

Efficient mode jumping MCMC for Bayesian variable selection in GLMM

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Introduction. Issues

- 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
- The number of models to select from is exponential in the number of candidate variables
- The search space in this context has numerous local extrema (potentially sparsely located)
- Hence efficient search algorithms have to be adopted for evaluating the posterior distribution within a reasonable amount of time

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 is the correlation structure between them through random effects
- $g(\cdot)$ 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

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

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

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

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

- 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:

$\theta = \{\vec{\beta}, \rho, \sigma_\epsilon^2\}$ 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:

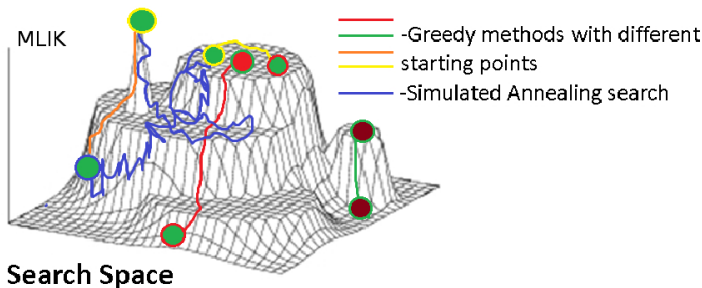
- $p(\gamma, \theta|\mathbb{D})$ posterior distribution of parameters and models
- $p(\gamma|\mathbb{D})$ marginal posterior distribution of the models
- Set of estimated models performing well in terms of some model selection criteria (MAP, WAIC, DIC, MLIK)

- **Note 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
- **Note 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
- Note 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
- Random walk 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**.

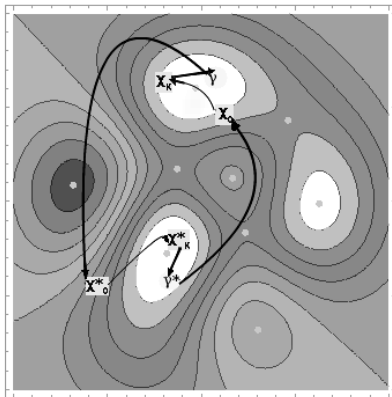


Figure: Locally optimized with randomization proposals

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

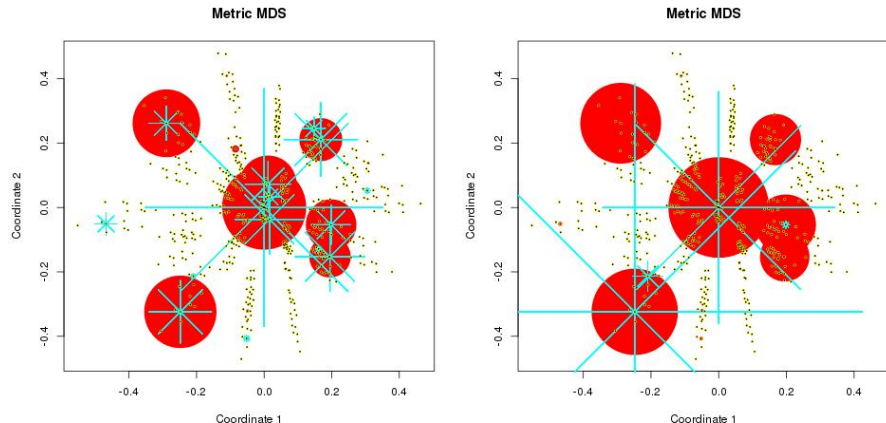


Figure: MDS plots with posterior modes of all found solutions for the approaches

Application to cosmological simulations. Cosmological hydro-simulation data (<http://yt-project.org/data/>).

Observations (Bernoulli classifiers):

- Galaxy is quenched (or not)
- Star hosts planet (or not)

Variables:

- Dark matter mass
- Gas mass
- Stellar mass
- Star formation rate
- Metallicity
- Gas molecular fraction
- Gas fraction
- Stellar fraction
- Stellar to gas mass ratio
- Other covariates, their interactions, polynomes and etc.

Application to NEO classification. NASA Space Challenge (<https://github.com/SpaceApps2016/Resources>).

Observations (Bernoulli classifiers):

- Asteroid is a NEO (PHA) object or not (Phocaea)

Variables:

- Rotation period
- Magnitude slope
- Mean anomaly
- Inclination
- Argument of perihelion
- Longitude of the ascending node
- Rms residual
- Semi major axis
- Eccentricity
- Mean motion
- Absolute magnitude
- Other covariates, their interactions, polynomes and etc.

Application to cosmological simulations or NEO objects classification

Logistic Bayesian regression addressed

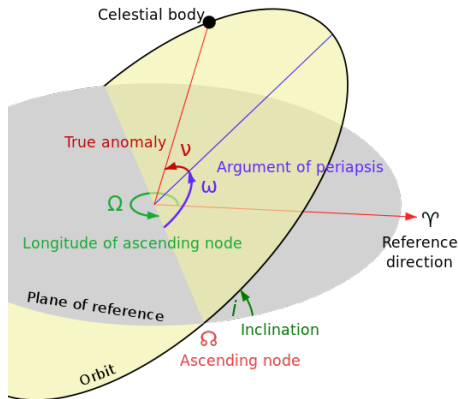
$$y_t = y | p_t \sim \text{Binom}(1, p_t) \quad (11)$$

$$p_t = \frac{e^{\gamma_0 \beta_0 + \sum_{i=1}^p \gamma_i \beta_i X_{t,i}}}{1 + e^{\gamma_0 \beta_0 + \sum_{i=1}^p \gamma_i \beta_i X_{t,i}}} \quad (12)$$

$$\beta | \gamma \sim N_{\sum_{i=1}^p \gamma_i}(\mu_\beta, \Sigma_\beta) \quad (13)$$

$$\gamma_i \sim \text{Binom}(1, q) \quad (14)$$

NEO objects classification. NASA space challenge



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Figure: Orbital elements(left) by Lasunncty (talk), CC BY-SA 3.0 and absolute vs apparent magnitude (right) by Mrscreath(<http://mrscreath.blogspot.com>)

NEO objects classification. NASA space challenge

20 covariates addressed in the experiment (both *reasonable* and *heuristic*): Mean anomaly $\in [0^\circ; 360^\circ)$; Argument of perihelion $\in [0^\circ; 360^\circ)$; Longitude of the ascending node $\in [0^\circ; 360^\circ)$; Inclination $\in [0^\circ; 180^\circ]$; Semi major axis $\in \mathbf{R}^+$; Eccentricity $\in \mathbf{R}^+$; Mean motion $\in \mathbf{R}^+$; Absolute magnitude $\in \mathbf{R}$ (brightness); Rms residual $\in \mathbf{R}^+$ (brightness error); Eccentricity² $\in \mathbf{R}^+$; Absolute magnitude² $\in \mathbf{R}^+$; Semi major axis² $\in \mathbf{R}^+$; Semi major axis³ $\in \mathbf{R}^+$; Mean anomaly \times Semi major axis; Mean anomaly \times Semi major axis² $\in \mathbf{R}^+$; Mean anomaly \times Semi major axis³ $\in \mathbf{R}^+$; Argument of perihelion \times Semi major axis $\in \mathbf{R}^+$; Argument of perihelion \times Semi major axis² $\in \mathbf{R}^+$; Argument of perihelion \times Semi major axis³ $\in \mathbf{R}^+$; Longitude of the ascending node \times Semi major axis $\in \mathbf{R}^+$.

Training set includes 32 NEO and 32 non-NEO objects, **test set** includes 20720 objects (14099 NEO, 6621 non-NEO), **validation sets** were used as some random subsets of a 100 elements from these 20720 **objects**

2²⁰ models in total, algorithm was run until ca **2500 models** and ca **10000 models** are visited.

NEO objects classification. Inference

Posterior inclusion probabilities and posterior model probabilities

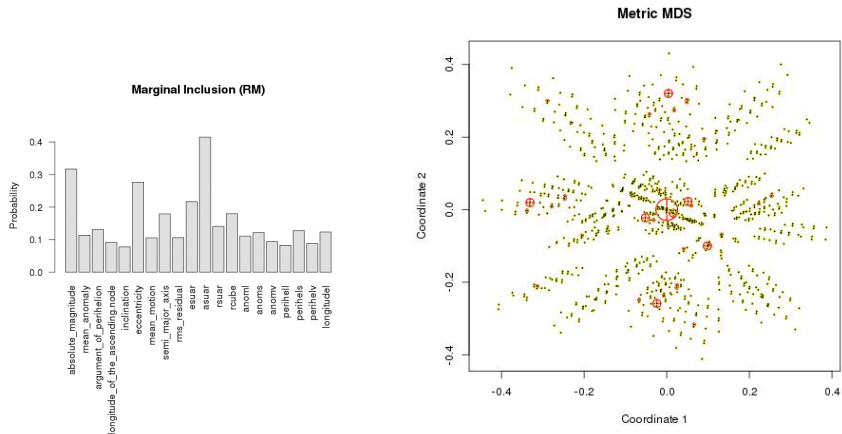


Figure: Comparison of marginal inclusion probabilities of the covariates (left) and models on the whole (right)

NEO objects classification. Bayesian classification

Choice of \mathbb{V}^* is crucial, $\mathbb{V}^* = \Omega_\gamma$ - often in-feasible, $\mathbb{V}^* = \mathbb{V}$ - very precise can be too slow, $\mathbb{V}^* = \mathbb{V} \cap p(\gamma|\mathbb{D}) \geq \alpha$ - often precise, but is a way faster!!!

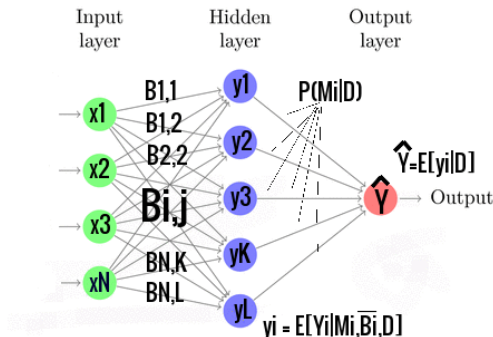


Figure: Bayesian Artificial Neuron Network for Classification

$$\hat{Y} = \mathbb{I}\{\hat{E}[Y|\mathbf{D}] \geq 0.5\}, \hat{E}[Y|\mathbf{D}] = \sum_{\gamma \in \mathbb{V}^*} \hat{E}[y_\gamma|\gamma, \mathbf{D}] \hat{p}(\gamma|\mathbf{D})$$

NEO objects classification. Results

Quite impressive actually... Surprisingly or not?.. Comments?..

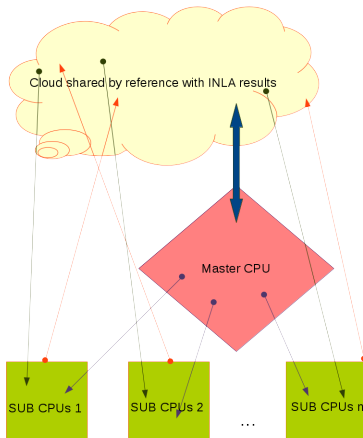
Remember: $||\text{training set}|| = 64$, $||\text{test set}|| = 20720$

Subset	$ \text{Hidden} $	Precision	FNR	FPR	Time	Time/it.
\mathbb{V}^1	10090	99.95656%	0.05670945 %	0.01510117 %	619.89 min	1.795 sec
\mathbb{V}^2	2512	99.80212%	0.05670945 %	0.49594239 %	172.66 min	0.499 sec
\mathbb{V}^3	412	99.46429%	0.04253813 %	1.56110622%	29.166 min	0.084 sec
\mathbb{V}^4	80	99.19402%	0.02836276%	2.40271201%	9.9812 min	0.029 sec
\mathbb{V}^5	4	90.00483%	0.04962427 %	23.7651171 %	4.7789 min	0.014 sec
$\text{argmax}_{\gamma \in \mathbb{V}^1} \{p_{\mathbb{V}}(\gamma \mathbb{D})\}$	1	82.83301%	0.07087675 %	34.8839473 %	4.5222 min	0.013 sec
Wake up NEO	?	93.86271%	1.00000000%	17.00000000%	-	-

Table: Comparison of performance (Precision, FDR, FNR, Time) of different models

N/B: the best model includes eccentricity², eccentricity, absolute magnitude², absolute magnitude

Multicore and shared memory issues



1. Share the work done by reference
2. Before assigning a job to a CPU check if the job is already done
3. Thus avoid re-completing jobs & minimize communication times
4. Important to control writing to the shared memory efficiently

Figure: Multiprocessing architecture

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.

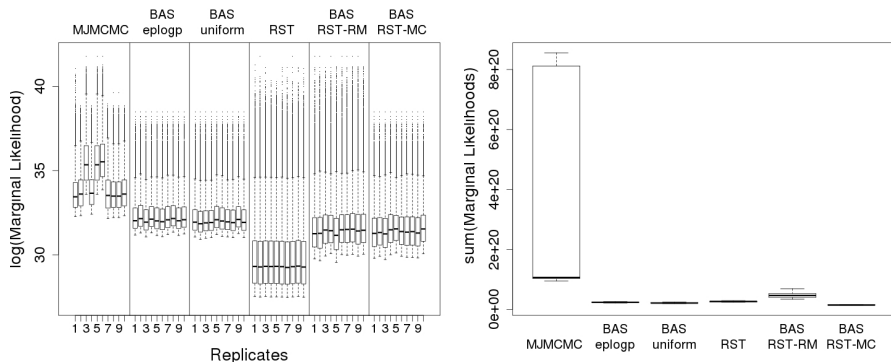


Figure: 100000 best mliks found (left) and posterior masses captured (right). Bayesian linear regression with a g-prior is addressed, since no other packages (to our awareness) manage model selection in GLMM

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

Checking convergence. Marginal inclusion probabilities

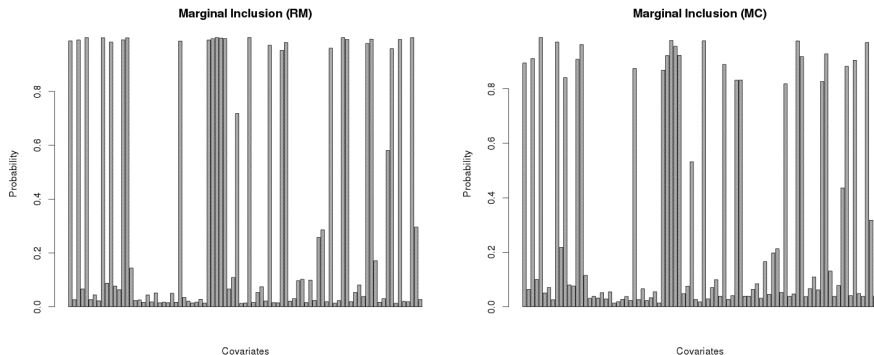


Figure: Comparison of marginal inclusion probabilities obtained by the Bayes formula and MCMC approximations from the best run of MJMCMC with $8.56e + 20$ posterior mass captured

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

References



M. Clyde, J. Ghosh, and M. Littman.

Bayesian adaptive sampling for variable selection and model averaging.
Journal of Computational and Graphical Statistics, 20(1):80–101, 2011.



A. Hubin and G.O. Storvik

Efficient mode jumping MCMC for Bayesian variable selection in GLMM.
arXiv:1604.06398v1, 2016.



H. Rue, S. Martino, and N. Chopin.

Approximate bayesian inference for latent gaussian models by using integrated nested laplace approximations.
Journal of the Royal Statistical Society, 71(2):319–392, 2009.



G.O. Storvik.

On the flexibility of metropolis-hastings acceptance probabilities in auxiliary variable proposal generation.
Scandinavian Journal of Statistics, 38:342–358, 2011.

The End.



Thank you.