

On mode jumping in MCMC for Bayesian variable selection within GLMM

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- GLMM are addressed for inference and prediction in a wide range of different applications providing a powerful scientific tool for the researchers and analysts from different fields
- More and more sources of data are becoming available introducing a variety of hypothetical explanatory variables for these models to be considered
- Selection of an optimal combination of these variables is crucial. Posterior model probabilities is one of the relevant measures to estimate quality of the models and perform proper Bayesian model averaging
- The number of models to select from is exponential in the number of candidate variables
- The search space has numerous sparsely located local extrema
- Hence efficient search algorithms have to be adopted for evaluating the posterior distribution within a reasonable amount of time

Bayesian vs. Frequentist statistics

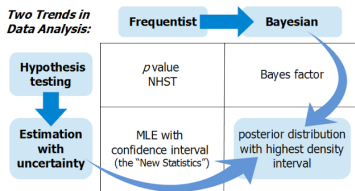
Frequentist: obtain $\hat{\theta}$ with CI by MLE, MM, MD etc.

vs.

Bayesian: obtain $p(\theta|\mathbb{D}) = \frac{p(\mathbb{D}|\theta)p(\theta)}{p(\mathbb{D})} = \frac{p(\mathbb{D}|\theta)p(\theta)}{\int_{\Omega_{\theta'}} p(\mathbb{D}|\theta')p(\theta')d\theta'}$

Frequentist vs. Bayesian

Two Trends in Data Analysis:



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Jerzy Neyman



Harold Jeffreys

Frequentist	Bayesian
Probability is a long-run average	Probability is a degree of belief
There is a true Model, the Data is a random realization	The Data is true/fixed, Models have probabilities
Probability of the data given a hypothesis (Likelihood)	Probability of a hypothesis given the data
Each repeated experiment/observation starts from ignorance	Can incorporate prior knowledge: probabilities can be updated

Figure: Paradigms shifts (left, adopted from John K. Kruschke, doingbayesiandataanalysis.blogspot.no) and differences between the paradigms (right, adopted from Andres Lopez-Sepulcre, www.slideshare.net/andreslopezsepulcre)

Bayesian Generalized Linear Mixed Model

$$Y_t | \mu_t \sim f(y | \mu_t), t \in \{1, \dots, T\} \quad (1)$$

$$\mu_t = g^{-1}(\eta_t) \quad (2)$$

$$\eta_t = \gamma_0 \beta_0 + \sum_{i=1}^p \gamma_i \beta_i X_{ti} + \delta_t \quad (3)$$

$$\boldsymbol{\delta} = (\delta_1, \dots, \delta_T) \sim N_T(\mathbf{0}, \boldsymbol{\Sigma}_b). \quad (4)$$

- $\beta_i \in \mathbb{R}, i \in \{0, \dots, p\}$ are regression coefficients
- $\boldsymbol{\Sigma}_b = \boldsymbol{\Sigma}_b(\boldsymbol{\psi}) \in \mathbb{R}^T \times \mathbb{R}^T$ is the covariance of the random effect δ_t
- $g(\cdot)$ is a proper link function
- $\gamma_i \in \{0, 1\}, i \in \{0, \dots, p\}$ are latent indicators defining if covariate X_{ti} is included into the model ($\gamma_i = 1$) or not ($\gamma_i = 0$)

We use a fully Bayesian approach, hence specify priors

$$\gamma_i \sim \text{Binom}(1, q) \quad (5)$$

$$q \sim \text{Beta}(\alpha_q, \beta_q) \quad (6)$$

$$\beta|\gamma \sim N_u(\mu_\beta, \Sigma_\beta), u = \sum_{i=1}^p \gamma_i \quad (7)$$

$$\psi \sim \varphi(\psi). \quad (8)$$

- q is the prior probability of including a covariate into the model
- α_q, β_q are hyper parameters for the prior on q
- μ_β, Σ_β are hyper parameters for the prior on $\beta|\gamma$
- ψ are the hyper parameters of the random effect

Inference on the model

Let:

$\theta = \{\beta, \Sigma_b\}$ define parameters of the model and $\gamma : \vec{\gamma}$ define a model itself, i.e. which covariates are addressed.

Then:

- $\theta|\gamma$ define parameters conditioned on fixed models
- $\exists 2^{p+1}$ different models

Goals:

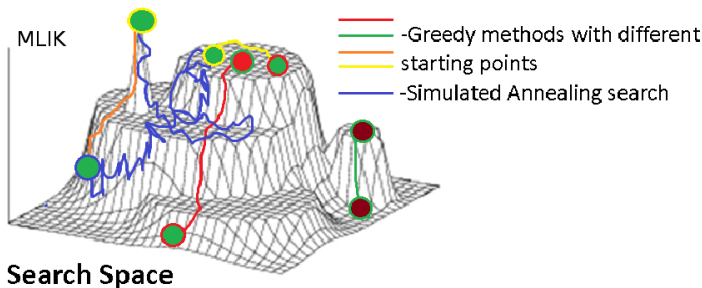
- $p(\gamma, \theta|\mathbb{D})$ posterior distribution of parameters and models
- $p(\gamma|\mathbb{D})$ marginal posterior probabilities of the models
- $p(\mathcal{G}|\mathbb{D})$ marginal posterior probabilities of the quantiles of interest \mathcal{G}

- **Notice that** $p(\gamma, \theta | \mathbb{D}) = p(\theta | \gamma, \mathbb{D}) p(\gamma | \mathbb{D})$
- $p(\theta | \gamma, \mathbb{D})$ and $\log p(\mathbb{D} | \gamma)$ can be efficiently obtained by INLA
- **Notice that** $p(\gamma | \mathbb{D}) = \frac{e^{\log p(\mathbb{D} | \gamma) + \log p(\gamma)}}{\sum_{\gamma' \in \Omega_\gamma} e^{\log p(\mathbb{D} | \gamma') + \log p(\gamma')}}$
- $\widehat{p}(\gamma | \mathbb{D}) = \frac{e^{\log p(\mathbb{D} | \gamma) + \log p(\gamma)}}{\sum_{\gamma' \in \mathbb{V}} e^{\log p(\mathbb{D} | \gamma') + \log p(\gamma')}}$
- \mathbb{V} is the **subspace** of Ω_γ to be **efficiently explored**
- **Notice that** for $p(\gamma) = p(\gamma') \forall \gamma, \gamma' \in \Omega_\gamma$:
- $p(\gamma | \mathbb{D}) \gg p(\gamma' | \mathbb{D})$ if $\log p(\mathbb{D} | \gamma) > \log p(\mathbb{D} | \gamma')$ often \implies
- **Near modal values in terms of log MLIK are particularly important** for construction of reasonable $\mathbb{V} \subset \Omega_\gamma$, **missing them can dramatically influence** posterior in the original space Ω_γ

Possible ways to explore $\mathbb{V} \subset \Omega_\gamma$

Main challenges are multimodality in Ω_γ and its size.

- Full enumeration of Ω_γ - infeasible for large dimensions
- Random walk in Ω_γ including simple MCMC - does not take advantage of the structure of $\Omega_\gamma \implies$ too slow
- Greedy optimization with numerous initial points - end up in local optima
- MCMC with mode jumping proposals seems to be a good idea



MCMC with locally optimized proposals

Tjelmeland and Hegstad [6] suggested continuous mode jumping proposals, **Storvik [5]** considers a more general setup, **we suggest mode jumping proposals** in the **discrete parameter spaces**.

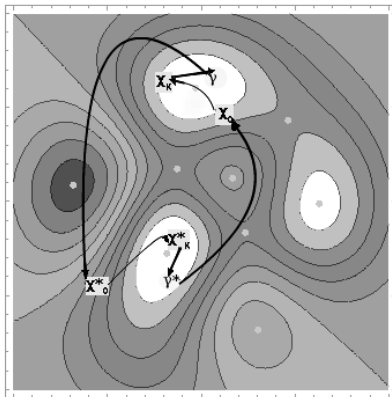


Figure: Locally optimized with randomization proposals

Application of MCMC with mode jumping proposals

We have shown that the detailed balance equation is satisfied for the following acceptance probabilities:

$$r_m(\gamma_j, \gamma_k) = \min \left\{ 1, \frac{p(\mathbb{D}|\gamma_k)p(\gamma_k)q_s(\gamma_j|\gamma_{j_{K-1}})}{p(\mathbb{D}|\gamma_j)p(\gamma_j)q_s(\gamma_k|\gamma_{k_{K-1}})} \right\}. \quad (9)$$

- $q_s(.|.)$ is the kernel of randomization at the end.

Hence we also obtain alternative MCMC estimators of posterior marginal probabilities

$$\tilde{p}(\gamma|\mathbb{D}) = \frac{\sum_{i=1}^W \mathbb{I}(\gamma_i = \gamma)}{W} \xrightarrow[W \rightarrow \infty]{d} p(\gamma|\mathbb{D}). \quad (10)$$

- W is the number of MCMC iterations (after burn-in)

How it looks like in reality

Modes are important: the standard MCMC procedure (right) misses two in this example. Visualization is challenging

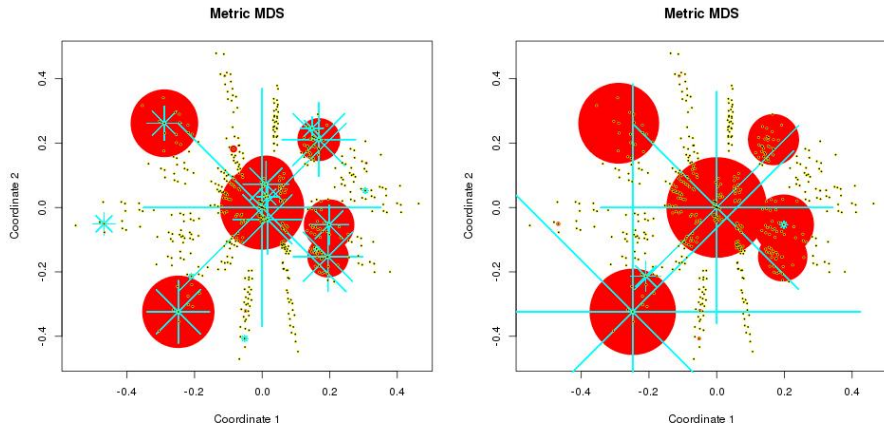


Figure: MDS plots with posterior modes of all found solutions for the approaches

The protein activity data. 2^{88} models. Multiple modes

Linear Bayesian regression with a Gelman's g-prior addressed:

$$y_t = y | m_t \sim N(m_t, \sigma_t) \quad (11)$$

$$m_t = \beta_0 + \sum_{i=1}^p \gamma_i \beta_i X_{t,i} \quad (12)$$

$$\beta | \gamma \sim N_u(\mu_\beta, \Sigma_\beta = g(X_\gamma' X_\gamma)^{-1}), u = \sum_{i=1}^p \gamma_i \quad (13)$$

$$\sigma_t \sim N(0, \sigma_b) \quad (14)$$

$$\gamma_i \sim \text{Binom}(1, q = 0.5). \quad (15)$$

Analytical integration is possible. Marginal likelihoods become:

$$p(\mathbb{D} | \gamma) \propto (1 + g)^{(T-p-1)/2} (1 + g[1 - R_\gamma^2])^{-(T-1)/2}. \quad (16)$$

Here R_γ^2 is the usual coefficient of determination of a linear regression model and g is the hyper-parameter of the g-prior. Notice that we set $g = T$.

The protein activity data. 2^{88} models. Multiple modes

Comparison to other algorithms: BAS, RS (simpler MCMC) on 2^{20} unique models visited for MJMCMC and BAS and 88×2^{20} iterations of RS.

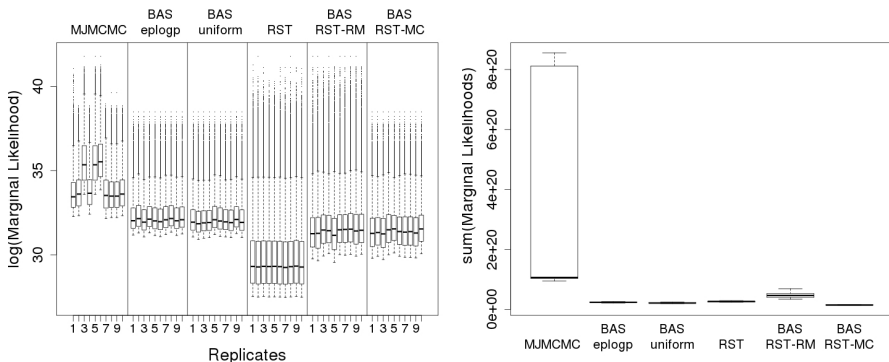


Figure: 100000 best mliks found (left) and posterior masses captured (right). Bayesian linear regression with a g-prior is addressed, since no other packages (to our awareness) manage model selection in GLMM

The protein activity data. 2^{88} models. Multiple modes

Checking convergence. Marginal inclusion probabilities

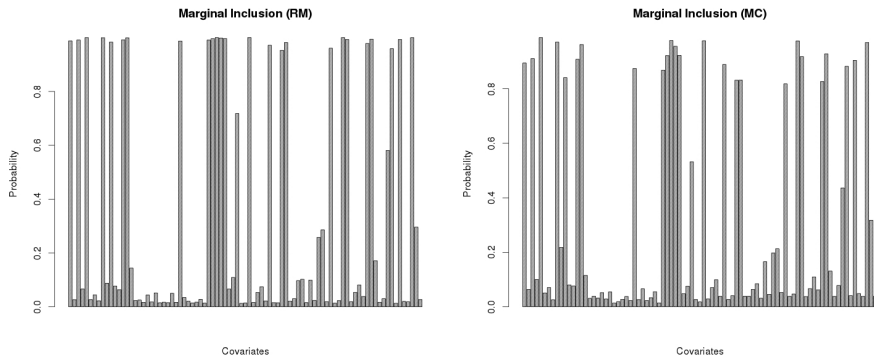


Figure: Comparison of marginal inclusion probabilities obtained by the Bayes formula and MCMC approximations from the best run of MJMCMC with $8.56e + 20$ posterior mass captured

Further (partly current) research

- Automatic creation of additional covariates based on the polynomes and interactions of the original ones as well as sigmoid functions of them (automatic feature extraction), based on an outer genetic algorithm (already implemented)

$I(\text{erf}(I(-(X37)((X54))))))$ added after 2^8 steps*

$I((I(-(X23)((X57))))))$ added after 2^{12} steps*

...

$I(\tanh(I((X73))))$ replaced $I((I((X81)((X68))))))$ after 2^{16} steps*

$I((I((X71)((X69))))))$ replaced $I(\text{erf}(I(((X54))))))$ after 2^{18} steps*

...

- Allowing the search over different choices of the random effect structures (to be addressed)
- Allowing the search over different choices of the response distributions (to be addressed)

Concluding remarks

- We introduced the MJMCMC approach for estimating posterior model probabilities and Bayesian model averaging and selection.
- It incorporates the ideas of MCMC with possibility of large jumps combined with local optimizers to generate proposals in the discrete space of models
- *EMJMCMC* R-package is developed and available from the GitHub repository: <http://aliaksah.github.io/EMJMCMC2016/>
- The developed package gives a user high flexibility in the choice of methods to obtain marginal likelihoods and model selection criteria within GLMM
- Extensive parallel computing for both MCMC moves and local optimizers is available within the developed package
- Based on the obtained in the experimental part results, we can claim MJMCMC to be a rather competitive novel algorithm that both performs well in terms of the search quality and addressed a more general class of statistical models than the competing approaches

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The End.



Thank you.