Abstract

The blmer package for R computes maximum a posteriori estimates for the covariance parameters in multilevel linear models, using weakly informative priors that guarantee a positive definite result. Additionally, fully Bayesian inference is possible through the specification of priors over additional parameters, a posterior sampler, and cross validation. It builds off of, and is cross-compatible with the popular multilevel/mixed effects regression R package lme4. blmer supports a variety of prior distributions and covariance decompositions, and incorporates an expressive syntax that is designed to be familiar to users of regression functions in R

1 Introduction

In multilevel models, maximum likelihood estimates of the covariance matrices for the modeled coefficients (also known as "random effects") can be at the boundary of the parameter space. Estimation in this case is problematic as the likelihood surface can be flat, slowing optimization and providing innaccurate estimates of standard errors. For a discussion of the the problems associated with degenerate covariance estimates in multilevel models, see (TODO: reference our other paper?).

As a solution, the **blmer** package for R [R Development Core Team, 2010] imposes prior distributions over the relevant covariance matrices such that there is zero probability mass associated with the boundary. Excepting this behavior, the prior distributions have been chosen to be otherwise vague and come with default settings that should be suitable in most applications. With these priors, **blmer** is able to gently shift estimates that are at the boundary away from 0 while leaving other parameters roughly unaffected. Furthermore, **blmer** permits the user to specify prior distributions over the remaining model parameters, obtain samples from the posterior, and estimate the prediction error for new samples using cross validation. Combined, these tools provide a fully Bayesian approach to multilevel linear models.

As there already exists for R a popular and efficient means of fitting multi-level models using maximum likelihood, one of our key computational goals was to be cross-compatible with, and to build off of the **lme4** package [Bates and Maechler, 2010]. Users of **lme4** will find in **blmer** a near-identical user interface and results contained in S4 objects that inherit from that package's mer object model.

Finally, we have attempted to create a prior specification language that mirrors the simplicity and expressiveness of R's model description syntax to setup the prior's structure, while combining the usefulness of named lists to set hyperparameters.

2 Multilevel linear models

While multilevel models have been well explicated elsewhere (TODO: references), we will briefly go over the model specification so that we can mathematically highlight how **blmer** differs from its predecessors. While what follows is for a linear model, generalized linear models are essentially similar in parameterization, except that they may lack an observation-level variance component.

Multilevel models apply to situations in which observational units can be naturally grouped together. There may be different grouping "factors" that apply. For example, a poll respondant might be grouped with other individuals by his or her race and/or state. Suppose that there are K such grouping factors, and that the number of potential groups at level k is denoted as J_k . Each observational unit then has K memberships, and we choose to denote which one of the J_k groups the ith observation belongs at the kth level by writing: $[i]_k$.

Now assume that we have $y_i, i = 1, ..., N$ observations and each is associated with a vector of predictors, x_i^{\top} . Furthermore, for each of the k = 1, ..., K factors and for each of the $j = 1, ..., J_k$ groups in that factor, we have another vector of predictors, z_{jk}^{\top} . A multilevel linear model would then be given by:

$$y_i \mid \theta \stackrel{\text{ind}}{\sim} N\left(x_i^{\top} \beta + \sum_{k=1}^K z_{[i]_k k}^{\top} \theta_{[i]_k k}, \sigma^2\right), i = 1, \dots, N,$$

$$\theta_{jk} \mid \Sigma_k \stackrel{\text{iid}}{\sim} N\left(0, \Sigma_k\right), j = 1, \dots, J_k, k = 1, \dots, K.$$

Our principle concern is with imposing priors $p(\Sigma_k)$ such that $\lim_{|\Sigma_k|\to 0} p(\Sigma_k) = 0$. We also otherwise generalize the above by imposing priors $p(\beta)$ and $p(\sigma^2)$.

As **lme4** maximizes the likelihood using numerical optimization on the covariance matrices of the latent variables, obtaining a posterior mode requires nothing more than "penalizing" that likelihood calculation by the contribution of the prior.

Priors and β and σ^2 have also been implemented. Conjugate families for these parameters are incorporated as pseudo-data, while non-conjugate families require expanding the parameter space used in optimization.

2.1 Covariance decompositions

In addition to imposing a prior directly on the covariance matrices of the model, we have also implemented two covariance decompositions which give the use more fine-grained control. The "correlation" decomposition attempts to treat the covariance matrix as a set of standard deviations and correlations, while the "spectral" decomposition breaks the matrix into its eigenvectors and eigenvalues.

The correlation decomposition is given by: $\Sigma = SRS$, for S a diagonal matrix of strictly positive elements and R a correlation matrix. As optimizing over a correlation matrix is a highly constrained problem, we instead let R be

any positive definite matrix. Consequently, the correlation decomposition corresponds to a redundant, multiplicative parameterization. (TODO: redundant, multiplicative parameterization are good + citation).

Alternatively, the spectral decomposition can be written as $\Sigma = Q\Lambda Q^{\top}$, where Q is an orthogonal matrix comprising the eigenvectors of Σ , and Λ is a diagonal matrix of eigenvalues.

Chosing one of the above decompositions alters the posterior mode returned by **blmer** to that of the decomposition itself. In the first case, this is necessary as the imposed prior involves an integral which may or may not be tractible. In the second, imposing priors on eigenvalues independently induces a prior on the original scale that has infinite mass in the limit as eigenvalues approach each other, which in turn complicates optimization. (TODO: reference as to why this is OK/good?)

3 Fitting models

blmer was designed to familiar to users of lme4. A blmer S4 object extends the mer class, and consequently inherits all of the same functionality. Fitting a model in blmer is achieved by modifying a call to the lmer() or glmer() function with the addition of several new arguments.

3.1 Calling blmer()

The prototype for the blmer() and bglmer() functions are given below:

```
blmer(formula, data, family = NULL, REML = TRUE, control = list(),
    start = NULL, verbose = FALSE, doFit = TRUE, subset, weights,
    na.action, offset, contrasts = NULL, model = TRUE, x = TRUE,
    cov.prior = NULL, fixef.prior = NULL, var.prior = NULL)

bglmer(formula, data, family = gaussian, start = NULL, verbose = FALSE,
    nAGQ = 1, doFit = TRUE, subset, weights, na.action, offset,
    contrasts = NULL, model = TRUE, control = list(),
    cov.prior = NULL, fixef.prior = NULL)
```

Note that except for the last lines, these are identical to the prototypes for lmer() and glmer(), as of version 0.999375-37 of the lme4 package.

The formats for the new arguments are all character strings (TODO: figure out if character strings are necessary) of a syntax that will be described below, but as an overview, the new arguments are:

- cov.prior: a prior on the covariance matrices of the modeled coefficients. The covariance matrices are denoted as Σ in the above formulation. Applies to both blmer() and bglmer().
- fixef.prior: a prior on the unmodeled regression coefficients, or fixed effects (β) . Also applies to both functions, but cannot be used in a call to blmer() if the REML argument is TRUE.

type	restriction	$\begin{array}{c} ext{posterior} \\ ext{mode} \end{array}$	families	options & defaults
none	none	Σ	$p(\Sigma) \propto 1$	none
direct	$\dim \Sigma = 1$	$\frac{\Sigma_{[11]} \text{ or}}{\sqrt{\Sigma_{[11]}}}$	gamma,	<pre>shape = 2, rate = 1 / sd(y), posterior.scale = 'sd'</pre>
			inverse.gamma	<pre>shape = 1 / 2, scale = 3 * sd(y) / 2, posterior.scale = 'sd'</pre>
direct	$\dim \Sigma > 1$	Σ	wishart,	<pre>df = dim(sigma) + 3, scale = diag(sd(y) / 2, dim(sigma))</pre>
			inverse.wishart	<pre>df = dim(sigma) - 1 / 2, inverse.scale = diag(3 * sd(y), dim(sigma))</pre>
correlation	none	S, R or	$S_{[jj]}\sim { t gamma},$	same as gamma above
		$S^{1/2}, R$	$S_{[jj]} \sim \text{inverse.gamma}$	same as inverse.gamma above
		where $\Sigma = SRS$,	$R \sim exttt{wishart} \ R \sim exttt{inverse.wishart}$	same as wishart above same as inverse.wishart above
		S = SRS, $S diagonal,$	Te vo inverse. wishaic	default families: $S_{[jj]} \stackrel{iid}{\sim} \text{gamma}, R \sim \text{wishart}$
		R pos. def.		default failiffes. $S[jj] = gamma, Ti = wishart$
spectral	none	Q, Λ or	$\Lambda_{[jj]} \sim exttt{gamma}$	same as above, but posterior.scale = 'var'
		$Q, \Lambda^{1/2}$ where	$\Lambda_{[jj]} \sim ext{inverse.gamma} \ p(Q) \propto 1$	<pre>same as above, but posterior.scale = 'var' none</pre>
		$\Sigma = Q\Lambda Q^{\top},$ Q orthogonal, Λ diagonal		default families: $\Lambda_{[jj]} \stackrel{iid}{\sim} gamma$

Table 1: Types, families, and options for priors on covariance components corresponding to the unobserved variables. The defaults correspond to fitting a standard, multilevel linear model. In the case of a generalized linear model, any reference to the standard deviation of the observations is replaced by 1. (TODO: seems reasonable for logistic. What about other glms?)

• var.prior: prior on the observation level variance component, σ^2 . Only applies to calls to blmer() as generalized linear models do not have this parameter (TODO: overdispersion?).

As priors require parameters of their own, we have adopted the namedelement list format used by R, mimicking the syntax for function calls.

3.2 Covariance prior

The principal difficulty in specifying a prior on Σ is that there are separately estimated covariance matrices for each of the K grouping factors. To afford the user more flexibility, priors can be specified as a default that will apply to all grouping factors or applied directly by the level name. To specify a prior that applies to a specific, named grouping factor, one passes to blmer() a character string of the format:

factor.name ~ prior.type(options.list)

Conversely, to specify a default prior that should apply to all grouping factors, the correct format is simply: prior.type(options.list).

The different prior types, options, and defaults are enumerated in Table 1. Direct prior types are specified by naming the prior family, while the correlation and spectral decompositions must be named explicitly. A list of examples covering the majority of use cases is presented below.

Specifying a direct, multivariate prior type with the default parameterization enables that prior to apply to the univariate case as well. Consequently, the Wishart can be used to specify a Gamma distribution and the Inverse-Wishart the Inverse-Gamma, although this forces the posterior mode to be calculated on the variance scale.

blmer permits fine tuning of the prior specification via a list of options placed in parentheses subsequent to naming the prior type. For a direct prior, the options should consist of prior parameters, such as the shape or scale of the distribution. For decompositions, the options should specify the names of the families to be applied to the individual components. These distributional families can be further controlled in the same fashion as a directly-applied prior.

3.3 Covariance examples

For the purposes of illustrating the means by which a covariance prior is specified in **blmer**, suppose that we have data consisting of a single predictor and two grouping factors. The outcomes are stored in y, the predictor in x, and the grouping factors are g.1 and g.2. Further suppose that it makes sense to model a different intercept for each of the different groups in the first factor, while we expect the intercept and the slope to vary in the second.

Likelihood fit

To fit a model in lme4, one might call:

```
lmer(y ~1 + x + (1 | g.1) + (1 + x | g.2))
```

Both of the following calls to blmer() produce the same estimate:

```
blmer(y ^{\sim} 1 + x + (1 | g.1) + (1 + x | g.2))
blmer(y ^{\sim} 1 + x + (1 | g.1) + (1 + x | g.2), cov.prior = ''none'')
```

Direct, univariate, default prior, standard deviation scale

The following places a univariate prior on the standard deviation of the contributions to the intercept for group 1:

```
blmer(y ^{\sim} 1 + x + (1 | g.1) + (1 + x | g.2), cov.prior = ''gamma'')
```

If the model consisted of any other grouping factors with only one input varying at that level, the prior would also apply.

Direct, multivariate, default prior, variance scale

If we install a Wishart prior as a default, it will downgrade to a gamma for the univariate case and consequently apply to the variances for groups 1 and 2.

```
blmer(y ~1 + x + (1 | g.1) + (1 + x | g.2), cov.prior = ''wishart'')
```

Direct, named grouping factors

We can mix the above by naming the grouping factors. We also change the prior on the first group so that this differs from the previous example.

```
blmer(y ~ 1 + x + (1 | g.1) + (1 + x | g.2),

cov.prior = ''g.1 ~ inverse.gamma, g.2 ~ wishart'')
```

Direct, default priors with options

For univariate families, it is easy to specify options for the default that will apply in more than one case. Just as in function calls, the naming is not essential, provided that the order matches the prototype. Consequently, the second call below is equivalent to the first.

This is complicated in the multivariate case, as the parameters will usually depend on the dimension of the covariance matrix. To apply the prior to all of the grouping factors with a multivariate prior and a parameterization that is not the default, each grouping factor should be named separately.

Decompositions, default options

Instead of naming a family directly, it is possible to specify a decomposition. The following installs a correlation or spectral decomposition as the default and applies it to all grouping factors.

```
blmer(y \tilde{\ }1 + x + (1 | g.1) + (1 + x | g.2), cov.prior = ''correlation'')
blmer(y \tilde{\ }1 + x + (1 | g.1) + (1 + x | g.2), cov.prior = ''spectral'')
```

Just as above, we can pick and choose which grouping factors receive which prior type:

Correlation options

We can modify the families used by both decompositions. The correlation prior requires both a univariate and matrix family, the first being applied independently to each component of the scale matrix and the second being applied to the center matrix.

Spectral options

Once again, it is possible to modify the options to a univariate prior and have it easily apply over all grouping factors. We illustrate by setting the prior family applied to the square roots of the eigenvalues in the spectral decomposition.

Coordinate priors

It is possible to apply different univariate priors to each component in the independent portions of the decompositions. The correlation prior enjoys the feature that the coordinates can be specified by name. Conversely, in a spectral decomposition permutations are possible so that one cannot guarantee that an eigenvalue goes with a specific input of the data. Consequently, to apply different univariate priors to the different coordinates in a spectral decomposition, specify the distributions by number.

Expressions as parameters

Finally, the expression to specify a parameter is evaluated in the environment that calls blmer(). It is thus possible to pass in variables or entire computations.

3.4 Fixed effect prior

TODO: implement this.

In order to move in a more fully Bayesian direction, it is also possible to impose a prior over the "fixed effects", β . To do so, a character string of the following format is passed to blmer() as the fixef.prior argument:

family	options & defaults		
none	none		
normal	<pre>mean = rep(0, dim(beta)),</pre>		
	<pre>var = diag(dim(beta))</pre>		
mvt	<pre>delta = rep(0, dim(beta)),</pre>		
	df = dim(beta) + 1,		
	sigma = diag(dim(beta))		
cauchy	<pre>location = rep(0, dim(beta)),</pre>		
•	<pre>scale = diag(dim(beta))</pre>		

Table 2: Families and options for priors on the "fixed effect" components of the model, β . TODO: what priors make sense? Took parameterization of multivariate-t from pmvt, which is in **mvtnorm**.

```
family.name(options.list)
```

The possible families and allowed options are listed in Table 2. It is not currently possible to apply different families to the different components of β .

3.5 Fixed effects examples

We reuse the model from the examples of the application of covariance priors above.

Maximum likelihood fit

Once again, by specifying none as the prior, it is possible to recover the maximum likelihood fit.

Normal prior, default options

The following imposes a simple, independent Gaussian prior over the fixed effects with zero mean and unit variance:

Alternative families with options

Using the options list construct, it is possible to set different parameters for the prior.

```
blmer(y ^{\sim} 1 + x + (1 | g.1) + (1 + x | g.2), REML = FALSE, fixef.prior = ''cauchy(location = c(5, 10))'')
```

family	options & defaults
none	none
gamma	shape = 0,
	rate = 0,
	<pre>posterior.scale = 'sd'</pre>
inverse.gamma	shape = 0,
	scale = 0,
	<pre>posterior.scale = 'sd'</pre>

Table 3: Families and options for priors on the observation-level variance component, σ^2 .

Note that, as above, expressions passed in are evaluated in the calling environment.

3.6 Observation variance prior

When the model to be fit is strictly linear, not generalized, it is possible to include a prior over the observation-level variance, σ^2 . The format follows that of a prior on the fixed effects, with the specification of a family name followed by an optional list of parameters. See table 3 for reference.

With variances and posterior inference, the question of the scale of the parameter arises. We opt to default to report the posterior mode of the standard deviation.

Finally, improper priors are also possible. Indeed, we default to the prior $p(\sigma) \propto \sigma^{-1}$, which is achieved by the limit of a gamma or inverse gamma as the parameters approach zero. These settings are detected by **blmer** and the proper functional form is applied.

4 Full Bayesian inference

Once a model has been fit in **blmer**, it is possible to obtain a set of simulations from the posterior by calling the sim() function. The prototype for sim() is:

```
sim(object, n.sims = 1000)
```

where object is a blmer S4 object obtained from blmer() or bglmer().

4.1 sim() results

The result from sim() is a named list of arrays corresponding to the parameters of the model to which priors have been applied, as well as the modeled coefficients. The list comprises:

• ranef: an array of dimensions: n.sims × the number of grouping factors × the number of modeled coefficients at each grouping factor, containing

samples of the modeled coefficients, θ . These are included in every set of simulations, as opposed to the other parameters which are only present if a prior is specified.

- fixef:n.sims \times number of unmodeled coefficients. These correspond to β .
- ranef.cov: n.sims × number of grouping factors × dimensions of covariance matrix of modeled coefficients at each grouping factor. In the above formulation, these are the different components of Σ . Posterior may be on a transformed scale if a decomposition is used.
- obs.var: n.sims $\times 1$. The observation level variance in a linear model, σ^2 . Posterior scale depends on prior scale, in that it is possible to obtain samples from the posterior of σ .

4.2 Posterior form

As we may be working with a model for which not every parameter has a prior, we need to specify the functional form from which we sample. In general, if the observations are y, the parameters with priors are η , and the unmodeled parameters are λ , we sample proportional to:

$$p(\eta \mid y, \hat{\lambda})$$

where $\hat{\lambda}$ is the maximum likelihood or maximum a posteriori estimate with a flat prior. For a model which is not fully "Bayesian", this represents an estimate of the posterior distribution.

5 Illustrative example

(COMMENT: the example should just show-case the use of the software package, but as we claim that the fit is close to lmer, I've included a few points of comparison)

In order to demonstrate the use of **blmer**, we downloaded data collected from a sequence of speed dating sessions conducted by Columbia University students between 2002 and 2004, available at: http://stat.columbia.edu/~gelman/arm/speed.dating/ (TODO: someone should get credit here, I assume). In each session, every male subject spends a brief amount of time with every female participant. At the end of each interview, both parties complete a score card based on his or her experience, ranking the potential partner on several axes and deciding whether or not to seek further communication. At the end, mutual matches were given each other's contact information.

We can use logistic regression to predict the probability that a respondant is interested in someone else based on his or her rankings of that potential partner. As each individual places different priorities on different attributes, in some sense we would like to make a distinct regression for everyone involved. However, as each person makes only a few decisions - no more than 22 in the most well-attended session, and 5 in the least - attempting to fit separate models leads to several cases of perfect separation. This motivates a multilevel model, grouping decisions based on the identification number of the decision maker.

Code to download and clean the data is presented in the supplementary materials. We have chosen to consider only those speed dating sessions that are specified as having similar experimental design. Doing so yields 5322 dating decisions made by 348 individuals.

5.1 Fitting the models

First, we specify the model and fit it in **lmer** as a point of comparison. As this is a generalized model, we fit it using the <code>glmer()</code> function. (TODO: explanation about model? Doesn't really matter, since it's just illustrative, but might be worth it. Model w/o sex as an interaction blows up as well, and would be simpler on the page)

The algorithm terminates in 122 iterations, and a quick check reveals that the derminant of the fitted covariance matrix is less than 2×10^{-22} . Taking a spectral decomposition of that matrix shows that, although there are 7 dimensions, the matrix is effectively of rank 5 with the smallest two eigenvalues being quite close to zero ($\leq 10^{-10}$).

Conversely, we calculate the posterior mode using the bglmer() while taking a spectral decomposition of the covariance matrix for the modeled coefficients. This is accomplished by running the code:

(COMMENT: if I run this with the spectral decomposition on the square roots of the eigenvalues, the fit is almost too close. I should probably rerun it with that, but I'll have to cut the contour plot because it becomes pretty boring).

The fit takes 135 iterations, the determinant of the new covariance matrix is 0.015, and the smallest two eigenvalues are 0.152 and 0.113 - showing some pull away from the boundary of the space.

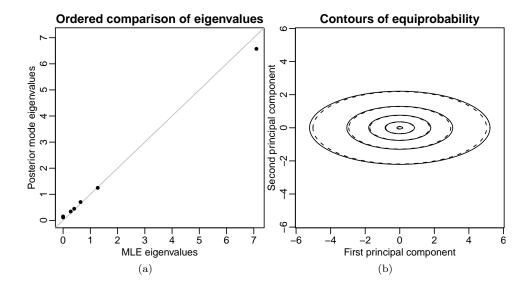


Figure 1: (a) Comparison of eigenvalues from the maximum likelihood fit and the posterior mode, using a spectral decomposition with $\Lambda_{[jj]} \sim \Gamma(2,1)$. (b) Comparison of contours of equiprobability, viewing the first two components of the estimated posterior mode in the first two principal components from the maximum likelihood estimate. Lines correspond to 0.05, 0.25, 0.5, 0.75, and 0.95 probability of new observations have more extreme distances from the origin.

(TODO: Some printout of the models, or perhaps a table? There is a neat story here with the results, in that attractiveness and shared interests are far and away the best predictors, and that women are far more choosy than men. But none of that is really relevant).

5.2 Comparison of results

In order to assess in a technical sense the distance between the two fits, Figure 1a visually shows the ordered eigenvalues. The eigenvalues demonstrate slight shrinkage towards the prior mode, which in this case is 1. Under the null hypothesis that the basic model is correct, the difference in deviances is 2.90. (TODO: I'm not sure how many degrees of freedom to use for this comparison, or really if it is even chi-squared).

Figure 1b shows a comparison of contours of equiprobability. The posterior mode fit, when viewed in the first two principal components of the maximum likelihood estimate, predicts a similar pattern of variation to that of the MLE.

However close the two fitted covariance matrices appear, more telling are the associated predictions for each model. Taking the empirical Bayes estimate of the modeled coefficients permits one to estimate the expected value for each

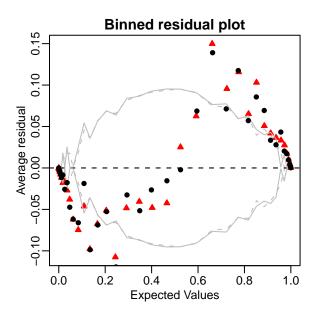


Figure 2: Binned residual plots for maximum likelihood and posterior mode estimates. The black dots and solid gray lines correspond to the binned residuals and approximate 95% confidence intervals for the MLE, while the red triangles and dashed lines are the same, respectively, for the posterior mode.

TODO: I think this plot should be redone, identifying which observation ends up in which bin and making sure that they stay consistent between the models. I suspect that the majority of the difference in the plots arises from observations jumping bin boundaries.

observation. From these, the Bayes estimator of any actual dating decision is y=1 if the expected value is greater than 0.5, 0 otherwise. Comparing these predictions, the models agree for all but 25 out of 4427 data points, or 99.4% of the time. Figure 2 overlays binned residual plots from both models, showing similar trends.

TODO: cross validation

5.3 Full Bayesian inference

TODO: section

6 Availability

- 6.1 Installing the package
- 6.2 Obtaining the source code
- 6.3 License

As blmer inherits code from lme4, it is available under the GNU General Public License, versions 2.0 and greater. For a copy of the license, visit http://www.gnu.org/licenses/gpl.html.

References

Douglas Bates and Martin Maechler. lme4: Linear Mixed-Effects Models Using S4 Classes, 2010. URL http://CRAN.R-project.org/package=lme4. R package version 0.999375-37.

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