Estimating Generalized (Non-)Linear Models with Group-Specific Terms with rstanarm

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Introduction

This vignette explains how to use the `stan_lmer`, `stan_glmer`, `stan_nlmer`, and `stan_gamm4` functions in the **rstanarm** package to estimate linear and generalized (non-)linear models with parameters that may vary across groups. Before continuing, we recommend reading the vignettes (glm.html) for the `stan_glm` function. The *Hierarchical Partial Pooling* vignette (pooling.html) also has examples of both `stan_glm` and `stan_glmer`.

GLMs with group-specific terms

Models with this structure are refered to by many names: multilevel models, (generalized) linear mixed (effects) models (GLMM), hierarchical (generalized) linear models, etc. In the simplest case, the model for an outcome can be written as

$$\mathbf{y} = \alpha + \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b} + \boldsymbol{\epsilon},$$

where $\mathbf{X}$ is a matrix predictors that is analagous to that in Generalized Linear Models and $\mathbf{Z}$ is a matrix that encodes deviations in the predictors across specified groups.

The terminology for the unknowns in the model is diverse. To frequentists, the error term consists of $\mathbf{Z}\mathbf{b} + \boldsymbol{\epsilon}$ and the observations within each group are *not* independent conditional on $\mathbf{X}$ alone. Since, $\mathbf{b}$ is considered part of the random error term, frequentists allow themselves to make distributional assumptions about $\mathbf{b}$, invariably that it is distributed multivariate normal with mean vector zero and structured covariance matrix $\boldsymbol{\Sigma}$. If ϵ_i is also distributed (univariate) normal with mean zero and standard deviation σ, then $\mathbf{b}$ can be integrated out, which implies

$$\mathbf{y} \sim \mathcal{N}\left(\alpha + \mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I} + \mathbf{Z}^\top\boldsymbol{\Sigma}\mathbf{Z}\right),$$

and it is possible to maximize this likelihood function by choosing proposals for the parameters $\alpha, \boldsymbol{\beta}$, and (the free elements of) $\boldsymbol{\Sigma}$.

Consequently, frequentists refer to $\mathbf{b}$ as the *random effects* because they capture the random deviation in the effects of predictors from one group to the next. In contradistinction, α and $\boldsymbol{\beta}$ are referred to as *fixed effects* because they are the same for all groups. Moreover, α and $\boldsymbol{\beta}$ persist in the model in hypothetical replications of the analysis that draw the members of the groups afresh every time, whereas $\mathbf{b}$ would differ from one replication to the next. Consequently, $\mathbf{b}$ is not a “parameter” to be estimated because parameters are unknown constants that are fixed in repeated sampling.

Bayesians condition on the data in-hand without reference to repeated sampling and describe their *beliefs* about the unknows with prior distributions before observing the data. Thus, the likelihood in a simple hierarchical model in **rstarnarm** is

$$\mathbf{y} \sim \mathcal{N}\left(\alpha + \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b}, \sigma^2\mathbf{I}\right)$$

and the observations are independent conditional on $\mathbf{X}$ and $\mathbf{Z}$. In this formulation, there are

- intercept(s) and coefficients that are *common across groups*
- deviations in the intercept(s) and / or coefficients that *vary across groups*

Bayesians are compelled to state their prior beliefs about all unknowns and the usual assumption (which is maintained in **rstanarm**) is that $\mathbf{b} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$, but it is then necessary to state prior beliefs about $\boldsymbol{\Sigma}$, in addition to $\alpha, \boldsymbol{\beta}$, and σ.

One of the many challenges of fitting models to data comprising multiple groupings is confronting the tradeoff between validity and precision. An analysis that disregards between-group heterogeneity can yield parameter estimates that are wrong if there is between-group heterogeneity but would be relatively precise if there actually were no between-group heterogeneity. Group-by-group analyses, on the other hand, are valid but produces estimates that are relatively imprecise. While complete pooling or no pooling of data across groups is sometimes called for, models that ignore the grouping structures in the data tend to underfit or overfit (Gelman et al.,2013). Hierachical modeling provides a compromise by allowing parameters to vary by group at lower levels of the hierarchy while estimating common parameters at higher levels. Inference for each group-level parameter is informed not only by the group-specific information contained in the data but also by the data for other groups as well. This is commonly referred to as *borrowing strength* or *shrinkage*.

In **rstanarm**, these models can be estimated using the `stan_lmer` and `stan_glmer` functions, which are similar in syntax to the `lmer` and `glmer` functions in the **lme4** package. However, rather than performing (restricted) maximum likelihood (RE)ML estimation, Bayesian estimation is performed via MCMC. The Bayesian model adds independent prior distributions on the regression coefficients (in the same way as `stan_glm`) as well as priors on the terms of a decomposition of the covariance matrices of the group-specific parameters. These priors are discussed in greater detail below.

Priors on covariance matrices

In this section we dicuss a flexible family of prior distributions for the unknown covariance matrices of the group-specific coefficients.

Overview

For each group, we assume the vector of varying slopes and intercepts is a zero-mean random vector following a multivariate Gaussian distribution with an unknown covariance matrix to be estimated. Unfortunately, expressing prior information about a covariance matrix is not intuitive and can also be computationally challenging. When the covariance matrix is not 1×1, it is often both much more intuitive and efficient to work instead with the **correlation** matrix and variances.

The variances are in turn decomposed into the product of a simplex vector (probability vector) and the trace of the implied covariance matrix, which is defined as the sum of its diagonal elements. Finally, this trace is set equal to the product of the order of the matrix and the square of a scale parameter. This implied prior on a covariance matrix is represented by the `decov` (short for decomposition of covariance) function in **rstanarm**.

Details

Using the decomposition described above, the prior used for a correlation matrix Ω is called the LKJ distribution and has a probability density function proportional to the determinant of the correlation matrix raised to a power of ζ minus one:

$$f(\Omega|\zeta) \propto \det(\Omega)^{\zeta-1}, \quad \zeta > 0.$$

The shape of this prior depends on the value of the regularization parameter, ζ in the following ways:

- If $\zeta = 1$ (the default), then the LKJ prior is jointly uniform over all correlation matrices of the same dimension as Ω.
- If $\zeta > 1$, then the mode of the distribution is the identity matrix. The larger the value of ζ the more sharply peaked the density is at the identity matrix.
- If $0 < \zeta < 1$, then the density has a trough at the identity matrix.

The $J \times J$ covariance matrix Σ of a random vector $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_J)$ has diagonal entries $\Sigma_{jj} = \sigma_j^2 = \text{var}(\theta_j)$. Therefore, the trace of the covariance matrix is equal to the sum of the variances. We set the trace equal to the product of the order of the covariance matrix and the square of a positive scale parameter τ:

$$\text{tr}(\Sigma) = \sum_{j=1}^{J} \Sigma_{jj} = J\tau^2.$$

The vector of variances is set equal to the product of a simplex vector $\boldsymbol{\pi}$ — which is non-negative and sums to 1 — and the scalar trace: $J\tau^2\boldsymbol{\pi}$. Each element π_j of $\boldsymbol{\pi}$ then represents the proportion of the trace (total variance) attributable to the corresponding variable θ_j.

For the simplex vector $\boldsymbol{\pi}$ we use a symmetric Dirichlet prior, which has a single *concentration* parameter $\gamma > 0$:

- If $\gamma = 1$ (the default), then the prior is jointly uniform over the space of simplex vectors with J elements.
- If $\gamma > 1$, then the prior mode corresponds to all variables having the same (proportion of total) variance, which can be used to ensure that the posterior variances are not zero. As the concentration parameter approaches infinity, this mode becomes more pronounced.
- If $0 < \gamma < 1$, then the variances are more polarized.

If all the elements of $\boldsymbol{\theta}$ were multiplied by the same number k, the trace of their covariance matrix would increase by a factor of k^2. For this reason, it is sensible to use a scale-invariant prior for τ. We choose a Gamma distribution, with shape and scale parameters both set to 1 by default, implying a unit-exponential distribution. Users can set the shape hyperparameter to some value greater than one to ensure that the posterior trace is not zero.

Comparison with **lme4**

There are several advantages to estimating these models using **rstanarm** rather than the **lme4** package. There are also a few drawbacks. In this section we briefly discuss what we find to be the two most important advantages as well as an important disadvantage.

Advantage: better uncertainty estimates

While **lme4** uses (restricted) maximum likelihood (RE)ML estimation, **rstanarm** enables full Bayesian inference via MCMC to be performed. It is well known that (RE)ML tends to underestimate uncertainties because it relies on point estimates of hyperparameters. Full Bayes, on the other hand, propogates the uncertainty in the hyperparameters throughout all levels of the model and provides more appropriate estimates of uncertainty for models that consist of a mix of common and group-specific parameters.

Advantage: incorporate prior information

The `stan_glmer` and `stan_lmer` functions allow the user to specify prior distributions over the regression coefficients as well as any unknown covariance matrices. There are various reasons to specify priors, from helping to stabilize computation to incorporating important information into an analysis that does not enter through the data.

Disadvantage: speed

The benefits of full Bayesian inference (via MCMC) come with a cost. Fitting models with (RE)ML will tend to be much faster than fitting a similar model using MCMC. Speed comparable to **lme4** can be obtained with **rstanarm** using approximate Bayesian inference via the mean-field and full-rank variational algorithms (see `help("rstanarm-package", "rstanarm")` for details). These algorithms can be useful to narrow the set of candidate models in large problems, but MCMC should always be used for final statistical inference.

Relationship to `glmer`

In the **lme4** package, there is a fundamental distinction between the way that Linear Mixed Models and Generalized Linear Mixed Models are estimated. In Linear Mixed Models, $\mathbf{b}$ can be integrated out analytically, leaving a likelihood function that can be maximized over proposals for the parameters. To estimate a Linear Mixed Model, one can call the `lmer` function.

Generalized Linear Mixed Models are appropriate when the conditional mean of the outcome is determined by an inverse link function, $\boldsymbol{\mu} = g\left(\alpha + \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b}\right)$. If $g\left(\cdot\right)$ is not the identity function, then it is not possible to integrate out $\mathbf{b}$ analytically and numerical integration must be used. To estimate a Generalized Linear Mixed Model, one can call the `glmer` function and specify the `family` argument.

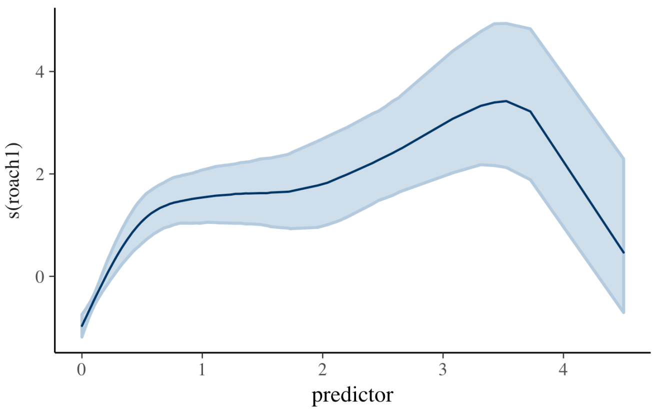
In the **rstanarm** package, there is no such fundamental distinction; in fact `stan_lmer` simply calls `stan_glmer` with `family = gaussian(link = "identity")`. Bayesians do not (have to) integrate $\mathbf{b}$ out of the likelihood and if $\mathbf{b}$ is not of interest, then the margins of its posterior distribution can simply be ignored.

Relationship to `gamm4`

The **rstanarm** package includes a `stan_gamm4` function that is similar to the `gamm4` function in the **gamm4** package, which is in turn similar to the `gamm` function in the **mgcv** package. The substring `gamm` stands for Generalized Additive Mixed Models, which differ from Generalized Additive Models (GAMs) due to the presence of group-specific terms that can be specified with the syntax of **lme4**. Both GAMs and GAMMs include nonlinear functions of (non-categorical) predictors called “smooths”. In the example below, so-called “thin-plate splines” are used to model counts of roaches where we might fear that the number of roaches in the current period is an exponentially increasing function of the number of roaches in the previous period. Unlike `stan_glmer`, in `stan_gamm4` it is necessary to specify group-specific terms as a one-sided formula that is passed to the `random` argument as in the `lme` function in the **nlme** package.

```
library(rstanarm)
data(roaches)
roaches$roach1 <- roaches$roach1 / 100
roaches$log_exposure2 <- log(roaches$exposure2)
post <- stan_gamm4 (../reference/stan_gamm4.html)(
  y ~ s(roach1) + treatment + log_exposure2,
  random = ~(1 | senior),
  data = roaches,
  family = neg_binomial_2,
  QR = TRUE,
  chains = CHAINS,
  cores = CORES,
  seed = SEED
)
```

```
plot_nonlinear (../reference/stan_gamm4.html)(post)
```



Here we see that the relationship between past and present roaches is estimated to be nonlinear. For a small number of past roaches, the function is steep and then it appears to flatten out, although we become highly uncertain about the function in the rare cases where the number of past roaches is large.

Relationship to `nlmer`

The `stan_gamm4` function allows designated predictors to have a nonlinear effect on what would otherwise be called the "linear" predictor in Generalized Linear Models. The `stan_nlmer` function is similar to the `nlmer` function in the **lme4** package, and essentially allows a wider range of nonlinear functions that relate the linear predictor to the conditional expectation of a Gaussian outcome.

To estimate an example model with the `nlmer` function in the **lme4** package, we start by rescaling the outcome and main predictor(s) by a constant

```
data("Orange", package = "datasets")
Orange$age <- Orange$age / 100
Orange$circumference <- Orange$circumference / 100
```

Although doing so has no substantive effect on the inferences obtained, it is numerically much easier for Stan and for **lme4** to work with variables whose units are such that the estimated parameters tend to be single-digit numbers that are not too close to zero. The `nlmer` function requires that the user pass starting values to the ironically-named self-starting non-linear function:

```
startvec <- c(Asym = 2, xmid = 7.25, scal = 3.5)
library(lme4)
nm1 <- nlmer (http://www.rdocumentation.org/packages/lme4/topics/nlmer)(circumference ~ SSlogis(age
             data = Orange, start = startvec)
summary(nm1)
```

```
Warning in vcov.merMod(object, use.hessian = use.hessian): variance-covariance matrix computed from
not positive definite or contains NA values: falling back to var-cov estimated from RX
```

```
Warning in vcov.merMod(object, correlation = correlation, sigm = sig): variance-covariance matrix c
not positive definite or contains NA values: falling back to var-cov estimated from RX
```

```
Nonlinear mixed model fit by maximum likelihood  ['nlmerMod']
Formula: circumference ~ SSlogis(age, Asym, xmid, scal) ~ Asym | Tree
   Data: Orange

     AIC      BIC   logLik deviance df.resid
   -49.2    -41.4     29.6    -59.2       30

Scaled residuals:
    Min      1Q  Median      3Q     Max
-1.9170 -0.5421  0.1754  0.7116  1.6820

Random effects:
 Groups   Name Variance Std.Dev.
 Tree     Asym 0.100149 0.31646
 Residual      0.006151 0.07843
Number of obs: 35, groups:  Tree, 5

Fixed effects:
     Estimate Std. Error t value
Asym   1.9205     0.1558   12.32
xmid   7.2791     0.3444   21.14
scal   3.4807     0.2631   13.23

Correlation of Fixed Effects:
     Asym  xmid
xmid 0.384
scal 0.362 0.762
```

Note the warning messages indicating difficulty estimating the variance-covariance matrix. Although **lme4** has a fallback mechanism, the need to utilize it suggests that the sample is too small to sustain the asymptotic assumptions underlying the maximum likelihood estimator.

In the above example, we use the `SSlogis` function, which is a lot like the logistic CDF, but with an additional `Asym` argument that need not be one and indicates what value the function approaches for large values of the first argument. In this case, we can interpret the asymptote as the maximum possible circumference for an orange. However, this asymptote is allowed to vary from tree to tree using the `Asym | Tree` syntax, which reflects an assumption that the asymptote for a randomly-selected tree deviates from the asymptote for the population of orange trees in a Gaussian fashion with mean zero and an unknown standard deviation.

The `nlmer` function supports user-defined non-linear functions, whereas the `stan_nlmer` function only supports the pre-defined non-linear functions starting with `SS` in the **stats** package, which are

```
 [1] "SSasymp"     "SSasympOff"  "SSasympOrig" "SSbiexp"     "SSfol"
 [6] "SSfpl"       "SSgompertz"  "SSlogis"     "SSmicmen"    "SSweibull"
```

To fit essentially the same model using Stan's implementation of MCMC, we add a `stan_` prefix

```
post1 <- stan_nlmer (../reference/stan_nlmer.html)(circumference ~ SSlogis(age, Asym, xmid, scal) ~
                    data = Orange, chains = CHAINS, cores = CORES, seed = SEED,
                    init_r = 0.5)
```

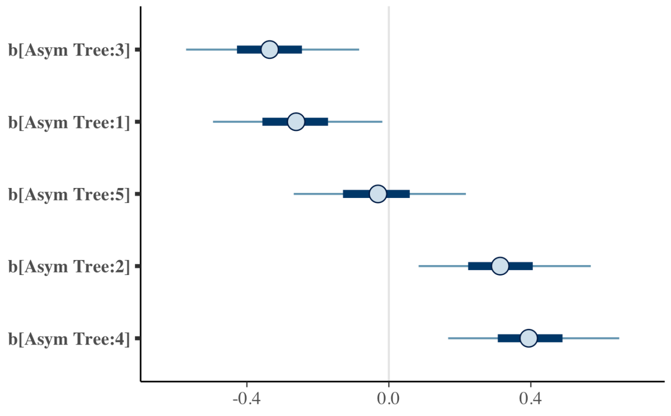
```
post1
```

```
stan_nlmer
 family:       gaussian [inv_SSlogis]
 formula:      circumference ~ SSlogis(age, Asym, xmid, scal) ~ Asym | Tree
 observations: 35
------
      Median MAD_SD
Asym  1.8    0.1   
xmid  6.8    0.3   
scal  3.2    0.3   
sigma 0.1    0.0   

Error terms:
 Groups   Name Std.Dev.
 Tree     Asym 0.314   
 Residual      0.091   
Num. levels: Tree 5 

Sample avg. posterior predictive distribution of y:
         Median MAD_SD
mean_PPD 1.2    0.0   

------
For info on the priors used see help('prior_summary.stanreg').
```

In `stan_nlmer`, it is not necessary to supply starting values; however, in this case it was necessary to specify the `init_r` argument so that the ranomly-chosen starting values were not more than 0.5 away from zero (in the unconstrained parameter space). The default value of 2.0 produced suboptimal results.

As can be seen, the posterior medians and estimated standard deviations in the MCMC case are quite similar to the maximum likelihood estimates and estimated standard errors. However, `stan_nlmer` produces uncertainty estimates for the tree-specific deviations in the asymptote, which are considerable.

```
plot(post1, regex_pars = "^[b]")
```

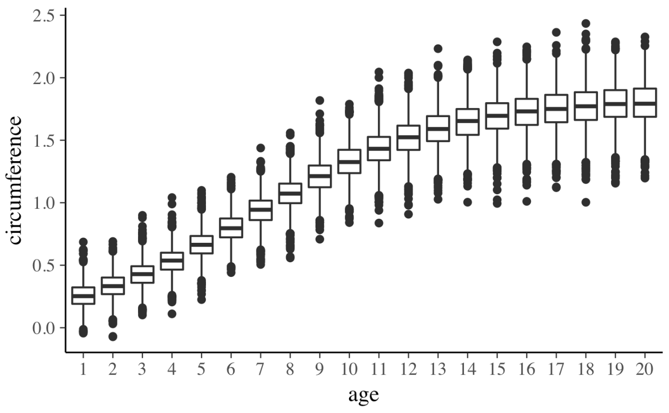


As can be seen, the age of the tree has a non-linear effect on the predicted circumference of the tree (here for a out-of-sample tree):

```
nd <- data.frame(age = 1:20, Tree = factor("6", levels = 1:6))
PPD <- posterior_predict (../reference/posterior_predict.stanreg.html)(post1, newdata = nd)
PPD_df <- data.frame(age = as.factor(rep(1:20, each = nrow(PPD))),
                     circumference = c(PPD))
ggplot(PPD_df, aes(age, circumference)) + geom_boxplot()
```

Developed by Jonah Gabry,

Site built with pkgdown (http://pkgdown.r-lib



If we were pharmacological, we could evaluate drug concentration using a first-order compartment model, such as

```
post3 <- stan_nlmer (../reference/stan_nlmer.html)(conc ~ SSfol(Dose, Time, lKe, lKa, lCl) ~
                    (0 + lKe + lKa + lCl | Subject), data = Theoph,
                    chains = CHAINS, cores = CORES, seed = SEED,
                    QR = TRUE, init_r = 0.25, adapt_delta = 0.999)
pairs(post3, regex_pars = "^l")
pairs(post3, regex_pars = "igma")
```

However, in this case the posterior distribution is bimodal Thus, you should always be running many chains when using Stan, especially `stan_nlmer`.

Conclusion

There are model fitting functions in the **rstanarm** package that can do essentially all of what can be done in the **lme4** and **gamm4** packages — in the sense that they can fit models with multilevel structure and / or nonlinear relationships — and propagate the uncertainty in the parameter estimates to the predictions and other functions of interest. The documentation of **lme4** and **gamm4** has various warnings that acknowledge that the estimated standard errors, confidence intervals, etc. are not entirely correct, even from a frequentist perspective.

A frequentist point estimate would also completely miss the second mode in the last example with `stan_nlmer`. Thus, there is considerable reason to prefer the **rstanarm** variants of these functions for regression modeling. The only disadvantage is the execution time required to produce an answer that properly captures the uncertainty in the estimates of complicated models such as these.