

Computational Statistics II

Unit B.1: Optimal scaling & adaptive Metropolis

Tommaso Rigon

University of Milano-Bicocca

Ph.D. in Economics and Statistics

Main concepts

- Optimal scaling for Metropolis-Hastings algorithm
 - Metropolis-within-Gibbs algorithm
 - Adaptive MCMC
 - Examples of adaptive MCMC algorithms
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- Associated **R** code: https://tommasorigon.github.io/CompStat/exe/un_B1.html

Random walk Metropolis-Hastings

- Let us consider a **random walk** Metropolis-Hastings (RWM) algorithm and let $\theta = \theta^{(r)}$ be the current status of the chain.
- It is called “random walk” because we sample θ^* from a **Gaussian proposal** distribution

$$(\theta^* | \theta^{(r)}) \sim N_p(\theta^{(r)}, \mathbf{S}), \quad \text{implying that} \quad q(\theta^* | \theta) = q(\theta | \theta^*).$$

- In this special case the **acceptance probability** simplifies and we get

$$\alpha = \min \left\{ 1, \frac{\pi(\theta^* | \mathbf{X})}{\pi(\theta | \mathbf{X})} \frac{q(\theta | \theta^*)}{q(\theta^* | \theta)} \right\} = \min \left\{ 1, \frac{\pi(\theta^*)\pi(\mathbf{X} | \theta^*)}{\pi(\theta)\pi(\mathbf{X} | \theta)} \right\}.$$

- This Gaussian proposal distribution is a sensible choice especially whenever the support of θ is unbounded.

Optimal choice of the proposal distribution

- Among all the possible proposal densities for $q(\theta \mid \theta^*)$, we restrict our focus on multivariate Gaussians centered on θ^* .
- Despite this important simplification, choosing the covariance matrix \mathbf{S} remains a difficult task and crucially affects the performance.
- In the **univariate / bivariate cases**, one could tune the variance of the proposal distribution \mathbf{S} by **trial and error** and with some patience.
- Unfortunately, whenever the parameter's dimension is large, the "manual" elicitation of the matrix \mathbf{S} is almost impossible.
- **Key question.** Can we identify an ideal covariance matrix \mathbf{S} that is optimal in some sense? Can we "estimate" it from the data?

Asymptotic variance

- For an arbitrary squared-integrable function $g(\cdot) : \mathbb{R}^p \rightarrow \mathbb{R}$, let us consider the Monte Carlo estimator

$$\hat{\eta}_g = \frac{1}{R} \sum_{r=1}^R g(\theta^{(r)}),$$

for the posterior expectation $\eta_g = \mathbb{E}\{g(\theta \mid \mathbf{X})\}$.

- If a central limit theorem holds, we have that

$$\sqrt{R} \frac{\hat{\mu}_g - \mu_g}{\sigma_g} \xrightarrow{d} N(0, 1),$$

where σ_g^2 is the so-called **asymptotic variance** of the MCMC algorithm.

- Intuitively, we seek a covariance matrix \mathbf{S} that minimizes the asymptotic variance σ_g^2 .
- Other measures of “optimality” can be defined, but it can be shown they are all equivalent asymptotically (for large values of p).

Asymptotic variance

- Let $\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \dots$ be a Markov chain, with $\theta^{(0)} \sim \pi(\theta \mid \mathbf{X})$ being a sample from the stationary distribution.
- The asymptotic variance can be written as follows

$$\sigma_g^2 = \text{var}\{g(\theta^{(0)} \mid \mathbf{X})\} \tau_g = \text{var}\{g(\theta^{(0)} \mid \mathbf{X})\} \left[1 + 2 \sum_{r=1}^{\infty} \text{Corr}\{g(\theta^{(0)}), g(\theta^{(r)})\} \right].$$

- The quantity τ_g is sometimes called **integrated autocorrelation time** and measures the **loss of efficiency** with respect to independent (iid) sampling ($\tau_g = 1$).
- When $\tau_g = 1$, the MCMC algorithm is “optimal” and there is no autocorrelation.
- Rarely, one could obtain $\tau_g < 1$, which is indeed an improvement over iid sampling.
- The `effectiveSize` **R** command produces an estimate of $R\tau_g^{-1}$ from the empirical samples of the chain.

Optimal scaling

- The relationship between the matrix \mathbf{S} and the asymptotic variance σ_g^2 is unclear. In addition, the variance σ_g^2 depends on the chosen function $g(\cdot)$.
- Let us initially assume that the posterior distribution has the following form

$$\pi(\boldsymbol{\theta} \mid \mathbf{X}) = \prod_{j=1}^p f(\theta_j), \quad \text{var}(\boldsymbol{\theta} \mid \mathbf{X}) = \sigma^2 I_p$$

meaning that the components of $\boldsymbol{\theta}$ are independent and identically distributed from some density f .

- Moreover, we consider the following proposal distribution

$$(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(r)}) \sim N_p(\boldsymbol{\theta}^{(r)}, s_p^2 I_p), \quad s_p^2 = \ell^2 / p.$$

- In this simplified setting, we seek an **optimal scaling** value for ℓ^2 .

Diffusion processes

- This problem simplifies remarkably in the **asymptotic** regime, as p diverges.
- Let us define a continuous-time stochastic process from the first component θ_1 of the $\theta = (\theta_1, \dots, \theta_p)$, namely:

$$Z^{(t)} = \theta_1^{([tp])}$$

where $[\cdot]$ denotes the integer part function.

- That is, $Z^{(t)}$ is a **speeded-up** continuous-time version of the original algorithm, parametrized to make jumps every p^{-1} time units.
- We need some smoothness conditions on the density f (Roberts et al., 1997), and in particular we assume that

$$\mathcal{I} = \mathbb{E} \left[\left\{ \frac{f'(\theta_1)}{f(\theta_1)} \right\}^2 \right] < \infty,$$

is well defined. The quantity \mathcal{I} equals σ^{-2} in the Gaussian case.

Diffusion processes

Theorem

Let $B^{(t)}$ be the standard Brownian motion and let $\Phi(\cdot)$ be the cdf of a standard Gaussian. The continuous-time stochastic process Z weakly converges to

$$Z \xrightarrow{d} W, \quad p \rightarrow \infty,$$

where W is a diffusion process satisfying the stochastic differential equation

$$dW^{(t)} = h(\ell)^{1/2} dB^{(t)} + \frac{h(\ell) \nabla \log f(W^{(t)})}{2} dt,$$

where the **speed of the diffusion** is

$$h(\ell) = \ell^2 2\Phi\left(-\frac{\mathcal{I}^{1/2}\ell}{2}\right).$$

- **Note.** All the involved quantities have a clear interpretation in terms of the original RWM algorithm.

Speed of the diffusion $h(\ell)$

- The speed of the diffusion $h(\ell)$ is strictly related to the asymptotic variance of the MCMC algorithm.
- Recall that we aim at finding an **optimal value** for ℓ that minimizes the autocorrelation.
- In first place, note that for small $\epsilon > 0$ it holds that

$$\text{Corr}\{g(W^{(0)}), g(W^{(\epsilon)})\} \approx 1 - \epsilon B_g h(\ell),$$

where B_g is a constant not depending on ℓ .

- Let $\tau_g(\ell)$ be the integrated autocorrelation of the RWM. Then for large p it holds that

$$\tau_g(\ell)^{-1} \approx h(\ell) e_g p^{-1},$$

where $e_g > 0$ is some constant depending only on $g(\cdot)$.

- **Remark.** The maximization of the speed of diffusion is equivalent to minimization of the autocorrelation for any function $g(\cdot)$.

Speed of diffusion and acceptance rate

- Let us define the acceptance rate of the original p -dimensional RWM as

$$A_p(\ell) = \lim_{R \rightarrow \infty} \frac{\text{"# of accepted moves"}}{R},$$

namely the long-term proportion of accepted moves.

- Then, it can be shown that

$$\lim_{p \rightarrow \infty} A_p(\ell) = A(\ell) = 2\Phi\left(-\frac{\mathcal{I}^{1/2}\ell}{2}\right).$$

- Moreover, recall the definition of the speed of diffusion

$$h(\ell) = \ell^2 2\Phi\left(-\frac{\mathcal{I}^{1/2}\ell}{2}\right) = \ell^2 A(\ell),$$

implying that the **speed of the diffusion** is strictly related to the **acceptance rate**.

Important consequences

- Hence, we consider ℓ maximizing the speed of diffusion $h(\ell)$, obtaining the **optimal scaling**

$$\ell_{\text{opt}} \approx \frac{2.38}{\mathcal{I}^{1/2}}.$$

- The acceptance rate, evaluated at the optimal scaling, is

$$A(\ell_{\text{opt}}) \approx 0.234,$$

corresponding to the **optimal acceptance rate**.

- This suggests the following optimal proposal variance for $(\theta^* \mid \theta^{(r)}) \sim N_p(\theta^{(r)}, s_p^2 I_p)$ for large values of p , with

$$s_p^2 = 2.38^2 (p \mathcal{I})^{-1},$$

where \mathcal{I} must be estimated / guessed in some way.

- If f is a Gaussian density with variance σ^2 , then we obtain $s_p^2 = 2.38^2 \sigma^2 p^{-1}$.

Getting practical

- These results are asymptotic (large p) and require that the posterior distributions has independent components.
- In practice, already when $p \approx 5$ the optimal acceptance rate is quite close to 0.234 based on simulation studies (Gelman et al., 1996).
- When $p = 1$ the optimal acceptance rate is higher and about 0.44.
- **Key extension.** If the posterior distribution is Gaussian with $p \times p$ covariance matrix Σ , it suffices to translate the components and **rotate the axes** according to Σ to make the components iid, leading to

$$(\theta^* \mid \theta^{(r)}) \sim N_p(\theta^{(r)}, \mathbf{S}), \quad \mathbf{S} = 2.38^2 \Sigma / p.$$

- This procedure is **optimal** for large p , although it requires the knowledge of Σ .

Binary regression

- Let $\mathbf{y} = (y_1, \dots, y_n)^\top$ be a vector of the observed **binary responses**.
- Let \mathbf{X} be the corresponding **design matrix** whose generic row is $\mathbf{x}_i = (1, x_{i2}, \dots, x_{ip})^\top$, for $i = 1, \dots, n$. All predictors have been **standardized**.
- We consider a generalized linear model such that

$$(y_i \mid \pi_i) \stackrel{\text{ind}}{\sim} \text{Bern}(\pi_i), \quad \pi_i = g(\eta_i), \quad \eta_i = \beta_1 x_{i1} + \dots + \beta_p x_{ip},$$

where $g(\cdot)$ is either the inverse logit transform or the cdf of a standard normal. We focus here on the **logistic regression case**.

- We aim at estimating the parameter vector $\beta = (\beta_1, \dots, \beta_p)^\top$ using RWM.
- We will employ a relatively vague prior centered at 0, namely

$$\beta \sim N_p(0, 100 I_p).$$

The Pima indian dataset

- During the course, we will test several algorithms on the “famous” **Pima indian dataset**, with $n = 532$ and $p = 8$.
- The purpose of this exercise is mainly presenting the implementation of the various MCMC algorithms and showing their performance in this specific example.
- **Warning.** The following results should not be generalized to any statistical models nor even to any logistic regression model.
- Depending on the sample size n , the dimension of the parameter space p as well as the dependence structure of the predictor, the results may vary significantly.
- Refer to the nice paper by Chopin & Ridgway (2017) for a more comprehensive discussion on this aspect.

Computational details

- Recall that at each step of the algorithm we need a sample from a multivariate Gaussian distribution $N_p(0, \mathbf{S})$.
- Albeit tempting, using built-in **R** functions such as `rmvnorm` and `mvrnorm` leads to a sensible **waste of computing time**.
- Indeed, in order to get a sample from $V \sim N_p(\mu, \mathbf{S})$, one needs to compute

$$V = \mu + \mathbf{A}\mathbf{Z},$$

where $\mathbf{Z} \sim N(0, I_p)$ is standard Gaussian and \mathbf{A} is a $p \times p$ matrix such that $\mathbf{A}\mathbf{A}^T = \mathbf{S}$.

- Hence, there is no need to compute \mathbf{A} at every step, as this can be done before running the MCMC.

```
A <- chol(S) # Cholesky decomposition of S (outside the MCMC)
V <- mu + crossprod(A, rnorm(2)) # Sample from V (inside the MCMC)
```

Naive covariance matrix

- Let us start with a **naive choice** for the proposal covariance $\mathbf{S} = \text{diag}\{10^{-3}, \dots, 10^{-3}\}$.
- Albeit being sub-optimal, this “random” choice of \mathbf{S} works decently.

```
# Covariance matrix of the proposal
S <- diag(1e-3, ncol(X))

# Running the MCMC (R = 30000, burn_in = 30000)
fit_MCMC <- as.mcmc(RMH(R, burn_in, y, X, S)) # Convert the matrix into a "coda" object

summary(effectiveSize(fit_MCMC)) # Effective sample size (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  174.9   205.0   258.5   259.6   320.7   333.1

summary(R / effectiveSize(fit_MCMC)) # Integrated autocorrelation time (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  90.06   93.56  119.31  122.76  146.43  171.52

summary(1 - rejectionRate(fit_MCMC)) # Acceptance rate
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  0.7191  0.7191  0.7191  0.7191  0.7191  0.7191
```

Approximating the posterior covariance matrix

- We know that a sensible choice for \mathbf{S} would be based on posterior covariance matrix Σ .
- The true Σ is unknown and therefore we need to rely on some (fast) **approximation**.
- A possibility is based on a **quadratic approximation** of the likelihood function, evaluated at the maximum likelihood estimate.

- This is particularly simple in the logistic regression case (do it as an exercise!), since we can set

$$\hat{\Sigma} = (\mathbf{X}^T \hat{\mathbf{H}} \mathbf{X})^{-1}, \quad \hat{\mathbf{H}} = \text{diag}\{\hat{\pi}_1(1 - \hat{\pi}_1), \dots, \hat{\pi}_n(1 - \hat{\pi}_n)\},$$

where $\hat{\pi}_i = [1 + \exp\{-(x_{i1}\hat{\beta}_{1,\text{ML}} + \dots + x_{ip}\hat{\beta}_{p,\text{ML}})\}]^{-1}$.

- This estimate $\hat{\Sigma}$ corresponds to the **Fisher information**, evaluated at the MLE.
- This is a variant of the **Laplace approximation** that ignores the prior contribution. Refer to Chopin and Ridgway (2017) for a more general and detailed explanation.

Laplace covariance matrix

- Let us use a covariance matrix based on the Laplace approximation $\mathbf{S} = 2.38^2 \hat{\Sigma} / p$.
- This choice for \mathbf{S} is almost optimal and indeed the effective sample size is much higher.

```
# Covariance matrix is selected using a Laplace approximation
fit_logit <- glm(type ~ X - 1, family = binomial(link = "logit"), data = Pima)
S <- 2.38^2 * vcov(fit_logit) / ncol(X) # The desired matrix is extracted using vcov
```

```
# Running the MCMC (R = 30000, burn_in = 30000)
fit_MCMC <- as.mcmc(RMH(R, burn_in, y, X, S))
```

```
summary(effectiveSize(fit_MCMC)) # Effective sample size
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  1107   1174   1206   1194   1228   1245
```

```
summary(R / effectiveSize(fit_MCMC)) # Integrated autocorrelation time (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  24.10  24.43  24.87  25.15  25.56  27.10
```

```
summary(1 - rejectionRate(fit_MCMC)) # Acceptance rate
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  0.2746  0.2746  0.2746  0.2746  0.2746  0.2746
```

- In several cases it is not possible to come up with a fast and reasonable estimate $\hat{\Sigma}$.
- Hence, a possibility is tuning the covariance matrix **S on the fly**, namely using the previously obtained samples.
- **Warning**. This is not anymore a MH algorithm and therefore the chain is not necessarily converging to the correct stationary distribution or converging at all.
- However, in many cases **ergodicity** of the chain is **preserved** as long as we adaptively tune **S** in a reasonable manner.
- The key condition is called **diminishing adaptation**, which essentially means that the changes in **S** are negligible as $R \rightarrow \infty$; see Roberts & Rosenthal (2009).

Adaptive Metropolis

- An example of adaptive MCMC is the so-called **adaptive Metropolis** (AM) algorithm.

- We implement here a **version** of the AM which makes use of the following proposal distribution

$$q_r(\beta^* | \beta) \sim N(\beta, 2.38^2/p \Sigma_r + \epsilon I_p),$$

where Σ_r is the covariance matrix of the previously r sampled values $\beta^{(1)}, \dots, \beta^{(r)}$.

- The constant $\epsilon > 0$ is some small value that avoid degeneracies. We will use $\epsilon = 10^{-6}$.
- Moreover, note that the following **recursive formula** holds true:

$$\Sigma_r = \frac{1}{r} \sum_{j=1}^r (\beta^{(j)} - \bar{\beta}^{(r)})^\top (\beta^{(j)} - \bar{\beta}^{(r)}) = \frac{r-1}{r} \Sigma_{r-1} + \frac{1}{r} (\beta^{(r)} - \bar{\beta}^{(r-1)})^\top (\beta^{(r)} - \bar{\beta}^{(r-1)}).$$

where $\bar{\beta}^{(r)} = (r-1)/r \bar{\beta}^{(r-1)} + \beta^{(r)}/r$ is the arithmetic means of the first r values.

- Several **variants** of this scheme exist, but the core idea is trying to estimate Σ .

Adaptive Metropolis

- We obtain results that are comparable to the MH based on the Laplace approximation in terms of effective sample size.
- However, the **computing time** is much **higher**, because we need to decompose \mathbf{S} at each iteration.

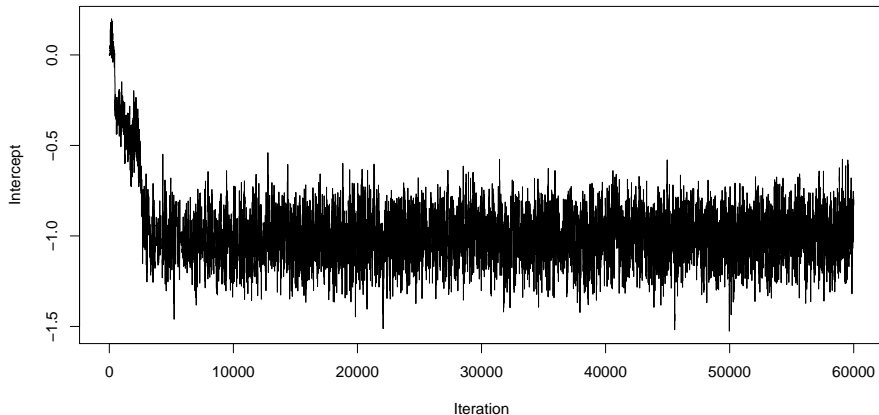
```
# Running the MCMC (R = 30000, burn_in = 30000)
fit_MCMC <- as.mcmc(RMH_Adaptive(R = R, burn_in = burn_in, y, X))

summary(effectiveSize(fit_MCMC)) # Effective sample size (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  869.3   962.0  1022.2  1037.5  1075.6  1284.7

summary(R / effectiveSize(fit_MCMC)) # Integrated autocorrelation time (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  23.35   27.98   29.35   29.36   31.24   34.51

summary(1 - rejectionRate(fit_MCMC)) # Acceptance rate (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  0.2058  0.2058  0.2058  0.2058  0.2058  0.2058
```

Traceplot of β_1 , including the burn-in



Metropolis-within-Gibbs (recap)

- The **Metropolis-within-Gibbs** algorithm is an MCMC algorithm that combines the MH and the Gibbs sampling algorithms.

- Let $\pi(\theta_j | -)$ be the so-called **full-conditional** of θ_j , that is

$$\pi(\theta_j | -) = \pi(\theta_j | \mathbf{X}, \theta_1, \dots, \theta_{j-1}, \theta_{j+1}, \dots, \theta_p), \quad j = 1, \dots, p,$$

namely the conditional distribution of θ_j given the data and the other parameters.

- In the Metropolis-within-Gibbs we proceed as in a standard Gibbs sampling but instead of drawing from the full conditional $\pi(\theta_j | -)$, we conduct a **Metropolis step**.
- We propose a value from $q(\theta_j^* | \theta_j)$, typically a univariate Gaussian random walk, that we accept / reject in the usual manner.
- This means that at each step of the chain some parameters are updated, some others are not. This produces **local moves** rather than **global moves**.

Metropolis-within-Gibbs

- We use random walk proposals $(\theta_j^* \mid \theta_j) \sim N_1(\theta_j, s_j^2)$, for $j = 1, \dots, p$.
- In this first experiment we set $s_1^2 = \dots = s_p^2 = 10^{-4}$.
- These results are **unacceptable**. We need a better specification for the variances s_j^2 .

```
p <- ncol(X) # Dimension of the parameter space
se <- sqrt(rep(1e-4, p)) # Standard deviations of the proposal distributions

# Running the MCMC (R = 30000, burn_in = 30000)
fit_MCMC <- as.mcmc(RMH_Gibbs(R = R, burn_in = burn_in, y, X, se))

summary(effectiveSize(fit_MCMC)) # Effective sample size (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
# 27.02  36.43  37.37  37.57  40.58  44.21
summary(R / effectiveSize(fit_MCMC)) # Integrated autocorrelation time (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
# 678.6  740.1  802.8  814.8  824.1 1110.1
summary(1 - rejectionRate(fit_MCMC)) # Acceptance rate (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
# 0.9682  0.9685  0.9697  0.9698  0.9710  0.9719
```

Adaptive Metropolis-within-Gibbs

- In order to get a better mixing, we could **adaptively** choose the variances s_j^2 as in Roberts and Rosenthal (2009).
- Since the updates are univariate, we can rely a more direct adaptive approach targeting the **optimal acceptance rate**, which is 0.44.
- Every 50 iterations (a batch), the algorithm increases or decreases the standard errors s_j according to the fraction of accepted values among the 50 batch values.
- It is convenient to work in the **logarithmic scale**, to facilitate the exploration of the space of suitable values.
- If the fraction of accepted values for the j th component is **higher/lower** than 0.44, then we **increase/decrease** the corresponding $\log s_j$ by the quantity $\min\{0.01, 1/\sqrt{r}\}$.
- Note that the **diminishing adaptation** condition is satisfied, as the correction is vanishing as r (the number of iterations) increases.

Adaptive Metropolis-within-Gibbs

- These results are comparable with the other suitably tuned MH approaches.
- However, the computing time is much higher.
- Note that the overall acceptance rates are indeed all close to 0.44.

```
fit_MCMC <- as.mcmc(RMH_Gibbs_Adaptive(R = R, burn_in = burn_in, y, X)) #  
  
summary(effectiveSize(fit_MCMC)) # Effective sample size (beta)  
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.  
# 653.2   733.1  1021.5  1009.3  1293.6  1373.3  
  
summary(R / effectiveSize(fit_MCMC)) # Integrated autocorrelation time (beta)  
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.  
# 21.84   23.19   31.43   32.76   41.07   45.93  
  
summary(1 - rejectionRate(fit_MCMC)) # Acceptance rate (beta)  
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.  
# 0.4451  0.4472  0.4479  0.4483  0.4494  0.4517
```

Summary of the results

- The following table compare the **average** results. Here ESS represents the estimated and average **effective sample size**.
- Among these competitors, the Laplace MH seems preferable.
- Note that we could sensibly speed up these results by using **Rcpp**!

	Seconds	ESS	ESS / Sec.	Acceptance rate
Vanilla MH	1.89	259.58	137.60	0.72
Laplace MH	1.77	1194.42	676.49	0.27
AM	4.54	1037.46	228.42	0.21
Metropolis-within-Gibbs	11.95	37.57	3.14	0.97
Ad. Metropolis-within-Gibbs	11.95	1009.32	84.48	0.45