The Art of Modeling

An Introduction to Linear Mixed Effects Models with R

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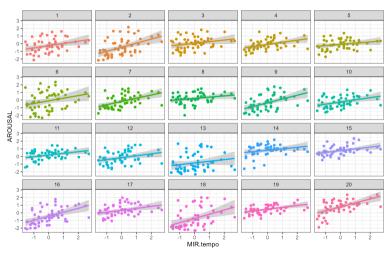
Agenda

- Motivation
- Setting up
- A bit of theory
- A Simulation Exercise
- The Art of Modeling
 - Model building
 - Model selection and comparison
 - Model checking
 - Model interpretation
 - Trouble Shooting
- Outlook; Generalized LMMs (logistic regression, ordinal)
- Hands on: Analyze your own data
- Wrap-up and Debrief

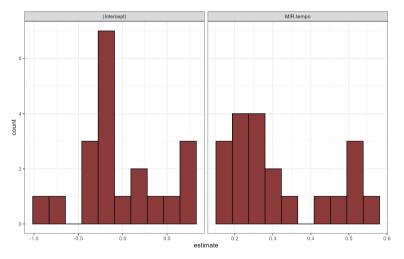
- In 2015, Elke Lange approached me with an idea for a cool study.
- Can perception of emotion expression in music be predicted by audio and other features?
- Setup: 20 audio engineers rated 60 musical excerpts (\approx 60 s on 22 variables (emotions, audio quality, modal analoguess).
- Extracted 86 audio features with the MIRToolbox.

- We reduced the six emotion variables to two variables AROUSAL and VALENCE using factor analysis.
- We found that tempo correlates moderately with AROUSAL, r = .31
- But is this true for all participants?
- Let's see!

The correlations by participants range from r = .19 to r = .54 (mean $\bar{r} = .37$).



Our first random effects!



Why Linear Mixed Effect Models?

- As the example shows, on many occasions, a constant effect of something on an individual seems not reasonable.
- Fixed effects are average effects.
- Are individual differences often more interesting?
- Specifics of experiments, such as stimuli, often simply a nuisance, from which one
 wants to abstract to achieve a better generalization.
- LMMs allow to model all this.

Why Linear Mixed Effect Models?

- The first reason to use LMMs was to deal with repeated measurement.
- When using a common (fully) crossed design, repeated measurement ANOVA is not the best option.
- Averaging loses power.
- LMMs allow modeling arbitrary complex models, when the independence assumption is violated due to repetitions or hierarchical nesting.
- Further benefits: Deals smoothly with NA, provide more detailed information.
- LMM is a very general model, unifying, t-tests, ANOVAS, rmANOVAS, ANCOVAS, and multiple linear regressions (and even χ^2 test and non-parametric tests based on ranks
- Elmar is lmer(), the function from the lme4 package to estimate LMMs, that we will use her.

Why Linear Mixed Models?

Hands On

- Team up with a partner, if you like
- Start R, load the accompanying RStudio project, install missing packages
- Git for project: https://github.com/klausfrieler/lmm_workshop
- Source the file setup.R
- Run setup_workspace()
- As a warm-up, create a scatter plot like that before for MIR.pulse_clarity and VALENCE. The data frame is mer in the workspace. Bonus question: how many of the individual correlations are significant compared to expectation?

A (column) vector of dimension N is a set of N numbers:

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix}$$

Also written as \mathbf{x} , or with components x_i .

A row vector is the transpose $\mathbf{x}^T = (x_1, x_2, \dots, x_N)$.

Vectors of same dimension can be added component-wise and mutliplied by numbers:

$$\mathbf{z} = \alpha \mathbf{x} + \beta \mathbf{y},$$

with components

$$z_i = \alpha x_i + \beta y_i$$

The scalar product is defined as

$$\vec{x} \cdot \vec{y} = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^N x_i y_i$$

The length of a vector is

$$||x|| = \sqrt{\sum_{i} x_i^2}$$

and the (Euclidian) distance between two vectors

$$d(x,y) = \|\mathbf{x} - \mathbf{y}\| = \sqrt{\sum_{i} (x_i - y_i)^2}$$

The (sample) standard deviation of a data vector is proportional to the distance to the vector of mean values

$$\hat{\sigma}(\mathbf{x}) = \frac{1}{\sqrt{N-1}} d(\mathbf{x}, \bar{\mathbf{x}}) = \frac{1}{\sqrt{N-1}} \|\mathbf{x} - \bar{\mathbf{x}}\|$$

For two data vectors of dimension N, \mathbf{x} , \mathbf{y} , the Pearson correlation r_{xy} is defined by the scalar product of the z-transformed vectors as:

$$r_{xy} = rac{1}{N-1} \mathbf{z}(x) \cdot \mathbf{z}(y) = rac{\mathbf{x} - ar{\mathbf{x}}}{\|\mathbf{x} - ar{\mathbf{x}}\|} \cdot rac{\mathbf{y} - ar{\mathbf{y}}}{\|\mathbf{y} - ar{\mathbf{y}}\|}$$

A **matrix X** of dimension $N \times M$ is a rectangular scheme of numbers, with N rows and M columns with elements x_{ij} .

$$X = \left(\begin{array}{ccc} x_{11} & \dots & x_{1M} \\ \vdots & \ddots & \vdots \\ x_{N1} & \dots & x_{NM} \end{array}\right)$$

A matrix can also be considered a N-dimensional row-vector of M-dimensional column vectors or a vice versa.

Matrices of same dimensions can be added and multiplied with a number just like vectors.

The transposed \mathbf{X}^T of a matrix \mathbf{X} switches row and columns, i. e., $x_{ji}^T = x_{ji}$

A N-dimensional vector \mathbf{x} can be regarded as a $N \times 1$ matrix. \mathbf{x}^T is then a $1 \times N$ vector.

Matrices $\bf A$ and $\bf B$ can multiplied $\bf C = \bf A \bf B$, if the number of columns of $\bf A$ is the same as the number of rows in $\bf B$. The elements of the result are defined as

$$c_{ij} = \sum_{k=1}^{M} a_{ik} b_{kj}$$

The elements of $\bf C$ are the scalar products of the *i*-th row vector of $\bf A$ with the *j*-th column vector of $\bf B$

$$c_{ij} = \mathbf{a}_i^T \mathbf{b}_j = \vec{a}_i \cdot \vec{b}_j$$

We have the following computation rules:

$$A(BC) = (AB)C,$$
 $A(B+C) = AB + AC$

Attention: matrix multiplication is, in general, not commutative : $AB \neq BA$

The quadratic $(N \times N)$ matrices are special as they can have an inverse matrix, i.e., if a matrix **A** there exists a matrix **A**⁻¹ such that

$$\mathbf{A}\mathbf{A}^{-1}=\mathbf{A}^{-1}\mathbf{A}=\mathbf{I}_{\mathcal{N}},$$

with the identity matrix I_N which has 1's on the diagonal and 0's everywhere else. The inverse exists, if A has full rank, i.e., no column or row vector is a linear combination of the other vectors or none of them is zero. This is equivalent to det $\mathbf{A} \neq 0$. Example of a non-invertible matrix:

$$\left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right) \cdot \left(\begin{array}{cc} a & b \\ c & d \end{array}\right) = \left(\begin{array}{cc} a & b \\ 0 & 0 \end{array}\right) \neq \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right)$$

Exercise

Let A be the followin matrix:

$$\mathbf{A} = \left(\begin{array}{ccc} 0 & 2 & -1 \\ 2 & -1 & 2 \\ -1 & 0 & 0 \end{array} \right)$$

and $\mathbf{y}^T = (1, -1, -1)$. Solve

$$(\mathbf{A}^T\mathbf{A})\mathbf{x} = \mathbf{y}$$

for x.

Use matrix operations in R, to create a matrix: matrix), t() for transposition, %*% for matrix multiplication, and solve for matrix inversion.

A linear regression model for one variable and N observations can be written as

$$y_i = \gamma + \beta x_i + \epsilon_i$$

with

- y_i the outcome for participant i, $1 \le i \le N$.
- ullet γ the overall intercept
- β the fixed effect coefficient,
- x_i the value of the predictor variable x.
- $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ the normal distributed residual error with mean 0 and variance σ^2 .

This can be extended to p predictors, each having their own beta coefficient.

$$y_i = \sum_{k}^{p} \beta_k x_{ik} + \epsilon$$

and be compactly written with vectors and matrices:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where **X** is the model-matrix, containing the measurements for each participant in rows, and variables are contained in columns.

The global intercept is represented here by adding a 0^{th} -column of ones to **X** and a 0^{th} -component to β , i. e., $\gamma = \beta_0$

Categorial predictors are encoded with numerical dummy variables, e.g., one-hot encoding ('constrast'). K categories add K-1 dummy variables to \mathbf{X} . This covers ANOVA and ANCOVA.

The β -coefficients can be estimated using various methods, e.g., ordinary least squares or maximum likelihood estimation.

In ordinary least squares, one seeks to find estimate $\hat{\mathbf{y}}$ that minimize the error to the observed y,

$$\sum_{i=1}^{N} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{N} \left(\sum_{k=1}^{p} x_{ik} \beta_k - y_i \right)^2 = f(\beta_0, \beta_2, \dots, \beta_p) = \min$$

This is a function of the unknown variables β_i , and a minimum can be found by setting partial derivations with respect to all variables to 0.

Calculating the partial derivative with respect to β_i yields

$$\frac{\partial}{\partial \beta_k} \sum_{i=1}^{N} \left(\sum_{k=1}^{p} x_{ik} \beta_k - y_i \right)^2 = 0$$

$$\sum_{i=1}^{N} 2 \left(\sum_{k=1}^{p} x_{ik} \beta_k - y_i \right) x_{ij} = 0$$

$$\sum_{i=1}^{N} \sum_{k=1}^{p} x_{ij} x_{ik} \beta_k - \sum_{i=1}^{N} y_i x_{ij} = 0$$

Using matrix notation this implies

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y},$$

and, finally,

$$\beta = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

This solution only exists, if the model matrix **X** is invertible, which means that it should have full rank. That's why multicollineriaty is a problem.

The maximum likelihood method has the same result, as it uses the logarithm of a normal distribution, which has a similar quadratic term.

Task: Use the data set scenario2 and calculate the beta coefficients using the formula above and compare to the linear model coef(lm(y x + z, data = scenario2))

A bit of theory: Hierarchical Linear regression

Now we incorporate the idea of varying beta coefficient. We use hierarchical models, introducing a linear equation for the betas. Consider

$$y_{ij} = \gamma + x_{ij}\beta_j + \epsilon_{ij}$$

where introduced a clustering index $1 \le j \le q$ for q clusters, indicating participants or stimuli etc. y_{ij} is the j-th value in cluster j.

The random effects assumption is that the intercepts and slopes are a normal distribution over the clusters, with mean values γ and β of the fixed effects . Hence, we can write for each cluster

$$\gamma_j = \gamma + u_j^{\gamma}
\beta_j = \beta + u_j^{\gamma}$$

A bit of theory: Hierarchical Linear regression

Inserting this into the original equation yields

$$y_{ij} = \gamma + \gamma_k + x_{ij}(\beta + \beta_j) + \epsilon_{ij}$$

= $(\gamma + x_{ij}\beta) + (\gamma_j + x_{ij}\beta_j) + \epsilon_{ij}$

Again using compact matrix notation, this yields to most commonly used formulation for a random effects model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{u} + \boldsymbol{\epsilon}$$

A bit of theory: Hierarchical Linear Regression

- In contrast to simple linear regression, no closed solution is available.
- Iterative method based maximum likelihood estimation (ML) or restricted maximum likelihood estimation (REML, default in lmer) needed.
- Algorithm might not find always a solution (see Trouble Shooting)
- The fixed coefficients are the same as when using simple linear regression.
- It is all about the standard errors! (= Type I errors).
- In fact, there are only random effects, where the mean of the random effects are the fixed effects.
- Model only identifiable under certain conditions, measurements need to allow estimation of the RE.
- Sometimes "boundary fits" are produced, which often indicates misspecification (see Trouble Shooting).

Simulation is the way to wisdom

As a preparation for the following, let's create some artificial data.

Exercise

- Scenario: N participants rate a set of M musical stimuli in two conditions/Variants, 'audio-only' (AO) and 'audio-visual' (AV) with respect to liking on a 5-point Likert scale (fully crossed design).
- Task: Write a function with parameters n_raters, n_stimuli, error (residual error) and beta (effect of condition) that generates liking ratings. (Approximate the 5-point Likert scale with a normal distribution with mean 3.)
- Tips: expand_grid or crossing create all combinations, rnorm produces normal-distributed random numbers for a given mean and standard deviation.
- Bonus Task: Set a parametrizable portion of values to NA. Add participant or stimulus-dependent covariates that correlate with liking to a certain (parametrizable) extent r.

The Art of Modeling

Roadmap

- 1. Data exploration
- 2. Model building
 - 2.1 Identifying variable types, random effects, fixed effects, covariates.
 - 2.2 Model optimization by way of model comparison
 - 2.3 Fixing converge and boundary fit issues
- 3. Model checking: are assumptions met?
- 4. Model interpretation: significance testing, marginal effects

Data exploration

- Know you data!
- First step should be always data exploration
- Particularly with complex data
- Histograms and scatterplots of all variables (e.g., psych::pairs.panels(), GGally::ggpairs()
- Data sanity: Missing values, outliers, 'pathological' distributions, unbalanced cluster/cell sizes etc.
- Altogether now: Know you data!

Model building

- There are certain researchers degrees of freedom to setup and estimate the "best" model fitting the data.
- No deterministic method to automatically find the best model, given the data.
- Approach: Model comparison with anova() and ranova() function.
- Generally: maximal, best fitting, and optimal models yield the best estimation of standard errors.
- Unbiased estimated only guaranteed, when assumptions are met (see Model Checking),

Model building

- Generally, all units with repeated measurement need to be included as random effects.
- Variables of Interest (VOI) should be identified, i. e., fixed effects as well as additional covariates.
- Fixed effects should be included as random slopes for the random effects) they apply (i.ė., if the vary across the cluster).
- Test necessity of random effects with the function ranova() from the lmerTest package.
- Model comparison is based on likelihood ratio tests
- For nested models, the difference of deviances (=-2logLik) is approximately χ^2 -distributed.
- AIC (and BIC) lower for better fitting models (no sig-test)

Model building

Exercise

- Simulate data with 10 raters or 10 items (strong/weak random effect with/without slope) using simulate_lmm()
- Test if inclusion of random effects (over rater and item) improves model fit significantly
- Tip: Establish that the simplest random effects is better using lmerTest::ranova(), then compare different models with anova()
- Bonus: repeated for different effect sizes and rater and item numbers, what is the difference?

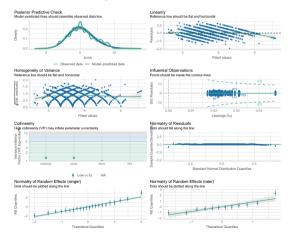
Model checking

Check the common assumptions using performance::check_model()

- Normality of residuals
- Linearity
- Homoscedasticity
- Influential observations
- Variance Inflation
- Normality of random effects

Model checking

Model check with performance::check_model() for the Covox data set with intercepts-only random effects of singer and rater.



lmerTest::lmer() Output

```
Linear mixed model fit by REML.
t-tests use Satterthwaite's method Formula:
liking ~ condition + (1 + condition | rater) + (1 + condition | item)
REML criterion at convergence: 379.9
Scaled residuals:
    Min 10 Median 30
-1 99790 -0 56716 -0 02668 0 58813 2 95504
Random effects:
Groups Name Variance Std.Dev. Corr
rater (Intercept) 0.1038 0.3222
        conditionAV 0.2291 0.4787
                                    0.57
item (Intercept) 0.0919 0.3032
        conditionAV 0.3157 0.5619
                                    0.01
Residual
                    0.2651 0.5149
Number of obs: 200, groups: rater, 10; item, 10
Fixed effects:
           Estimate Std. Error df t value Pr(>|t|)
(Intercept) 2.5529 0.1491 14.3158 17.13 6.16e-11 ***
conditionAV 0.7701 0.2445 14.9130 3.15 0.00665 **
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '1
```

```
lmerTest::lmer() Output General Info
Linear mixed model fit by REML.
t-tests use Satterthwaite's method Formula:
liking ~ condition + (1 + condition | rater) + (1 + condition | item)
REML criterion at convergence: 379.9
Scaled residuals:
    Min 10 Median 30 Max
-1.99790 -0.56716 -0.02668 0.58813 2.95504
```

```
lmerTest::lmer() Output Random Effects
Random effects:
Groups
         Name
                     Variance Std.Dev. Corr
rater (Intercept) 0.1038
                              0.3222
         conditionAV 0.2291 0.4787
                                      0.57
item
         (Intercept) 0.0919 0.3032
         conditionAV 0.3157 0.5619
                                      0.01
Residual
                     0.2651 0.5149
Number of obs: 200, groups: rater, 10; item, 10
```

True values are .5 for all intercepts and slopes standard deviations and for intercept- slope correlations. Residual error is $\epsilon = .5$.

```
lmerTest::lmer() Fixed Effects
Fixed effects:
           Estimate Std. Error df t value Pr(>|t|)
(Intercept) 2.5529 0.1491 14.3158 17.13 6.16e-11 ***
condition2 0.7701 0.2445 14.9130 3.15 0.00665 **
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 ', 0.1 ' 1
Correlation of Fixed Effects:
           (Intr)
conditionAV 0.177
```

True values are Intercept = 3.0, $\beta_{\mbox{cond}} = 1.0. \Rightarrow \mbox{Very small sample size!}$

Test for overall significance using anova(). Compute model fit as marginal R_m^2 , variance explained by fixed effects, and conditional R_c^2 , variance explained by full model. Usually $R_c^2 \gg R_m^2$.

lmerTest::lmer() Further metrics

Sometimes MuMIn::r.squaredGLMM() is needed. Try also sjPlot::tab_model().

Model interpretation: A Note on Significances

- Even though the main resaon to use LMMs is getting the standard errors 'right', there is a bit or problem with p-values for coefficients.
- The 1me4 deliberately does not provide p-value estimates for the fixed effect coefficients. Problem is to get the degrees of freedom right.
- Alternative methods to establish significance are model comparison, parametric bootstrap, profiled confidence intervals, MCMM sampling or simply looking at t>2, if sameple size is large enough.
- The ImerTest package adds p-values for betas using Satterthwaite's degrees of freedom method or the Kenward-Rogers method, both are not beyond discussion.

Model interpretation: Extracting stuff

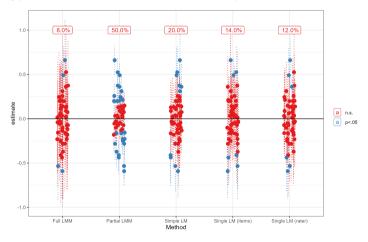
- coef(): Retrieves all coefficients as list of data frames per random effect. Includes fixed effects. Data frames of same size of data, except excluded cases.
- fixef(): Retrieves fixed effect coefficients as vector.
- lme4::ranef(): Retrieves random effects as data frame.
- AIC(), BIC(), logLik(), deviance(REML = FALSE) for global model fit parameters
- vcov()/VarCorr() for fixed/random effects variance-covariance matrices
- predict(), residuals() Get predictions/residuals.
- confint(), get conifidence intervals for all random and fied effects coefficients...
- broom.mixed::tidy(), broom.mixed::glance() retrieves coefficients / model fit as tibble, usefull for aggregation

Work on one or more of these problems.

Exercise

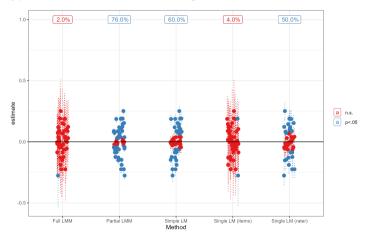
- Simulate N data sets with M raters and K items using simulate_lmm(), aggregate the fixed effects coefficients and calculate mean and sd, plot histograms.
- Simulate a data set of you liking with simulate_lmm(). Fit a simple model fit <lmer(liking condition + (1|rater)) Compare the standard deviations of
 individual random effect estimates with those given by the summary
 (summary(fit)\$varc or VarCorr(fit))? What is going on?
- Simulate a data set with zero fixed effect simulate_lmm(fixef = 0). Fit three
 models with condition as fixed effects and either intercept + slope, intercept-only,
 simple linear regression. Compare the results (using, e.g., sjPlot::plot_models().

Estimates and Type I errors for null effect, small sample size.



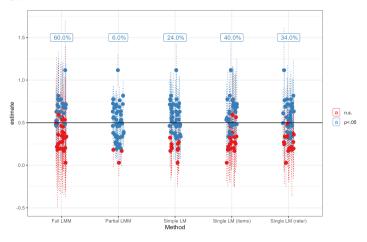
$$N_{\mathrm{sim}} =$$
 50, $N_{\mathrm{raters}} =$ 10, $N_{\mathrm{items}} =$ 10, $\beta_{\mathrm{cond}} =$ 0.0

Estimates and Type I errors for null effect, large sample size.



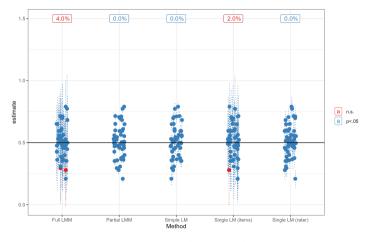
$$N_{\mathrm{sim}} =$$
 50, $N_{\mathrm{raters}} =$ 200, $N_{\mathrm{items}} =$ 20, $\beta_{\mathrm{cond}} =$ 0.0

Estimates and Type II errors for weak effect, small sample size.



$$N_{\mathsf{sim}} = 50$$
, $N_{\mathsf{raters}} = 10$, $N_{\mathsf{items}} = 10$, $\beta_{\mathsf{cond}} = 0.5$

Estimates and Type II errors for weak effect, large sample size.



$$N_{\mathsf{sim}} = 50$$
, $N_{\mathsf{raters}} = 200$, $N_{\mathsf{items}} = 20$, $\beta_{\mathsf{cond}} = 0.5$

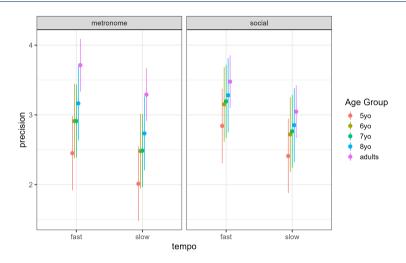
Model interpretation: Marginal effects

- For post-hoc testing and visualization you could use two packages: emmeans (older) and marginaleffects (modern and fancy).
- These allow to aggregate model predictions across conditions and mean covariates etc. taking care of standard errors etc.

Example

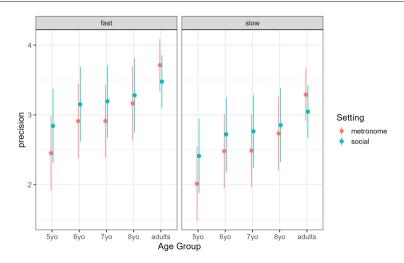
We use the kid_beats data set and fit the following model precision age_group * setting + tempo + beat_prod + beat_perc + 1 | experimenter) + (1 | p_id) Participants from five different age_groups tapped along to a metronome or a human (setting) in two different tempo conditions (fast: 400 ms, slow: 600 ms)) and the precision of the tapping was measured (logarith of standard deviation of IOIs). For each participant, there were also two beat-related covariates beat_prod and beat_perc.

Model interpretation: Marginal effects



marginaleffects::plot_predictions(kid_beats_model, by = c("tempo", "age_group", "setting"))

Model interpretation: Marginal effects



 ${\tt Call: marginal effects::plot_predictions(kid_beats_model, \ by = c("age_group", "setting", "tempo"))}$

Trouble Shooting

- Frequently, 1mer does not converge or shows scary warning messages.
- Singular fit is actually a feature not a bug. It mostly means that some random
 effects are estimated to 0 or could not estimated at all, which means the model is
 overspecified. Solution: Inspect the random effects results, possibly simplify the
 model or decide to ignore.)
- Model does not converge. This also mostly means that the model is overspecified or the data do not support the identification of the model or are otherwise peculiar.
 Solution: Try another optimizer first, or increase tolerance and iteration steps. If that does not work: simplify model.
- An often helpful optimizer is "bobyqa". Usage: lmer(..., control = lmerControl(optimizer = "bobyqa"))
- Warning: for large datasets and complicated random effects (random slopes!), the
 estimation can take a VERY long time. Setting control = lmerControl(calc.deriv
 = FALSE) can speed up things.

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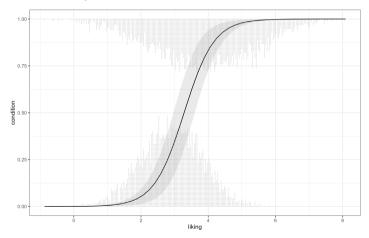
Outlook and Wrap-Up

Outlook: Generalized LMMs

- Generalized Linear Models can be applied to binary (and other) data types, using the lme4::glmer function. Syntax is very similar but it needs specification of a "link" function.
- The link function transforms the outcome to something continuous that can be modeled using LMMs.
- Involves extra steps of transformation, prediction and interpretation might be a bit different, as well as model parameter
- Mixed effects logistic regression uses family = binomial.
- Mixed-effects ordinal regression with package ordinal, multinomial mixe regression with mclogit::mblogit.
- Bayesian mixed models (e.g. the brms package), also possible provides different numerical estimation method
- And much more . . .

Example: Logistic Regression

Predicting condition from liking with simulated data and strong random effects with slope (200 Rater, 20 Stimuli).



Hands On: Your own models

Try it yourself!

- Take some of your own data and run some models. Show us the results!
- Or explore the mer, covox, kid_beats or scenario2 data sets in the repository

Wrap-up

- LMM are state-of-start statistic models, substituting most other methods.
- Need to be used in case of repeated measurements, particularly, the common fully crossed designs
- Mainly affects estimation of standard error, better inference.
- Comes with some complexities and subtleties, but this is basically true for all statistical models . . .
- Happy modeling!

Debrief

- How did you like the workshop?
- Did you learn something?
- Will you use linear mixed effect models in the future?
- What could be improved?
- Further comments and questions

The End