance.

```
PROC NLMIXED;
PARMS b0=3.8 bSmkEvent=-.3 bSmkMean=-1.2 alpha00=.8 c01=-.4
      alpha10=-.9  bNmr=0 bNmrSmk=0 alpha01=0 alpha11=0 vare=3;
z = (b0 + u0) + (bSmkEvent + u1)*SmkEvent
      + bSmkMean*SmkMean + bNmr*Nmr + bNmrSmk*Nmr*SmkEvent;
varu0 = EXP(alpha00 + alpha01*Nmr);
varu1 = EXP(alpha10 + alpha11*Nmr);
MODEL NegAff ~ NORMAL(z,vare);
RANDOM u0 u1 ~ NORMAL([0,0], [varu0,c01,varu1]) SUBJECT=id;
```

Users must provide starting values for all parameters on the PARMS statement. To do so, it is beneficial to run the model in stages using estimates from a prior stage as starting values and setting the additional parameters to zero or some small value. For example, one can start by estimating a random-intercepts model with fixed effects (β), random intercept variance (alpha00), and error variance (vare). Estimates of these parameters can then be specified as starting values in a model that adds in the random slope effect (alpha11). Finally, the full model with the additional parameters associated with the covariate (bNmr, bNmrSmk, alpha01, alpha11) can be estimated. In practice, this approach works well with PROC NLMIXED, which sometimes has difficulties in converging to a solution for complex models. In the example above, the starting values are based on the estimates for the model without the covariate effects.

Output

Below is the output that is obtained from this run using PROC NLMIXED. The `Specifications` section indicates the dependent variable (`NegAff`), the subject variable (`id`), the random effects (`u0` and `u1`), and some particulars about the default estimation method. The `Dimensions` section indicates that 8179 observations are nested within 234 subjects, and that the maximum number of nested observations is 79 (i.e., one or more subjects had 79 observations in the dataset). The number of parameters in this model equals 11. The starting values for these are then listed in the `Parameters` section. The `Iteration History` gives details of the iterative maximum likelihood solution. In particular, at model convergence , the message that the convergence criterion is satisfied is given. The results from models that do not converge are not to be relied upon, and so it is critical that this message is obtained.

The model deviance (-2 log likelihood value) is provided under the `Fit Statistics` section, as are several variants of the deviance statistic that are sometimes used in model selection. The deviance value itself is what is used to perform the likelihood-ratio test of relative model fit, as reported in Table 2 of the paper, for example. Notice that the deviance value of this model is 33111, whereas the model in Table 2 lists a deviance of 33089 (for Model II with NMR, considering Negative Affect as the dependent variable). The difference is attributable to the six day-of-week indicators that are not included in the current model, but were included in the model in the paper. Thus, the likelihood ratio test statistic equals 33111-33089 = 22 on six degrees of freedom, which is significant at the .005 level. This indicates that the excluded day-of-week indicators are jointly statistically significant. Here for simplicity, these day-of-week indicators were excluded, however the model in the paper did include them.

Finally, the `Parameter Estimates` section provides the estimated parameters, standard errors, t-values, and p-values for the model parameters. Additionally, a 95% confidence interval (`Lower` and `Upper`) is listed for each parameter. Because the current model does not include the six day-of-week indicators, the results are not identical to those in the paper, however, they are very close. For example, in Table 3, the main effect of `Nmr` is listed as -.790, se=.128. p<.001, and below it is given as -.7941, se=.1284, p<.0001.

The NLMIXED Procedure

Specifications

Data Set	WORK.LOC
Dependent Variable	NegAff
Distribution for Dependent Variable	Normal
Random Effects	u0 u1
Distribution for Random Effects	Normal
Subject Variable	id
Optimization Technique	Dual Quasi-Newton
Integration Method	Adaptive Gaussian Quadrature

Dimensions

Observations Used	8179
Observations Not Used	0
Total Observations	8179
Subjects	234
Max Obs Per Subject	79
Parameters	11
Quadrature Points	1

Parameters

b0	bSmk Event	bSmkMean	alpha00	c01	alpha10	bNmr	bNmrSmk	alpha01
3.8	-0.3	-1.2	0.8	-0.4	-0.9	0	0	0

Parameters

alpha11	vare	NegLogLike
0	3	16576.2923

Iteration History

Iter	Calls	NegLogLike	Diff	MaxGrad	Slope
1	3	16573.6752	2.617063	13.71446	-385.585
2	4	16572.8466	0.828579	23.79174	-2.3485
3	6	16571.6432	1.203389	22.55616	-1.19072
4	8	16565.8421	5.801109	54.36423	-1.66505
5	10	16558.1306	7.711568	20.4593	-7.28426
6	12	16557.4444	0.686163	5.177624	-1.09432
7	14	16557.3388	0.105574	4.88083	-0.10278
8	16	16556.7815	0.557294	18.26876	-0.13846
9	17	16555.9108	0.870683	5.927052	-0.96989
10	19	16555.7303	0.180542	5.521026	-0.23988
11	20	16555.5762	0.15411	3.555233	-0.08382
12	22	16555.5205	0.055643	2.560761	-0.08058
13	23	16555.4689	0.051677	1.829615	-0.02059
14	25	16555.4514	0.017475	0.692705	-0.0246
15	27	16555.4484	0.00302	0.552165	-0.00297
16	29	16555.4192	0.029191	1.643918	-0.00199
17	31	16555.408	0.011207	0.117259	-0.01456
18	33	16555.4079	0.000103	0.138147	-0.00014

NOTE: GCONV convergence criterion satisfied.

Fit Statistics

-2 Log Likelihood	33111
AIC (smaller is better)	33133
AICC (smaller is better)	33133
BIC (smaller is better)	33171

Parameter Estimates

Parameter	Estimate	Standard Error	DF	t Value	Pr > |t|	Alpha	Lower	Upper	Gradient

b0	5.6903	0.3495	232	16.28	<.0001	0.05	5.0017	6.3788	-0.02125
bSmkEvent	-0.4307	0.2978	232	-1.45	0.1495	0.05	-1.0176	0.1561	0.004534
bSmkMean	-0.9534	0.7137	232	-1.34	0.1829	0.05	-2.3595	0.4527	0.084348
alpha00	1.0564	0.3415	232	3.09	0.0022	0.05	0.3835	1.7293	-0.02701
c01	-0.4033	0.1107	232	-3.64	0.0003	0.05	-0.6215	-0.1852	-0.01249
alpha10	-0.8078	1.1669	232	-0.69	0.4894	0.05	-3.1069	1.4912	-0.13815
bNmr	-0.7941	0.1284	232	-6.18	<.0001	0.05	-1.0471	-0.5411	-0.0333
bNmrSmk	0.05819	0.1169	232	0.50	0.6192	0.05	-0.1722	0.2885	0.041661
alpha01	-0.1928	0.1334	232	-1.45	0.1497	0.05	-0.4555	0.06998	0.028638
alpha11	-0.04040	0.4421	232	-0.09	0.9273	0.05	-0.9114	0.8306	0.027324
vare	3.0534	0.04914	232	62.13	<.0001	0.05	2.9565	3.1502	-0.00842