

Understanding mixed effects models through data simulation

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Abstract


Experimental designs that sample both subjects and stimuli from a larger population need to account for random effects of both subjects and stimuli using mixed effects models. However, much of this research is analyzed using ANOVA on aggregated responses because researchers are not confident specifying and interpreting mixed effects models. The tutorial will explain how to simulate data with random effects structure and analyse the data using linear mixed effects regression (with the lme4 R package), with a focus on interpreting the output in light of the simulated parameters. Data simulation can not only enhance understanding of how these models work, but also enables researchers to perform power calculations for complex designs. All materials associated with this article can be accessed at <https://osf.io/3cz2e/>.


Keywords: simulation, mixed effects models, power, lme4, R

Word count: 5572

Background

In this article, we walk through the simulation and analysis of multilevel data with crossed random effects of subjects and stimuli. The article's target audience is researchers who work with experimental designs that sample subjects and stimuli, such as is the case for a large amount of experimental research in face perception, psycholinguistics, or social cognition. Simulation is useful not only for helping understand how models work, but also for estimating power when planning a study or performing a sensitivity analysis. The tutorial assumes basic familiarity with R programming.

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Generalizing to a population of encounters

Many research questions in psychology and neuroscience are questions about certain types of *events*: What happens when people encounter particular types of stimuli? For example: Do people recognize abstract words faster than concrete words? What impressions do people form about a target person’s personality based on their vocal qualities? Can people categorize emotional expressions more quickly on the faces of social ingroup members than on the faces of outgroup members? How do brains respond to threatening versus non-threatening stimuli? In all of these situations, researchers would like to be able to make general statements about phenomena that go beyond the particular participants and particular stimuli that they happen to have chosen for the specific study. Traditionally, people speak of such designs as having *crossed random factors* of participants and stimuli, and think of the goal of inference as being simultaneous generalization to both populations. However, it may be more intuitive to construe the goal as generalizing to a single population of events: in particular, to a population of *encounters* between the units from the sampled populations (Barr, 2018).

Most analyses using conventional statistical techniques, such as analysis of variance and t-test, commit the fallacy of treating stimuli as fixed rather than random. For example, imagine a sample of participants are rating the trustworthiness of a sample of faces, with the goal being to determine whether the faces of people born on even numbered days look more trustworthy than those born on odd-numbered days. Obviously, they don’t. At the extreme, imagine we only sample a single face from each category, but have 100 people rate each face. If our analysis treats the sample of faces as *fixed*, or a perfect representation of the larger population of faces on Earth, we will be almost guaranteed a significant difference in one direction or the other. We will have sufficient power to detect even tiny differences in apparent trustworthiness, so this result will be highly replicable with large samples of raters. As you increase the number of faces in the sample, the problem gets better, but if you increase the number of raters, it gets worse again.

The problem, and the solutions to the problem, have been known in psycholinguistics for over 50 years (Clark, 1973; Coleman, 1964), and most psycholinguistic journals require authors to demonstrate generality of findings over stimuli as well as over subjects. Even so, the quasi- F statistics for ANOVA (F' and min- F') that Clark proposed as a solution were widely recognized as unreasonably conservative (Forster & Dickinson, 1976), and until fairly recently, most psycholinguists performed separate by-subjects (F_1) and by-items analyses (F_2), declaring an effect “significant” only if it was significant for both analyses. This $F_1 \times F_2$ approach has been widely used, despite the fact that Clark had already shown it to be invalid, since both F statistics have higher than nominal false positives in the presence of a null effect— F_1 due to unmodeled stimulus variance, and F_2 due to unmodeled subject variance.

Recently, psycholinguists have adopted linear mixed-effects modeling as the standard for the statistical analysis, given numerous advantages over ANOVA, including the ability to simultaneously model subject and stimulus variation, to gracefully deal with missing data or unbalanced designs, and to accommodate arbitrary types of continuous and categorical predictors or response variables (Baayen, Davidson, & Bates, 2008; Locker, Hoffman,

58 & Bovaird, 2007). This development has been facilitated by the `lme4` package for R
59 (Bates, Mächler, Bolker, & Walker, 2015), which provides powerful functionality for model
60 specification and estimation. With an appropriately specified model, mixed-effects models
61 yield major improvements in power over quasi- F approaches and avoid the increased false
62 positive rate associated with separate F_1 and F_2 (Barr et al., 2013).

63 Despite mixed-effects modeling becoming the *de facto* standard for analysis in psy-
64 cholinguistics, the approach has yet to take hold in other areas where stimuli are routinely
65 sampled, even in spite of repeated calls for improved analyses in social psychology (Judd,
66 Westfall, & Kenny, 2012) and neuroimaging (Bedny, Aguirre, & Thompson-Schill, 2007;
67 Westfall, Nichols, & Yarkoni, 2016). One of the likely reasons for the limited uptake outside
68 of psycholinguistics is because mixed-effects models expose the analyst to a level of statistical
69 and technical complexity far beyond most researchers' training. While some of this com-
70 plexity is specific to mixed-effects modeling, some of it is simply hidden away from users of
71 traditional techniques by GUIs and function defaults. The novice mixed modeler is suddenly
72 confronted with the need to make decisions about how to specify categorical predictors,
73 which random effects to include or exclude, which of the statistics in the voluminous output
74 to attend to, and whether and how to re-configure the optimizer function when a convergence
75 error or singularity warning appears.

76 We are optimistic that the increasing adoption of the mixed-effects approach will
77 improve the generality and thus reproducibility of studies in psychology and related fields,
78 but empathize with the frustration — and sometimes, exasperation — expressed by many
79 novices when they attempt to grapple with these models in their research. A profitable
80 way to build understanding and confidence is through data simulation. If you can create
81 a datasets by sampling from a population where you know the ground truth about the
82 population parameters you are interested in (e.g., means and standard deviations of each
83 group), you can check how often and under what circumstances a statistical model will
84 give you the correct answer. Knowing the ground truth also allows you to experiment with
85 various modeling choices and observe their impact on a model's performance.

Box 1. Glossary of terms

crossed random factors	Refers to a design with multiple random factors, such as subjects and items, the levels of which are crossed (e.g., each subject encounters each stimulus)
data-generating process (DGP)	The mathematical model capturing assumptions about the processes giving rise to the data
fixed effect	An effect whose value is constant across realizations of the experiment
random effect	An effect whose value varies across potential realizations of the experiment (e.g., due to sampling)
random intercept	A random effect capturing the deviation of a sampling unit (subject or item) from the model intercept
random slope	A random effect capturing the deviation of a sampling unit (subject or item) from the model slope
variance components	Parameters describing the distribution of random effects in the population

86

87

Data, materials, and online resources

88 The code to reproduce the analyses reported in this article and appendices with
 89 extended examples are publicly available via the Open Science Framework and can be
 90 accessed at <https://osf.io/3cz2e>. This code is supplemented by two web apps at http://shiny.psy.gla.ac.uk/lmem_sim and <http://shiny.psy.gla.ac.uk/crossed> that perform data
 91 simulation without requiring knowledge of R code. These apps allow you to change parameters
 92 and inspect the results of LMEM and ANOVA analyses, as well as calculate power and false
 93 positive rates for these analyses.
 94

95

Simulating data with crossed random factors

96 Data simulation can play a powerful role in statistics education, enhancing under-
 97 standing of the use and interpretation of statistical models and the assumptions behind
 98 them. The data simulation approach to learning about statistical models differs from
 99 the standard approach in most statistics textbooks, where the learner is presented with a
 100 step-by-step analysis of a sample of data from some population of interest. Such exercises
 101 usually culminate in inferences about characteristics of the population of interest from model
 102 estimates. Although this reflects the typical uncertain situation of the analyst, the learner
 103 cannot fully appreciate the performance of the model without knowing the ground truth.
 104 In a data simulation approach, the learner starts out knowing the ground truth about the
 105 population and writes code to simulate the process of taking and analyzing samples from
 106 that population. Giving learners knowledge of the underlying population parameters as well
 107 as the ability to explore how population parameters are reflected in model estimates can
 108 yield powerful insight into the appropriate specification of models and the interpretation of
 109 statistical output.

Data simulation also has a wide variety of scientific uses, one of which is to estimate properties of statistical models in situations where algorithms for computing those properties are unknown or can only be applied with difficulty. For instance, Forster and Dickinson (1976) used Monte Carlo simulation to explore the behavior of the quasi- F statistics for ANOVA (F' and min- F') under various conditions. In a Monte Carlo simulation, the long run properties of a process are estimated by generating and analyzing many simulated datasets—usually, thousands or tens of thousands of them.

One of the most important applications of Monte Carlo simulation is in the estimation of power for complex models. The notion of power appears most frequently in the context of study planning, where a power analysis is used to determine the target N for a study. Power is the proportion of time that a specified statistical test will generate a significant result for a sample of data of a specified size taken from a population with a specified effect. Therefore, as long as you can characterize the distributions of variables in the population, you can sample data from this simulated population and run your analysis. The proportion of times that this procedure produces a significant result is the power of your test. You can adjust any parameters in this simulation in order to estimate other parameters, such as the minimum effect size that your analysis can detect with 80% power and an N of 200 per group. You can also set the population effect size to zero and calculate the proportion of significant results to check if your analysis procedure inflates *false positives*.

For most traditional statistical procedures such as t -test or ANOVA, there are analytical procedures for estimating power. Westfall, Kenny, and Judd (2014) present analytic power curves for simple mixed effects designs such as the one described in this tutorial (with a corresponding app at <https://jakewestfall.shinyapps.io/crossedpower>). But even where analytical solutions exist, simulation can still be useful to estimate power or false positive rates, because real psychological data nearly always deviates from the statistical assumptions behind traditional procedures. For instance, most statistical procedures used in psychology assume a continuous and unbounded dependent variable, but it is often the case that researchers use discrete (e.g., Likert) response scales. When assumptions are not met, power simulations can provide a more reliable estimate than analytical procedures.

To give an overview of the simulation task, we will simulate data from a design with crossed random factors of subjects and stimuli, fit a model to the simulated data, and then see whether the resulting sample estimates are similar to the population values we specified when simulating the data. In this hypothetical study, subjects classify the emotional expressions of faces as quickly as possible, and we use their response time as the primary dependent variable. Let's imagine that the faces are of two types: either from the subject's ingroup or from an outgroup. For simplicity, we further assume that each face appears only once in the stimulus set. The key question is whether there is any difference in classification speed across the type of face.

Required software

The simulation will be presented in the R programming language (R Core Team, 2018). To run the code, you will need to have some add-on packages available.

```
# load required packages
library("lme4")      # model specification / estimation
library("lmerTest")  # provides p-values in the output
library("tidyverse") # data wrangling and visualisation
```

151 Because the code uses random number generation, if you want to reproduce the exact
 152 results below you will need to set the random number seed at the top of your script and
 153 ensure you are using R version 3.6.0 or higher. If you change the seed or are using a lower
 154 version of R, your exact numbers will differ, but the procedure will still produce a valid
 155 simulation.

```
# ensure this script returns the same results on each run
set.seed(8675309)
```

156 Establishing the data-generating parameters

157 The first thing to do is to set up the parameters that govern the process we assume to
 158 give rise to the data, the *data-generating process* or DGP. In this hypothetical study, each of
 159 100 subjects will respond to all 50 stimulus items (25 ingroup and 25 outgroup), for a total
 160 of 5000 observations.

161 **Specify the data structure.** We want the resulting data to be in long format,
 162 with the structure shown below, where each row is a single observation for each trial. The
 163 variable `subj_id` runs from S001 to S100 and indexes the subject number; `item_id` runs
 164 from I01 to I50 and indexes the item number; `category` is whether the face is ingroup or
 165 outgroup, with items 1-25 always ingroup and items 26-50 always outgroup; and `RT` is the
 166 participant's response time for that trial. Note that a trial is uniquely identified by the
 167 combination of the `subj_id` and `item_id` labels.

Table 2
The target data structure.

row	subj_id	item_id	category	RT
1	S001	I01	ingroup	750.2
2	S001	I02	ingroup	836.1
...
49	S001	I49	outgroup	811.9
50	S001	I50	outgroup	801.8
51	S002	I01	ingroup	806.7
52	S002	I02	ingroup	805.9
...
5000	S100	I50	outgroup	859.9

168 Note that for independent variables in designs where subjects and stimuli are crossed,
 169 you can't think of factors as being solely "within" or "between" because we have two sampling
 170 units; you must ask not only whether independent variables are within- or between- subjects,
 171 but also whether they are within- or between- stimulus items. Recall that a within-subjects

factor is one where each and every subject receives all of the levels, and a between-subjects factor is one where each subject receives only one of the levels. Likewise, a within-items factor is one for which each stimulus receives all of the levels. For our current example, the category factor is within subjects but between items, given that each stimulus item is either ingroup or outgroup.

Specify the fixed effects. Getting an appropriately structured dataset is the easy part. The difficult part is generating the RT values. For this, we need to establish an underlying statistical model. Let us start with a basic model and build up from there. We want a model of RT for subject s and item i that looks something like:

$$RT_{si} = \beta_0 + \beta_1 X_i + e_{si}. \quad (1)$$

According to the formula, response RT_{si} for subject s and item i is defined as sum of an intercept term β_0 , which in this example is the grand mean reaction time for the population of stimuli, plus β_1 , the mean RT difference between ingroup and outgroup stimuli, plus random noise e_{si} . To make β_0 equal the grand mean and β_1 equal the mean outgroup minus the mean ingroup RT, we will code the `category` variable as `-.5` for the ingroup category and `+.5` for the outgroup category.

In the model formula, we use Greek letters (β_0 , β_1) to represent population parameters that are being directly estimated by the model. In contrast, Roman letters represent observed values (`RT_{si}`) or quantities derived from observed values along with model estimates, such as residual error (e_{si}).

Although this model is incomplete, we can go ahead and choose parameters for β_0 and β_1 . For this example, we set a grand mean of 800 ms and a mean difference of 50 ms. You will need to use disciplinary expertise and/or pilot data to choose these parameters; by the end of this tutorial you will understand how to extract those parameters from an analysis.

```
# set fixed effect parameters
b0 <- 800 # intercept; i.e., the grand mean
b1 <- 50 # slope; i.e., effect of category
```

The parameters β_0 and β_1 are *fixed effects*: they characterize properties of the population of encounters between subjects and stimuli. Thus, we set the mean RT for a “typical” subject encountering a “typical” stimulus to 800 ms, and assume that responses are typically 50 ms slower for outgroup than ingroup faces.

Specify the random effects. This model is completely unrealistic, however, because it doesn’t allow for any individual differences among subjects or stimuli. Subjects are not identical in their response characteristics: some will be faster than average, and some slower. We can characterize the difference from the grand mean for each subject s in terms of a *random effect* T_{0s} , where the first subscript, 0, indicates that the deflection goes with the intercept term, β_0 . This *random intercept* term captures the value that must be added or subtracted to the intercept for subject s , which in this case corresponds to how much slower or faster this subject relative to the average reaction time of 800 ms. Just as it is unrealistic to expect the same intercept for every subject, it is also unrealistic to assume this

for stimuli; in other words, that it is equally easy to categorize emotional expressions across all faces in the dataset. It will be easier to do so for some faces than others, and we can incorporate this assumption by including by-item random intercepts O_{0i} , with the subscript 0 reminding us that it is a deflection from the β_0 term, and the i indexing each of the 50 stimulus items (faces). Each face is assigned a unique *random intercept* that characterizes how much slower or faster responses to this particular face tend to be relative to the average reaction time of 800 ms. Adding these terms to our model yields:

$$RT_{si} = \beta_0 + T_{0s} + O_{0i} + \beta_1 X_i + e_{si} \quad (2)$$

Now, whatever values of T_{0s} and O_{0i} we end up with in our sampled dataset will depend on the luck of the draw, i.e., on which subjects and stimuli we happened to have sampled from their respective populations. Unlike fixed effects, we assume these values will differ across different realizations of the experiment where subjects and/or stimuli are different. In practice, we often re-use the same stimuli across many studies, but we still need to treat the stimuli as sampled if we want to be able to generalise our findings to the whole population of stimuli.¹

It is an important conceptual feature of mixed-effects models that they do not directly estimate the individual random effects (T_{0s} and O_{0i} values), but rather, they estimate the random effects parameters that characterize the distributions from which these effects are drawn. It is this feature that enables generalization beyond the particular subjects and stimuli in the experiment. We assume that each T_{0s} comes from a normal distribution with a mean of zero and unknown standard deviation, τ_0 (`tau_0` in the code). The mean of zero reflects the assumption that each random effect is a deflection from the grand mean. Similarly, for the by-item random intercepts, we assume the O_{0i} values to be sampled from a normal distribution also with a mean of zero and with an unknown standard deviation, ω_0 (`omega_0`). (The subscript 0 reflects that these parameters are associated with β_0 , the intercept).² In our simulation, we will set the by-subject random intercept SD to 100, and the by-item random intercept SD to 80.

```
# set random effect parameters
tau_0    <- 100 # by-subject random intercept sd
omega_0  <- 80  # by-item random intercept sd
```

There is still a deficiency in our data-generating model related to β_1 , the fixed effect of category. Currently our model assumes that each and every subject is exactly 80 ms faster to categorize emotions on ingroup faces than on outgroup faces. Clearly, this assumption is totally unrealistic; some participants will be more sensitive to ingroup/outgroup differences than others. We can capture this in an analogous way to which we captured variation in the intercept, namely by including by-subject *random slopes* T_{1s} .

¹To ensure a finding is generalizable, when attempting a replication it is useful to sample new items, just as one would typically sample new participants.

²You will sometimes see the assumption of random effects drawn from a normal distribution notated mathematically as, e.g.: $O_{0i} \sim N(0, \omega_0^2)$, which you can read as "the random intercept O_{0i} for each subject i is drawn from a normal distribution with mean of zero and variance of ω_0^2 ". Variance is just the square of the standard deviation.

$$RT_{si} = \beta_0 + T_{0s} + O_{0i} + (\beta_1 + T_{1s}) X_i + e_{si} \quad (3)$$

The random slope T_{1s} is an estimate of how much faster or slower subject s is in categorizing ingroup/outgroup faces than the population mean effect β_1 , which we already set to 50 ms. Given how we coded the X_i variable, the mean effect for subject s is given by the $\beta_1 + T_{1s}$ term. So, a participant who is 90 ms faster on average to categorize ingroup than outgroup faces would have a random slope T_{1s} of 40 ($\beta_1 + T_{1s} = 50 + 40 = 90$). As we did for the random intercepts, we assume that the T_{1s} effects are drawn from a normal distribution, with a mean of zero and standard deviation of τ_1 (`tau_1` in the code). For this example, we assume the standard deviation is 40 ms.

But note that we are sampling *two* random effects for each subject s , a random intercept T_{0s} and a random slope T_{1s} . It is possible for these values to be correlated, in which case we should not sample them independently. For instance, perhaps people who are faster than average overall (negative random intercept) also show a smaller than average effect of the ingroup/outgroup manipulation (negative random slope) due to allocating less attention to the task. We can capture this by allowing for a small correlation between the two factors, `rho`, which we assign to be 0.2.

Finally, we need to characterize the trial-level noise in the study (e_{si}) in terms of its standard deviation. Here we simply assign this parameter value `sigma` to be twice the size of the by-subject random intercept SD. Later, we will

```
# set more random effect and error parameters
tau_1 <- 40 # by-subject random slope sd
rho <- .2 # correlation between intercept and slope
sigma <- 200 # residual (error) sd
```

To summarize, we established a reasonable statistical model underlying the data having the form:

$$RT_{si} = \beta_0 + T_{0s} + O_{0i} + (\beta_1 + O_{1s}) X_i + e_{si} \quad (4)$$

The response time for subject s on item i , RT_{si} , is decomposed into a population grand mean β_0 , a by-subject random intercept T_{0s} , a by-item random intercept O_{0i} , a fixed slope β_1 , a by-subject random slope T_{1s} , and a trial-level residual e_{si} . Our data-generating process is fully determined by seven parameters. There are two fixed effects parameters, the fixed intercept β_0 (`b0`) and fixed slope β_1 (`b1`). There are four variance parameters governing the random effects: the standard deviation of the by-subject random intercepts, τ_0 (`tau_0`); the standard deviation of by-subject random slopes, τ_1 (`tau_1`), the correlation between the by-subject random intercepts and random slopes, ρ (`rho`); and the standard deviation of the by-item random intercepts, ω_0 (`omega_0`). Finally, the seventh parameter σ (`sigma`) reflects any remaining trial-by-trial variation not already captured by the model. In the next section we will apply this data-generating process to simulate the sampling of subjects, items, and trials (encounters).

272 Simulating the sampling process

273 Let's first define parameters related to the number of observations. In this example,
 274 we will simulate data from 100 subjects responding to 25 ingroup faces and 25 outgroup
 275 faces. There are no between-subject factors, so we can set `nsubj` to 100. We set `n_ingroup`
 276 and `n_outgroup` to the number of stimulus items in each condition.

```
# set number of subjects and items
n_subj <- 100 # number of subjects
n_ingroup <- 25L # 25 ingroup stimuli
n_outgroup <- 25L # 25 outgroup stimuli
```

277 **Simulate the sampling of stimulus items.** We need to create a table listing
 278 each item, which category it is in, and simulated values for its random effects.

```
# simulate a sample of items
# total number of items = n_ingroup + n_outgroup
items <- data.frame(
  item_id = seq_len(n_ingroup + n_outgroup),
  category = rep(c("ingroup", "outgroup"), c(n_ingroup, n_outgroup)),
  O_0i = rnorm(n = n_ingroup + n_outgroup, mean = 0, sd = omega_0)
)
```

279 For the first variable in the dataset, `item_id`, we have used `seq_len()` to assign a
 280 unique integer to each of the 50 stimulus faces; these IDs function like names. The `category`
 281 variable designates whether the face is ingroup or outgroup, with the first 25 items being
 282 ingroup and the last 25 being outgroup. Finally, we sample the values of O_{0i} from a normal
 283 distribution using the `rnorm()` function, with a mean of 0 and SD of ω_0 .

284 Let us introduce a numerical predictor to represent what category each stimulus item
 285 i appears in (i.e., for the X_i in our model). Since we predict that responses to ingroup faces
 286 will be faster than outgroup faces, we set ingroup to -0.5 and outgroup to +0.5. We will
 287 later multiply this *effect coded* factor by the fixed effect of category ($b_1 = 50$) to simulate
 288 data where the ingroup faces are on average -25 ms different from the grand mean, while
 289 the outgroup faces are on average 25 ms different from the grand mean.

```
# effect-code category
items$X_i <- recode(items$category, "ingroup" = -0.5, "outgroup" = +0.5)
```

290 In R, most regression procedures can handle two-level factors like `category`. By
 291 default, the procedure will create a new numeric predictor that codes one level of the factor
 292 as zero and the other as one. Why not just use the defaults? The short explanation is that
 293 the default of 0, 1 coding is not well-suited to the kinds of factorial experimental designs
 294 often found in psychology and related fields. For the current example, using the default
 295 coding for the X predictor would change the interpretation of β_0 : instead of the grand
 296 mean, it would reflect the mean for the group coded as zero. One could change the default,
 297 but we feel it is better to be explicit in the code about what values are being used (see
 298 <https://talklab.psy.gla.ac.uk/tvw/catpred> for further discussion).

Table 3
The resulting table of item parameters.

item_id	category	O_0i	X_i
1	ingroup	-79.7	-0.5
2	ingroup	57.7	-0.5
3	ingroup	-49.4	-0.5
4	ingroup	162.4	-0.5
5	ingroup	85.2	-0.5
6	ingroup	79	-0.5
...
44	outgroup	54.7	0.5
45	outgroup	-20.2	0.5
46	outgroup	-12.1	0.5
47	outgroup	-70	0.5
48	outgroup	-158.2	0.5
49	outgroup	19	0.5
50	outgroup	2.9	0.5

Simulate the sampling of subjects. Now we will simulate the sampling of individual subjects, resulting in a table listing each subject and their two correlated random effects. This will be slightly more complicated than what we just did, because we cannot simply sample the T_{0s} values from a univariate distribution using `rnorm()` independently from the T_{1s} values. Instead, we must sample $\langle T_{0s}, T_{1s} \rangle$ pairs—one pair for each subject—from a bivariate normal distribution. To do this, we will use the `mvrnorm()` function, a multivariate version of `rnorm()` from the MASS package that comes pre-installed with R. We specify the three parameters describing this distribution—two variances and a correlation—by entering them into a 2x2 *variance-covariance* matrix using the `matrix()` function, and then passing this matrix to `mvrnorm()` using the `Sigma` argument. This requires converting the standard deviations into variances (by squaring them) and calculating the covariance, which is simply the product of the correlation and two standard deviations, i.e., $\rho \times \tau_0 \times \tau_1$.

We only need this one function from MASS, so we can call it directly using the `package::function()` syntax instead of loading the library (specifically, `MASS::mvrnorm()` instead of `library(MASS)`).³

```
# simulate a sample of subjects

# calculate random intercept / random slope covariance
covar <- rho * tau_0 * tau_1

# put values into variance-covariance matrix
cov_mx <- matrix(
```

³Note that MASS package has a function we don't need named 'select()', but loading it using 'library()' would overwrite the function of the same name from the 'dplyr' package that we often do need, so in general it is a good idea to avoid loading MASS.

```

c(tau_0^2, covar,
  covar, tau_1^2),
nrow = 2, byrow = TRUE)

# generate the by-subject random effects
subject_rfx <- MASS::mvrnorm(n = n_subj,
                             mu = c(T_0s = 0, T_1s = 0),
                             Sigma = cov_mx)

# combine with subject IDs
subjects <- data.frame(subj_id = seq_len(n_subj),
                       subject_rfx)

```

Table 4
The resulting table of subject parameters.

subj_id	T_0s	T_1s
1	-14.7	11.1
2	-8.4	-36.7
3	87.7	-47.5
4	209.3	62.9
5	-23.6	21.5
6	90.1	56.7
...
94	99.5	-31
95	44.3	69.3
96	12.2	37.1
97	-121.9	42.3
98	-49.9	-41.1
99	-134.5	16.6
100	-30.2	37.5

314 **Simulate trials (encounters).** Since all subjects respond to all items, we can set
 315 up a table of trials by making a table with every possible combination of the rows in the
 316 subject and item tables using the tidyverse function `crossing()`. Each trial has random
 317 error associated; we simulate this from a normal distribution with a mean of 0 and SD of
 318 `sigma`.

```

# cross subject and item IDs; add an error term

trials <- crossing(subjects, items) %>%
  mutate(e_si = rnorm(n_subj * (n_ingroup + n_outgroup), # N subj x N stimuli
                      mean = 0, sd = sigma)) %>%
  select(subj_id, item_id, category, X_i, everything())

```

Table 5
The resulting table of trials (encounters).

subj_id	item_id	category	X_i	T_0s	T_1s	O_0i	e_si
1	1	ingroup	-0.50	-14.65	11.13	-79.73	-66.54
1	2	ingroup	-0.50	-14.65	11.13	57.75	-34.74
1	3	ingroup	-0.50	-14.65	11.13	-49.38	-37.49
1	4	ingroup	-0.50	-14.65	11.13	162.35	231.26
1	5	ingroup	-0.50	-14.65	11.13	85.23	-187.64
1	6	ingroup	-0.50	-14.65	11.13	78.98	104.81
...
100	44	outgroup	0.50	-30.15	37.52	54.73	-3.38
100	45	outgroup	0.50	-30.15	37.52	-20.16	18.47
100	46	outgroup	0.50	-30.15	37.52	-12.08	87.92
100	47	outgroup	0.50	-30.15	37.52	-69.99	25.47
100	48	outgroup	0.50	-30.15	37.52	-158.15	91.23
100	49	outgroup	0.50	-30.15	37.52	19.01	78.14
100	50	outgroup	0.50	-30.15	37.52	2.89	-34.31

Calculate the response values. Note how this resulting table contains the full decomposition of effects that we need to compute the response according to the linear model we defined above:

$$RT_{si} = \beta_0 + T_{0s} + O_{0i} + (\beta_1 + O_{1s}) X_i + e_{si} \quad (5)$$

Thus, we will calculate the response variable RT by adding together:

- the grand intercept (**b0**),
- each subject-specific random intercept (**T_0s**),
- each item-specific random intercept (**O_0i**),
- each sum of the category effect (**b1**) and the random slope (**T_1s**), multiplied by the numerical predictor (**X_i**), and
- each residual error (**e_si**).

After this we will use `dplyr::select()` to keep the columns we need. Note that the resulting table has the structure that we set as our goal at the start of this exercise, with the additional column **X_i**, which we will keep to use in the estimation process, described in the next section.

```
# calculate the response variable
dat_sim <- trials %>%
  mutate(RT = b0 + T_0s + O_0i + (b1 + T_1s) * X_i + e_si) %>%
  select(subj_id, item_id, category, X_i, RT)
```

Table 6
The final simulated dataset.

subj_id	item_id	category	X_i	RT
1	1	ingroup	-0.5	609
1	2	ingroup	-0.5	778
1	3	ingroup	-0.5	668
1	4	ingroup	-0.5	1148
1	5	ingroup	-0.5	652
1	6	ingroup	-0.5	939
...
100	44	outgroup	0.5	865
100	45	outgroup	0.5	812
100	46	outgroup	0.5	889
100	47	outgroup	0.5	769
100	48	outgroup	0.5	747
100	49	outgroup	0.5	911
100	50	outgroup	0.5	782

333 **Data simulation function.** To make it easier to try out different parameters or
 334 to generate many datasets for the purpose of power analysis, you can put all of the code
 335 above into a custom function. Set up the function to take all of the parameters we set
 336 above as arguments. We'll set the defaults to the values we used, but you can choose your
 337 own defaults. The code below is just all of the code above, condensed a bit. It returns one
 338 dataset with the parameters you specified.

```
# set up the custom data simulation function
my_sim_data <- function(
  nsubj      = 100,  # number of subjects
  n_ingroup  = 25,   # number of ingroup stimuli
  n_outgroup = 25,   # number of outgroup stimuli
  b0         = 800,  # grand mean
  b1         = 50,   # effect of category
  omega_0    = 80,   # by-item random intercept sd
  tau_0      = 100,  # by-subject random intercept sd
  tau_1      = 40,   # by-subject random slope sd
  rho        = 0.2,  # correlation between intercept and slope
  sigma      = 200) { # residual (standard deviation)

  items <- data.frame(
    item_id = seq_len(n_ingroup + n_outgroup),
    category = rep(c("ingroup", "outgroup"), c(n_ingroup, n_outgroup)),
    X_i = rep(c(-0.5, 0.5), c(n_ingroup, n_outgroup)),
    O_0i = rnorm(n = n_ingroup + n_outgroup, mean = 0, sd = omega_0))

  # variance-covariance matrix
```

```

cov_mx <- matrix(
  c(    tau_0^2,          rho * tau_0 * tau_1,
      rho * tau_0 * tau_1,    tau_1^2          ),
  nrow = 2, byrow = TRUE)

subjects <- data.frame(subj_id = seq_len(nsubj),
                       MASS::mvrnorm(n = nsubj,
                                     mu = c(T_0s = 0, T_1s = 0),
                                     Sigma = cov_mx))

crossing(subjects, items) %>%
  mutate(e_si = rnorm(n_subj * (n_ingroup + n_outgroup),
                     mean = 0, sd = sigma),
         RT = b0 + T_0s + 0_0i + (b1 + T_1s) * X_i + e_si) %>%
  select(subj_id, item_id, category, X_i, RT)
}

```

339 Now you can generate a dataset with the default parameters using `my_sim_data()` or,
 340 for example, a dataset with 500 subjects and no effect of category using `my_sim_data(nsubj`
 341 `= 50, b1 = 0)`.

342 Analyzing the simulated data

343 Setting up the formula

344 Now we're ready to analyse our simulated data. The first argument to `lmer()` is a
 345 model formula that defines the structure of the linear model. The formula for our design
 346 maps onto how we calculated the response above.

347 `RT ~ 1 + X_i + (1 | item_id) + (1 + X_i | subj_id)`

- 348 • RT is the response
- 349 • 1 corresponds to the grand intercept (`b0`),
- 350 • `X_i` is the predictor for the ingroup/outgroup manipulation for item *i*;
- 351 • `(1 | item_id)` specifies a by-subject random intercept (`I0i`),
- 352 • `(1 + X_i | subj_id)` specifies a subject-specific random intercept (`S0s`) plus the
 353 subject-specific random slope of category (`S1s`),
- 354 • the error term is automatically included in all models, so is left implicit

355 The “fixed” part of the formula, `RT ~ 1 + X_i`, establishes the $RT_{si} + \beta_0 + \beta_1 X_i + e_{si}$
 356 part of our linear model. Every model has an intercept (β_0) term and residual term (e_{si}) by
 357 default, so you could alternatively leave the 1 out and just write `RT ~ X_i`.

358 The terms in parentheses with the `|` separator define the random effects structure. For
 359 each of these bracketed terms, the left-hand side of the `|` names the effects you wish to allow
 360 to vary and the right hand side names the variable identifying the levels of the random factor
 361 over which the terms vary (e.g., subjects or items). The first term, `(1 | item_id)` allows

the intercept (1) to vary over the random factor of items (`item_id`). This is an instruction to estimate the parameter underlying the 0_{0i} values, namely ω_0 . The second term, $(1 + X_i | \text{subj_id})$, allows both the intercept and the effect of category (coded by X_i) to vary over the random factor of subjects (`subj_id`). It is an instruction to estimate the three parameters that underlie the T_0 s and T_1 s values, namely τ_0 , τ_1 , and ρ .

Interpreting the lmer summary

The other arguments to the `lme4` function are the name of the data frame where the values are found (`dat_sim`), and `REML = FALSE` which selects maximum-likelihood estimation, which is preferable to the default estimation technique when testing fixed effects. Use the `summary()` function to view the results.

```
# fit a linear mixed-effects model to data
mod_sim <- lmer(RT ~ 1 + X_i + (1 | item_id) + (1 + X_i | subj_id),
               data = dat_sim, REML = FALSE)

summary(mod_sim, corr = FALSE)
```

```
## Linear mixed model fit by maximum likelihood . t-tests use Satterthwaite's
## method [lmerModLmerTest]
## Formula: RT ~ 1 + X_i + (1 | item_id) + (1 + X_i | subj_id)
## Data: dat_sim
##
##          AIC          BIC    logLik deviance df.resid
## 67769.5    67815.1 -33877.7   67755.5     4993
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -3.7355 -0.6744  0.0076  0.6705  3.5521
##
## Random effects:
## Groups   Name                Variance Std.Dev. Corr
## subj_id  (Intercept)         8366     91.47
##          X_i                 3286     57.32  0.12
## item_id  (Intercept)         3943     62.79
## Residual                    41285    203.19
## Number of obs: 5000, groups:  subj_id, 100; item_id, 50
##
## Fixed effects:
##              Estimate Std. Error    df t value Pr(>|t|)
## (Intercept)   807.72      13.07 122.48  61.809  <2e-16 ***
## X_i           39.47      19.53  58.49   2.021  0.0478 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Let's break down the output step-by-step and try to find estimates of the seven parameters

we used to generate the data: `b0`, `b1`, `tau_0`, `tau_1`, `rho`, `omega_0` and `sigma`. If you analyze existing data with a mixed effects model, you can use these estimates to help you set reasonable values for random effects in your own simulations.

After providing general information about the model fit, the output is divided into a **Random effects** and a **Fixed effects** section. The fixed effects section should be familiar from other types of linear models.

```
## Fixed effects:
##           Estimate Std. Error    df t value Pr(>|t|)
## (Intercept)  807.72     13.07 122.48  61.809  <2e-16 ***
## X_i          39.47     19.53  58.49   2.021   0.0478 *
```

The **Estimate** column gives us parameter estimates for the fixed effects in the model, i.e., $\hat{\beta}_0$ and $\hat{\beta}_1$, which are estimated at about 807.72 and 39.47. The next columns give us the standard errors, estimated degrees of freedom (using the Satterthwaite approach), t value, and finally, p value.

The **Random effects** section is specific to mixed-effects models, and will be less familiar to the reader.

```
## Random effects:
## Groups   Name          Variance Std.Dev. Corr
## subj_id  (Intercept)  8366     91.47
##          X_i          3286     57.32  0.12
## item_id  (Intercept)  3943     62.79
## Residual                41285    203.19
```

These are the estimates for the *variance components* in the model. Note that there are no p -values associated with these effects. If you wish to determine whether a random effect is significant, you need to run the model with and without the random effect term and compare the log-likelihoods of the models. To avoid confusion, it is best to think of the information in this table as coming from three separate tables divided up by the values in the **Groups** column.

The first subtable, where the value of **Groups** is `subj_id`, gives the estimates for the variance parameters defining the by-subject random effects.

```
## Groups   Name          Variance Std.Dev. Corr
## subj_id  (Intercept)  8366     91.47
##          X_i          3286     57.32  0.12
```

We have estimates for the variance of the intercept and slope (`X_i`) in the **Variance** column, which is just the square of the standard deviation in the **Std.Dev.** column. We obtain estimates for `tau_0` and `tau_1` of 91.47 and 57.32 respectively. The **Corr.** column gives us the estimated correlation between the by-subject random intercepts and slopes, estimated here as 0.12.

The second subtable gives us the by-item random effect parameter estimates of which there is only one, 62.79, corresponding to `omega_0`. Again, the **Variance** column is just this

439 value squared.

```
440 ## Groups   Name          Variance Std.Dev. Corr
441 ## item_id (Intercept) 3943      62.79
```

442 The last subtable gives us the estimate of the residual term, 203.19.

```
443 ## Groups   Name          Variance Std.Dev. Corr
444 ## Residual              41285     203.19
```

445 We have found all seven parameters in the output. Let's compare them to the values
446 that we put in.

Table 7

The simulation parameters compared to the model estimations.

variable	explanation	simulated value	estimated by model
b0	intercept (grand mean)	800.0	807.72
b1	fixed effect of category	50.0	39.47
tau_0	by-subject random intercept SD	100.0	91.47
rho	correlation between intercept and slope	0.2	0.12
tau_1	by-subject random slope SD	40.0	57.32
omega_0	by-item random intercept SD	80.0	62.79
sigma	residual (error) SD	200.0	203.19

447 You can also use `broom.mixed::tidy()` to output fixed and/or random effects in a
448 tidy table. This is especially useful when you need to combine the output from hundreds of
449 simulations to calculate power. The code below adds a column with the simulated parameters
450 we set above so you can compare them to the estimated parameters from this simulated
451 dataset.

```
# get a tidy table of results
broom.mixed::tidy(mod_sim) %>%
  mutate(sim = c(b0, b1, tau_0, rho, tau_1, omega_0, sigma)) %>%
  select(1:3, 9, 4:8)
```

Table 8

The output of the tidy function from broom.mixed.

effect	group	term	sim	estimate	std.error	statistic	df	p.value
fixed	NA	(Intercept)	800.0	807.72	13.1	61.8	122.5	0.000
fixed	NA	X_i	50.0	39.47	19.5	2.0	58.5	0.048
ran_pars	subj_id	sd__(Intercept)	100.0	91.47	NA	NA	NA	NA
ran_pars	subj_id	cor__(Intercept).X_i	0.2	0.12	NA	NA	NA	NA
ran_pars	subj_id	sd__X_i	40.0	57.32	NA	NA	NA	NA
ran_pars	item_id	sd__(Intercept)	80.0	62.79	NA	NA	NA	NA
ran_pars	Residual	sd__Observation	200.0	203.19	NA	NA	NA	NA

Setting Parameters

Now that you see where each parameter we used to generate the data appears in the analysis output, you can use the analysis of pilot data to get estimates for these parameters for further simulation. For example, if you have pilot data from 10 participants on this task, you can analyse their data using the same code as above, and estimate values for `b0`, `b1`, `tau_0`, `tau_1`, `rho`, `omega_0`, and `sigma` for use in a power calculation or a sensitivity analysis (see appendix 1C).

Calculate Power

Data simulation is useful not only for illuminating modeling approaches, but also for calculating power when planning a study. The basic idea of a power simulation is to generate a large number of datasets encoding your assumptions about likely parameter values, fit models to each dataset, and then calculate the proportion of models that reject the null hypothesis as a measure of power.

First we create a function that analyses the simulated data and test it by running it once with default parameters.

```
# set up the power function
my_lmer_power <- function(...) {
  # ... is a shortcut that forwards any arguments to
  # my_sim_data(), the function created above
  dat_sim <- my_sim_data(...)
  mod_sim <- lmer(RT ~ X_i + (1 | item_id) + (1 + X_i | subj_id),
    dat_sim, REML = FALSE)

  broom.mixed::tidy(mod_sim)
}

# run one model with default parameters
my_lmer_power()
```

Table 9

The output of lmer_power().

effect	group	term	estimate	std.error	statistic	df	p.value
fixed	NA	(Intercept)	812.96	14.3	56.9	115.4	0.000
fixed	NA	X_i	83.41	21.8	3.8	53.3	0.000
ran_pars	subj_id	sd__(Intercept)	94.45	NA	NA	NA	NA
ran_pars	subj_id	cor__(Intercept).X_i	0.19	NA	NA	NA	NA
ran_pars	subj_id	sd__X_i	41.39	NA	NA	NA	NA
ran_pars	item_id	sd__(Intercept)	73.18	NA	NA	NA	NA
ran_pars	Residual	sd__Observation	199.23	NA	NA	NA	NA

You can also change parameters. For example, what would happen if you increase the number of items to 50 in each group and decrease the effect of category to 20 ms?

```
# run one model with new parameters
my_lmer_power(n_ingroup = 50, n_outgroup = 50, b1 = 20)
```

Table 10

The output of lmer_power() with 50 items per group and a category effect of 20 ms.

effect	group	term	estimate	std.error	statistic	df	p.value
fixed	NA	(Intercept)	793.23	13.6	58.2	169.8	0.000
fixed	NA	X_i	22.21	16.0	1.4	106.6	0.168
ran_pars	item_id	sd__(Intercept)	75.75	NA	NA	NA	NA
ran_pars	subj_id	sd__(Intercept)	111.60	NA	NA	NA	NA
ran_pars	subj_id	cor__(Intercept).X_i	0.28	NA	NA	NA	NA
ran_pars	subj_id	sd__X_i	31.64	NA	NA	NA	NA
ran_pars	Residual	sd__Observation	199.51	NA	NA	NA	NA

469 You can use the `purrr::map_df` function to run the simulation repeatedly and save
 470 the results to a data table. This will take a while, so test using just a few repetitions (`reps`)
 471 first, then make sure you save the full results to a CSV file so you can comment out this
 472 code and load from the saved data for the rest of your script in the future. You can use
 473 these data to calculate power for each fixed effect.

```
# run simulations and save to a file
reps <- 100
sims <- purrr::map_df(1:reps, ~my_lmer_power())
write_csv(sims, "sims.csv")

# read saved simulation data
sims <- read_csv("sims.csv", col_types = cols(
  # makes sure plots display in this order
  group = col_factor(ordered = TRUE),
  term = col_factor(ordered = TRUE)
))

# calculate mean estimates and power for specified alpha
alpha <- 0.05

sims %>%
  filter(effect == "fixed") %>%
  group_by(term) %>%
  summarise(
    mean_estimate = mean(estimate),
    mean_se = mean(std.error),
    power = mean(p.value < alpha)
  )
```

Table 11
Power calculation for fixed effects.

term	Mean Estimate	Mean Std. Error	Power
(Intercept)	803.6	15.4	1.00
cat	47.6	23.6	0.53

Conclusion

Mixed-effects modeling is a powerful technique for analyzing data from complex designs. The technique is close to ideal for analyzing data with crossed random factors of subjects and stimuli: it gracefully and simultaneously accounts for subject and item variance within a single analysis, and outperforms traditional techniques in terms of type I error and power. However, this additional power comes at the price of technical complexity. Through this article, we have attempted to make mixed-effects models more approachable using data simulation.

We considered only a simple, one-factor design. However, the general principles are the same for higher-order designs. For instance, consider a 2x2 design, with factors *A* and *B* both within subjects, but *A* within items and *B* between items. For such a design, you would have four instead of two by-subject random effects: the intercept, main effect of *A*, main effect of *B*, and the *AB* interaction. You would also need to specify correlations between each of these effects. You would also have two by-item random effects: one for the intercept and one for *A*. Our supplemental online materials (<https://osf.io/3cz2e/>) include such an extension of the example in this paper with `category` as a within-subject and between-item factor and adding `expression` as a within-subject and within-item factor. For further guidance and discussion on how to specify the random effects structure in complex designs, see (Barr, 2013).

Here we only considered a design with a normally distributed response variable. However, generalised linear mixed effect models allow for response variables with different distributions, such as binomial. Our supplemental online materials (<https://osf.io/3cz2e/>) illustrate the differences in simulation required for the study design in this paper with a binomial accuracy score (correct/incorrect) as the response variable.

We also have not said much in this tutorial about estimation issues, such as what to do when the fitting procedure fails to converge. Further guidance on this point can be found in (Barr et al., 2013), and by consulting the help materials in the `lme4` package (`?lme4::convergence`). We have also assumed that the random effects specification for the `lmer()` function should be based on the study design. However, we note that others have argued in favor of data-driven approaches for random effects specification (Matuschek, Kliegl, Vasishth, Baayen, & Bates, 2017).

In this tutorial, we have introduced the main concepts needed to get started with mixed effects models. Through data simulation of your own study designs, you can develop your understanding and perform power calculations to guide your sample size plans.

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