Adaptive Markov Chain Monte Carlo Theory, Methodology and Practice

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OxWaSP - module 1 - Oct 2018

Adaptive MCMC in 3 minutes (what it is?)

- Most MCMC algorithms need **tuning** to be efficient and reliable in large scale applications
- Tuning requires **computing time** and **human time** (performing and assessing trial runs) and typically **expert knowledge**
- Hand **tuning may not be practical**: too many variables, when to stop tuning, tuning criterion not clear, etc.
- **Adaptive MCMC is about tuning MCMC without human intervention**
- It uses the **trajectory so far** to tune the sampling kernel **on the fly** (so it is not a Markov chain anymore)

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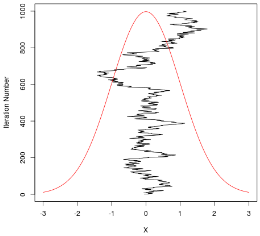
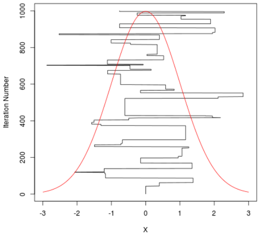
Adaptive MCMC in 3 minutes (3 examples)

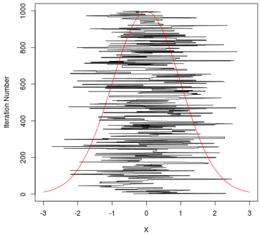
- Random Walk Metropolis with proposal increments

$$Y_{n+1} \sim q_\sigma(X_n, \cdot) = X_n + \sigma N(0, Id).$$

Plots for different σ - Goldilock's principle







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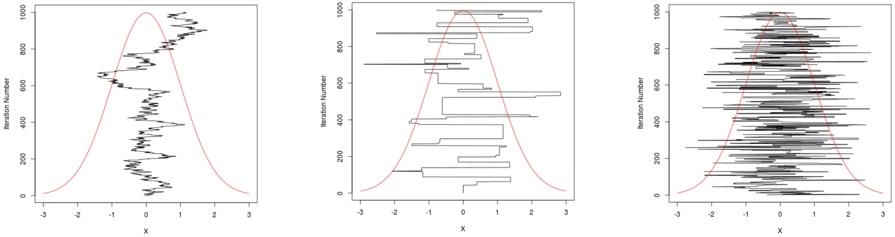

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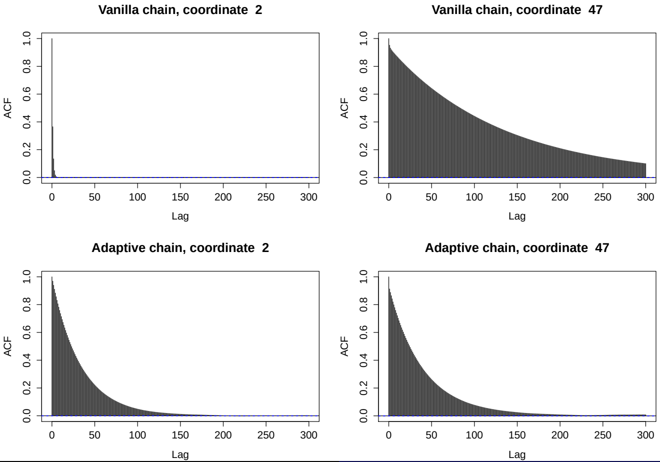
Adaptive MCMC in 3 minutes (3 examples)

- Random Scan Gibbs Sampler for 50d Truncated Multivariate Normals
  Are uniform $1/d$ selection probabilities optimal?



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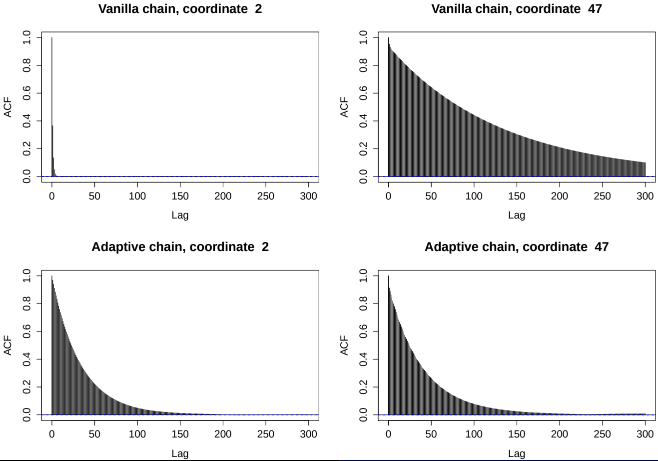
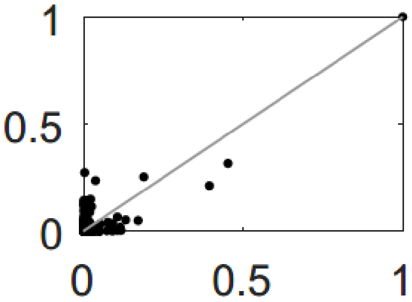
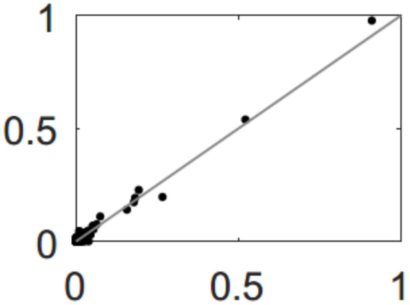


Adaptive MCMC in 3 minutes (3 examples)

- Variable selection (p = 22576) - Metropolis type algorithms
  Plots of posterior inclusion probabilities Run 1 vs Run 2 (checking agreement)
  Standard Add-Swap-Delete proposal vs. an optimized non-local proposal





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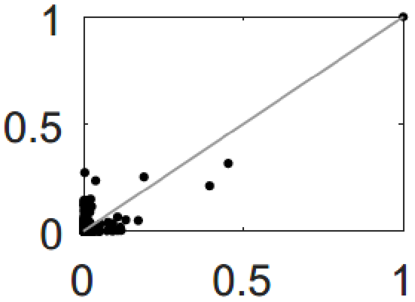

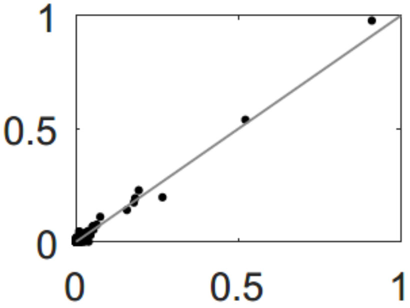

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Adaptive MCMC in 5 minutes (ingredients that we need)

- For a given MCMC class we need **a parameter to optimize**
- An optimization rule that is **mathematically sound**
- An optimization rule that is **computationally cheap**
- Need underpinning theory to **verify it is ergodic**
  (it is not Markovian - how do we know bizarre things don't happen??)
- It needs to **work in practice**

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the usual MCMC setting

- let π be a target probability distribution on $\mathcal{X}$, typically arising as a posterior distribution in Bayesian inference,
- the goal is to evaluate

$$I := \int_{\mathcal{X}} f(x)\pi(dx).$$

- direct sampling from π is not possible or inefficient
  for example π is known up to a normalising constant
- MCMC approach is to simulate $(X_n)_{n\geq 0}$, an ergodic Markov chain with **transition kernel** P and limiting distribution π, and take ergodic averages as an estimate of I.
- the usual estimate

$$\hat{I} := \frac{1}{n}\sum_{k=t}^{t+n} f(X_k)$$

- **SLLN** for Markov chains holds under very mild conditions
- **CLT** for Markov chains holds under some additional assumptions and is verifiable in many situations of interest

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Reversibility and stationarity

- How to design P so that X_n converges in distribution to π ?
- **Definition.** P is reversible with respect to π if

$$\pi(x)P(x,y) = \pi(y)P(y,x)$$

  as measures on $\mathcal{X} \times \mathcal{X}$
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The Metropolis algorithm

- **Idea.** Take any transition kernel Q with transition densities $q(x, y)$ and make it reversible with respect to π
- **Algorithm.** Given X_n
  sample $Y_{n+1} \sim Q(X_n, \cdot)$
- with probability $\alpha(X_n, Y_{n+1})$ set $X_{n+1} = Y_{n+1}$, otherwise set $X_{n+1} = X_n$
- where

$$\alpha(x, y) = \min\{1, \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}\}.$$

- Under mild assumptions on Q the algorithm is ergodic.
- However it's performance depends heavily on Q
- is is **difficult** to design the proposal Q so that P has **good convergence properties**, especially if $\mathcal{X}$ is high dimensional

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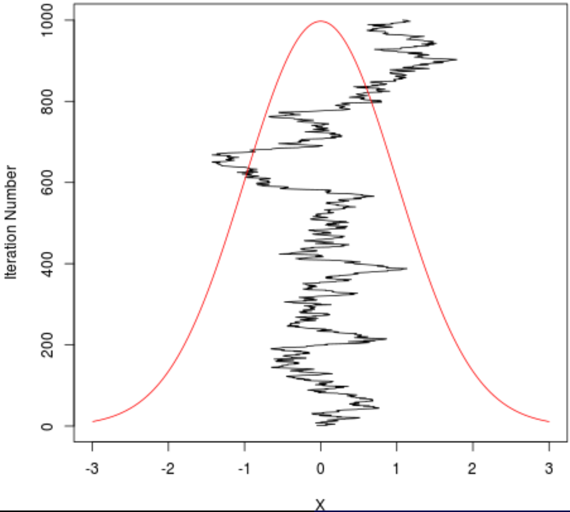

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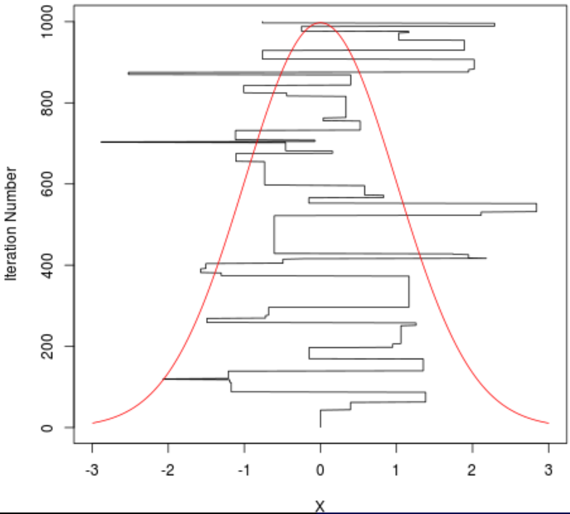

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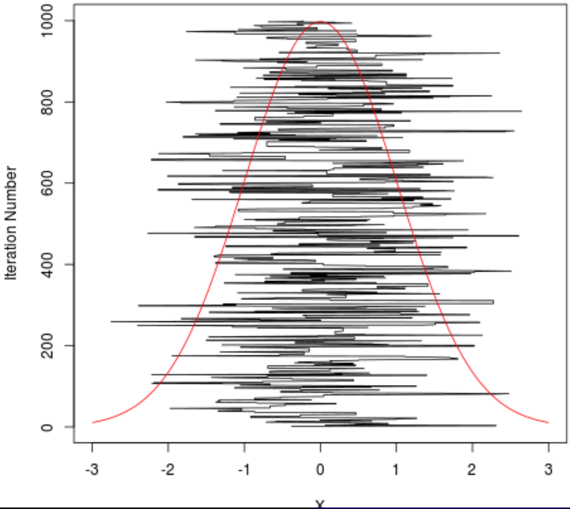

diffusion limit [RGG97]

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- but how to choose it?
- if the dimension of $\mathcal{X}$ goes to ∞, e.g. $\mathcal{X} = \mathbb{R}^d$, and $d \to \infty$,
- if the proposal is set as $Q = N(x, \frac{l^2}{d} I_d)$ for fixed $l > 0$,
- if we consider
$$Z_t = d^{-1/2} X^{(1)}_{\lfloor dt \rfloor}$$
- then Z_t converges to the Langevin diffusion
$$dZ_t = h(l)^{1/2} dB_t + \frac{1}{2} h(l) \nabla \log \pi(Z_t) dt$$

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optimal acceptance rate [RGG97]

- Z_t converges to the Langevin diffusion

$$dZ_t = h(l)^{1/2} dB_t + \frac{1}{2} h(l) \nabla \log \pi(Z_t) dt$$

- where $h(l) = 2l^2 \Phi(-Cl/2)$ is the speed of the diffusion and $A(l) = 2\Phi(Cl/2)$ is the asymptotic acceptance rate.
- maximising the speed $h(l)$ yields the optimal acceptance rate

$$A(l) = 0.234$$

  which is independent of the target distribution π
- it is a remarkable result since it gives a simple criterion (and the same for all target distributions π) to assess how well the Random Walk Metropolis is performing.

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$$dZ_t = h(l)^{1/2} dB_t + \frac{1}{2} h(l) \nabla \log \pi(Z_t) dt$$

- where $h(l) = 2l^2 \Phi(-Cl/2)$ is the speed of the diffusion and $A(l) = 2\Phi(Cl/2)$ is the asymptotic acceptance rate.
- maximising the speed $h(l)$ yields the optimal acceptance rate

$$A(l) = 0.234$$

which is independent of the target distribution π

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the scaling problem cd

- take Random Walk Metropolis with proposal increments
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$$Y_{n+1} \sim q_\sigma(X_n, \cdot) = X_n + \sigma N(0, Id).$$
- so the theory says the optimal average acceptance rate
$$\bar{\alpha} := \int\int \alpha(x,y) q_\sigma(x, dy)\pi(dx)$$
should be approximately $\alpha^* = 0.234$
- however it is not possible to compute σ^* for which $\bar{\alpha} = \alpha^*$.
- It is very tempting to adjust σ on the fly while simulation progress
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  - when to stop estimating $\bar{\alpha}$? (to increase or decrease σ)
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$$\log \sigma_{n+1} = \log \sigma_n + \gamma_n(\alpha(X_n, Y_{n+1}) - \alpha^*)$$
where $\gamma_n \to 0$.

- Recall we follow a very precise mathematical advice from diffusion limit analysis [RGG97]
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- The adaptation rule is mathematically appealing (diffusion limit)
- The adaptation rule is computationally simple (acceptance rate)
- It works in applications (seems to improve convergence significantly)
- Improves convergence even in settings that are neither high dimensional, nor satisfy other assumptions needed for the diffusion limit
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- **YES.** Similar optimal scaling results are available for MALA, HMC, etc.
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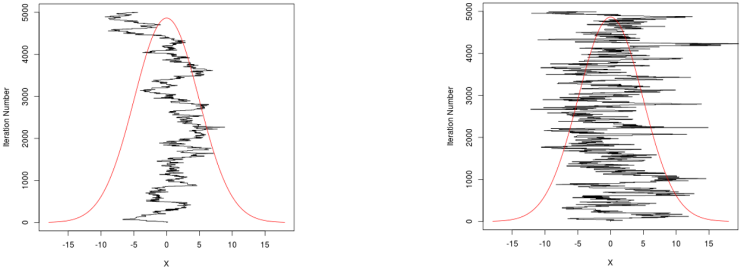
Adaptive Metropolis algorithm

- Optimal scaling is not the whole story for optimizing the RWM!
- Take target π to be a 20-dimensional $N(0, \Sigma)$ with highly irregular Σ.
- Both of these Metropolis-Hastings are optimally scaled to have acc rate ≈ 0.23



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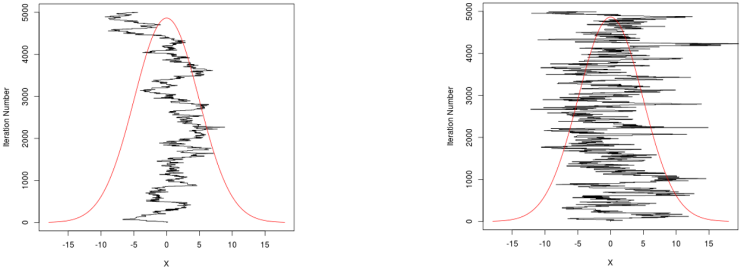

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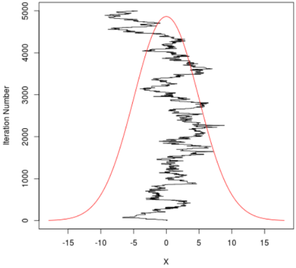

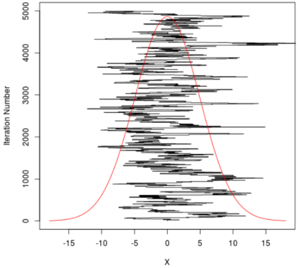

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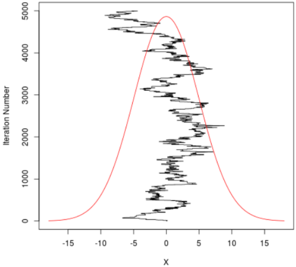

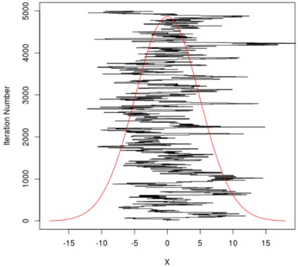

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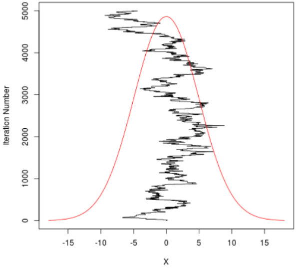

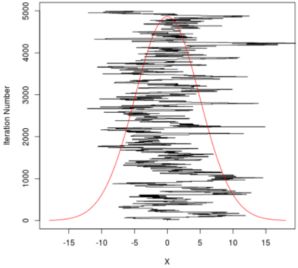

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- And if $\pi = N(0, \Sigma)$, is a $d-$dimensional Gaussian, then [RR01]

$$q_\theta = N(0, \frac{(2.38)^2}{d}\Sigma)$$

- Moreover, if wrong covariance matrix is used, i.e.

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  then the slowdown of the algorithm is given by the following inhomogeneity factor [RR01]

$$b = d\frac{\sum_{j=1}^d \lambda_j}{(\sum_{j=1}^d \lambda_j^{1/2})^2}$$

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- This suggests **we should estimate Σ on the fly** and gives rise to the Adaptive Metropolis algorithm [HST01]
- Σ_n - the covariance matrix used at time n is updated by an **iterative formula**.
- The AM version of [HST01] (the original one) uses

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  P_θ - Random Scan Gibbs Sampler with coordinate selection probabilities
  $$\theta = (\alpha_1, \ldots, \alpha_n)$$
- In each case values of θ will affect efficiency of P_θ

parametric family of transition kernels P_θ

- typically we can design a family of ergodic transition kernels P_θ, $\theta \in \Theta$.
- Ex 1a. $\Theta = R_+$
  P_θ - Random Walk Metropolis with proposal increments
  $$q_\theta = \theta N(0, Id)$$
- Ex 1b. $\Theta = R_+ \times \{d \text{ dimensional covariance matrices}\}$
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The typical Adaptive MCMC setting

- In a typical Adaptive MCMC setting the parameter space Θ is large
- there is an optimal $\theta_* \in \Theta$ s.t. P_{θ_*} converges quickly.
- there are arbitrary bad values in Θ, say if $\theta \in \bar{\Theta} - \Theta$ then P_θ is not ergodic.
- if $\theta \in \Theta_* :=$ a region close to θ_*, then P_θ shall inherit good convergence properties of P_{θ_*}.
- When using adaptive MCMC we hope θ_n will eventually find the region Θ_* and stay there essentially forever. And that the adaptive algorithm $\mathcal{A}$ will inherit the good convergence properties of Θ_* in the limit.
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You can actually run your Adaptive MCMC algorithm $\mathcal{A}$, and it will do what it is supposed to do! (under verifiable conditions)

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Adaptive Gibbs Sampler - a generic algorithm

- `AdapRSG`
  1. Set $p_n := R_n(p_{n-1}, X_{n-1}, \ldots, X_0) \in \mathcal{Y} \subset [0,1]^d$
  2. Choose coordinate $i \in \{1, \ldots, d\}$ according to selection probabilities p_n
  3. Draw $Y \sim \pi(\cdot | X_{n-1,-i})$
  4. Set $X_n := (X_{n-1,1}, \ldots, X_{n-1,i-1}, Y, X_{n-1,i+1}, \ldots, X_{n-1,d})$
- Given target distribution π, **what are the optimal selection probabilities** p?
- Similarly clean and operational criteria as in the Metropolis-Hastings case, are not available
- Little guidance in literature
- We need something that
  - has universal appeal,
  - is easy enough to compute and code,
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Adaptive Random Scan Metropolis within Gibbs

`AdapRSMwG`

1. Set $p_n := R_n(p_{n-1}, X_{n-1}, \ldots, X_0) \in \mathcal{Y}$
2. Choose coordinate $i \in \{1, \ldots, d\}$ according to selection probabilities p_n
3. Draw $Y \sim Q_{X_{n-1,-i}}(X_{n-1,i}, \cdot)$
4. With probability

$$\min\left(1, \quad \frac{\pi(Y|X_{n-1,-i})\; q_{X_{n-1,-i}}(Y, X_{n-1,i})}{\pi(X_{n-1}|X_{n-1,-i})\; q_{X_{n-1,-i}}(X_{n-1,i}, Y)}\right), \tag{1}$$

accept the proposal and set

$$X_n = (X_{n-1,1}, \ldots, X_{n-1,i-1}, Y, X_{n-1,i+1}, \ldots, X_{n-1,d})\,;$$

otherwise, reject the proposal and set $X_n = X_{n-1}$.

Adaptive RS adaptive Metropolis within Gibbs

AdapRSadapMwG

1. Set $p_n := R_n(p_{n-1}, X_{n-1}, \ldots, X_0, \gamma_{n-1}, \ldots, \gamma_0) \in \mathcal{Y}$
2. Set $\gamma_n := R'_n(\alpha_{n-1}, X_{n-1}, \ldots, X_0, \gamma_{n-1}, \ldots, \gamma_0) \in \Gamma_1 \times \ldots \times \Gamma_n$
3. Choose coordinate $i \in \{1, \ldots, d\}$ according to selection probabilities α, i.e. with $\Pr(i = j) = p_j$
4. Draw $Y \sim Q_{X_{n-1,-i}, \gamma_{n-1}}(X_{n-1,i}, \cdot)$
5. With probability (2),

$$\min\left(1, \quad \frac{\pi(Y|X_{n-1,-i})\, q_{X_{n-1,-i},\gamma_{n-1}}(Y, X_{n-1,i})}{\pi(X_{n-1}|X_{n-1,-i})\, q_{X_{n-1,-i},\gamma_{n-1}}(X_{n-1,i}, Y)}\right),$$

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Adapting the Gibbs Sampler: IF... IF...[CLR18a]

- If π was Gaussian...
- If we knew the covariance matrix Σ of π
- Then for $RSGS(p)$ and the target

$$\pi = N(\mu, \Sigma),$$

- we could compute the Spectral Gap (L_2-convergence rate) of RSGS(p) (building on Amit 1991, 1996 and Roberts and Sahu 1997)
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$$G(p) = \frac{1}{\lambda_{max}\Big(M(\Sigma, p)\Big)},$$

  where $M(\cdot,\cdot)$ is a known $d \times d$ matrix-valued function.
- So one could take

$$p^{opt} = \operatorname{argmax}_p G(p) \;=\; \operatorname*{argmin}_{p \in \Delta_{d-1}} \lambda_{max}\Big(M(\Sigma, p)\Big),$$

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- Gradient of G at p:
$$\nabla G(p) = F(\Sigma, p, x),$$
where F is a known $d-1$ dimensional vector-valued function and x is in the eigenspace of the maximal eigenvalue, i.e.
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Guidance from the Gaussian case

- We can use the guidance from the Gaussian case to optimise general posteriors
- Many posterior distributions in Bayesian inference will be close to Gaussians by the Bernstein-von Mieses Theorem
- We can estimate Σ_n on the fly.
- Solving

$$\text{argmax}_p \Big(G(p) \Big)$$

  is expensive and we can not afford a full solution after every update of Σ_n.
- In [CLR18a] a version of sub-gradient stochastic optimisation algorithm for convex functions is developed that progresses gradually stochastic optimisation as Σ_n stabilises.
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- $$\mathrm{Corr} = \begin{pmatrix} 1 & -\rho_1 & 0 & 0 & \cdots & 0 \\ -\rho_1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & -\rho_2 & \cdots & 0 \\ 0 & 0 & -\rho_2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & 1 & -\rho_k \\ 0 & \cdots & \cdots & 0 & -\rho_k & 1 \end{pmatrix}$$
- Speedup of up to $k = d/2$ times.

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Toy Example 2 - a star-like correlation structure

- $$\Sigma = \begin{pmatrix} 1 & c & c & c & \cdots & c \\ c & 1 & 0 & 0 & \cdots & 0 \\ c & 0 & 1 & 0 & \cdots & 0 \\ c & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ c & \cdots & \cdots & 0 & 1 & 0 \\ c & \cdots & \cdots & 0 & 0 & 1 \end{pmatrix}.$$
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Simulations

- Consider coordinate-wise RSGS in $d-$dimensions. Denote

$$h_i = \frac{x_i}{\sqrt{Var_\pi(x_i)}}$$

  to be normalized linear functions depending on one coordinate only.
- We will focus on the worst performing coordinate in the sense of CLT asymptotic variance

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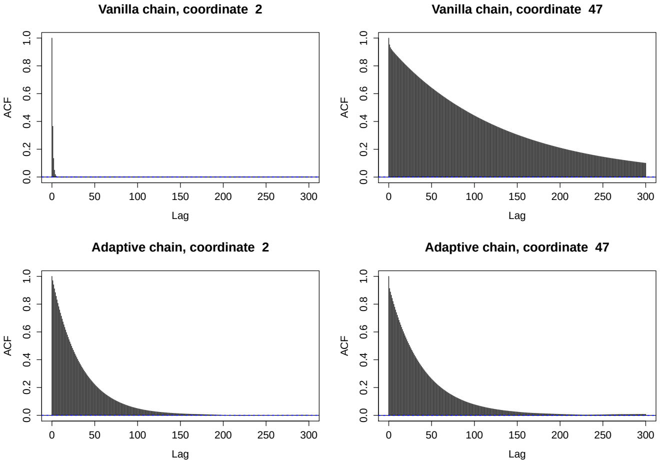
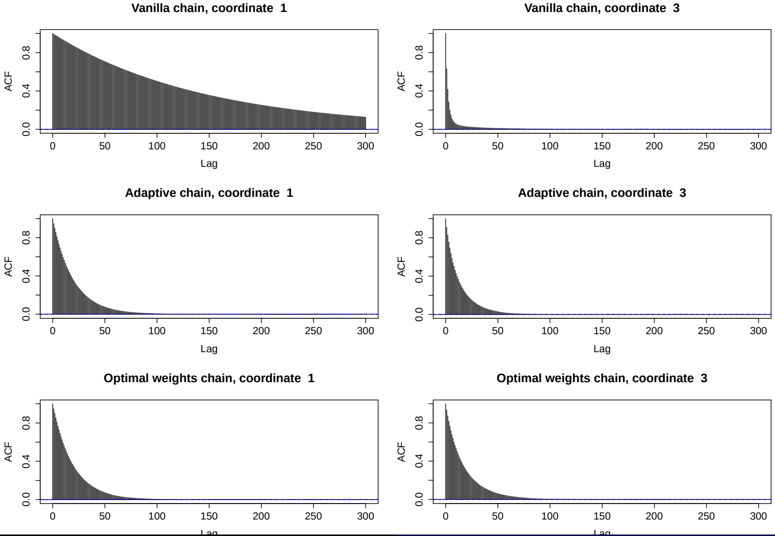
Truncated Multivariate Normals, d=50



Truncated Multivariate Normals, d=50

	$1/G(p)$	$\max_i \sigma^2_{as}(h_i)$
vanilla	6384	248
adaptive	1850	72
$\frac{\text{vanilla}}{\text{adaptive}}$	3.45	3.44

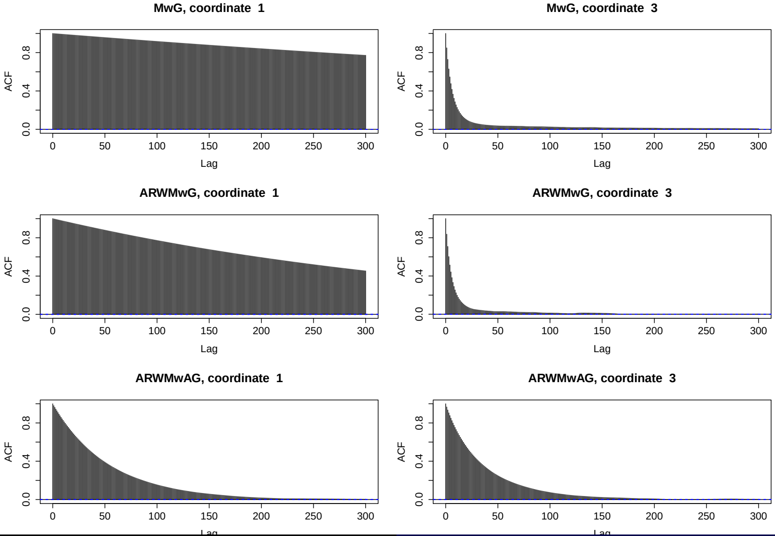
Poisson Hierarchical Model, d=50, Gibbs Sampler



Poisson Hierarchical Model, d=50, Gibbs Sampler

	$1/G(p)$	$\max_i \sigma^2_{as}(h_i)$
vanilla	13435	482
adaptive	1355	52
$\frac{\text{vanilla}}{\text{adaptive}}$	9.9	9.27

Poisson Hierarchical, d=50, Metropolis within Gibbs



Poisson Hierarchical, d=50, Metropolis within Gibbs

	$1/G(p)$	$\max_i \sigma^2_{as}(h_i)$
RWMwG (vanilla)	13244	1993
ARWMwG (partially adaptive)	13244	971
ARWMwAG (adaptive)	1376	138
$\frac{\text{partially adaptive}}{\text{adaptive}}$	9.63	7
$\frac{\text{vanilla}}{\text{adaptive}}$	9.63	14.45

Computational cost for the Poisson Hierarchical Model

	$\max_i \sigma_{as}^2(h_i)$	Cost per 5000 iterations	Cost of adaptation
ARSGS	52	0.37	0.0025
ARWMwAG	138	0.028	0.0025

Summary of Adaptive Gibbs

- The Adaptive Gibbs Sampler uses a principled optimisation strategy based on the Gaussian model and the Spectral Gap to guide adaptation
- ARSGS and ARWMwAG are useful even if the target is not normal or even not continuous
- [CLR18a] provides full implementations of the algorithms that can be readily used in applications
- Adaptation can be done in parallel with the sampling (and it is only a fraction of the sampling cost anyway)
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Variable selection setting

- $$y = \alpha\mathbf{1} + X_\gamma\beta_\gamma + \epsilon, \qquad \epsilon \sim N(0, \sigma^2 I_n)$$
  where y is an $(n \times 1)$-dimensional vector of responses, $X = (x_1, \ldots, x_p)$ is an $(n \times p)$-dimensional data matrix and $\gamma = (\gamma_1, \ldots, \gamma_p) \in \Gamma = \{0, 1\}^p$ is a vector of indicator variables in which γ_i denotes whether the i-th variable is included in the model (when $\gamma_i = 1$).
- Bayesian variable selection involves placing a prior on the parameters of the regression model above, $(\alpha, \beta_\gamma, \sigma^2)$, as well as on the model γ.
- Sampling from the posterior model space is often difficult (exponential growth)
- Has been addressed via adaptive MCMC in a number of papers [NK05, JS13, CGL11].
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The individual adaptation algorithm [GLS17]

- The probability of proposing to move from model γ to γ' is given in a product form

$$q_\eta(\gamma, \gamma') = \prod_{j=1}^{p} q_{\eta,j}(\gamma_j, \gamma_j')$$

  where $\eta = (A, D) = (A_1, \dots, A_p, D_1, \dots, D_p)$,
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Synthetic data example

- Consider the synthetic data example analysed in [YWJ16]
- The speedup over the vanilla sampler of [YWJ16] is as follows

		5 chains				25 chains			
		SNR				SNR			
(n, p)		0.5	1	2	3	0.5	1	2	3
(500, 500)	IA	4.9	1.8	5.5	5.1	1.2	1.5	2.4	2.3
	ASI	1.7	21.3	31.8	7.5	2.0	36.0	42.7	12.6
(500, 5000)	IA	8.7	2.2	718.0	81.5	7.1	2.9	2267.2	147.2
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(1000, 5000)	IA	2.2	2.2	9167.2	11.3	5.6	2.5	15960.7	199.8
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- adaptive MCMC algorithms learn about π on the fly and use this information during the simulation
- the transition kernel P_n used for obtaining $X_n|X_{n-1}$ is allowed to depend on $\{X_0, \ldots, X_{n-1}\}$
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ergodicity: a toy counterexample

- Let $\mathcal{X} = \{0, 1\}$ and π be uniform.
- $$P_1 = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} \quad \text{and} \quad P_2 = (1-\varepsilon)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \varepsilon P_1 \quad \text{for some} \quad \varepsilon > 0.$$
- π is the stationary distribution for both, P_1 and P_2.
- Consider X_n , evolving for $n \geq 1$ according to the following adaptive kernel:
$$Q_n = \begin{cases} P_1 & \text{if} \quad X_{n-1} = 0 \\ P_2 & \text{if} \quad X_{n-1} = 1 \end{cases}$$
- Note that after two consecutive 1 the adaptive process X_n is trapped in 1 and can escape only with probability ε.
- Let $\bar{q}_1 := \lim_{n\to\infty} P(X_n = 1)$ and $\bar{q}_0 := \lim_{n\to\infty} P(X_n = 0)$.
- Now it is clear, that for small ε we will have $\bar{q}_1 \gg \bar{q}_0$ and the procedure fails to give the expected asymptotic distribution.

Adaptive Gibbs sampler - a generic algorithm

AdapRSG

1. Set $\alpha_n := R_n(\alpha_{n-1}, X_{n-1}, \dots, X_0) \in \mathcal{Y} \subset [0,1]^d$
2. Choose coordinate $i \in \{1, \dots, d\}$ according to selection probabilities α_n
3. Draw $Y \sim \pi(\cdot|X_{n-1,-i})$
4. Set $X_n := (X_{n-1,1}, \dots, X_{n-1,i-1}, Y, X_{n-1,i+1}, \dots, X_{n-1,d})$

- It is easy to get tricked into thinking that if step 1 is not doing anything "crazy" then the algorithm must be ergodic.
- Theorem 2.1 of [LC06] states that ergodicity of adaptive Gibbs samplers follows from the following two conditions:
  - (i) $\alpha_n \to \alpha$ a.s. for some fixed $\alpha \in (0,1)^d$; and
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- The above theorem is simple, neat and wrong.

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a cautionary example that disproves [LC06]

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- with target distribution given by $\pi(i,j) \propto j^{-2}$
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  for some choice of the sequence $(a_n)_{n=0}^{\infty}$ satisfying $8 < a_n \nearrow \infty$
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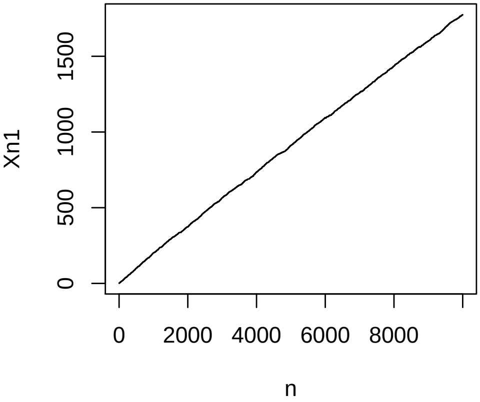

Ergodicity of an adaptive algorithm - framework

- $\mathcal{X}$ valued process of interest X_n
- Θ valued random parameter θ_n
  representing the choice of kernel when updating X_n to X_{n+1}
- Define the filtration generated by $\{(X_n, \theta_n)\}$

$$\mathcal{G}_n = \sigma(X_0, \ldots, X_n, \theta_0, \ldots, \theta_n),$$

- Thus

$$P(X_{n+1} \in B \mid X_n = x, \theta_n = \theta, \mathcal{G}_{n-1}) = P_\theta(x, B)$$

- The distribution of θ_{n+1} given $\mathcal{G}_n$ depends on the algorithm.
- Define

$$A^{(n)}(x, \theta, B) = P(X_n \in B \,\|\, X_0 = x, \theta_0 = \theta)$$
$$T(x, \theta, n) = \|A^{(n)}(x, \theta, \cdot) - \pi(\cdot)\|_{TV}$$

- We say the adaptive algorithm is ergodic if

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- The family $\{P_\gamma : \gamma \in \mathcal{Y}\}$ is Simultaneously Geometrically Ergodic if
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Adaptive random scan Metropolis within Gibbs

`AdapRSMwG`

1. Set $\alpha_n := R_n(\alpha_{n-1}, X_{n-1}, \dots, X_0) \in \mathcal{Y}$
2. Choose coordinate $i \in \{1, \dots, d\}$ according to selection probabilities α_n
3. Draw $Y \sim Q_{X_{n-1,-i}}(X_{n-1,i}, \cdot)$
4. With probability

$$\min\left(1, \quad \frac{\pi(Y|X_{n-1,-i})\, q_{X_{n-1,-i}}(Y, X_{n-1,i})}{\pi(X_{n-1}|X_{n-1,-i})\, q_{X_{n-1,-i}}(X_{n-1,i}, Y)}\right), \tag{2}$$

accept the proposal and set

$$X_n = (X_{n-1,1}, \dots, X_{n-1,i-1}, Y, X_{n-1,i+1}, \dots, X_{n-1,d});$$

otherwise, reject the proposal and set $X_n = X_{n-1}$.

Adaptive random scan adaptive Metropolis within Gibbs

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2. Set $\gamma_n := R'_n(\alpha_{n-1}, X_{n-1}, \ldots, X_0, \gamma_{n-1}, \ldots, \gamma_0) \in \Gamma_1 \times \ldots \times \Gamma_n$
3. Choose coordinate $i \in \{1, \ldots, d\}$ according to selection probabilities α, i.e. with $\Pr(i = j) = \alpha_j$
4. Draw $Y \sim Q_{X_{n-1,-i},\gamma_{n-1}}(X_{n-1,i}, \cdot)$
5. With probability (2),

$$\min\left(1, \ \frac{\pi(Y|X_{n-1,-i})\, q_{X_{n-1,-i},\gamma_{n-1}}(Y, X_{n-1,i})}{\pi(X_{n-1}|X_{n-1,-i})\, q_{X_{n-1,-i},\gamma_{n-1}}(X_{n-1,i}, Y)}\right),$$

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- Assuming that `RSG(`β`)` is uniformly ergodic and $|\alpha_n - \alpha_{n-1}| \to 0$, we can prove ergodicity of
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- Recall the Adaptive Metropolis Algorithm with proposals

$$Y_{n+1} \sim q_{\sigma_n}(X_n, \cdot) = X_n + N(0, \Sigma_n),$$

- The theory suggests increment

$$N(0, (2.38)^2 \Sigma_n / d)$$

- The AM version of [HST01] (the original one) uses

$$N(0, \Sigma_n + \varepsilon Id)$$

- Modification due to [RR09] is to use

$$Q_n = (1-\beta) N(0, (2.38)^2 \Sigma_n / d) + \beta N(0, \varepsilon Id / d).$$

- the above modification appears more tractable: containment has been verified for both, exponentially and super-exponentially decaying tails (Bai et al 2009).
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a new class: `AdapFail` Algorithms

- an adaptive algorithm $\mathcal{A} \in$ `AdapFail`, if with positive probability, it is asymptotically less efficient then ANY MCMC algorithm with fixed θ.
- more formally, `AdapFail` can be defined e.g. as follows: $\mathcal{A} \in$ `AdapFail`, if

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$$\forall_{\epsilon_* > 0}, \quad \exists_{0<\epsilon<\epsilon_*}, \quad \text{s.t.} \quad \lim_{K\to\infty} \inf_{\theta\in\Theta} \lim_{n\to\infty} P\Big(M_\epsilon(X_n, \theta_n) > K M_\epsilon(\tilde{X}_n, \theta)\Big) > 0\,,$$

  where $\{\tilde{X}_n\}$ is a Markov chain independent of $\{X_n\}$, which follows the fixed kernel P_θ.
- Lemma [ŁR14]:If containment doesn't hold for $\mathcal{A}$ then $\mathcal{A} \in$ AdapFail.

The fly in the ointment

- Theoretical properties of adaptive MCMC have been studied using a range of techniques, such as: coupling, martingale approximations, stability of stochastic approximation (Roberts, Rosenthal, Moulines, Andrieu, Vihola, Saksman, Fort, Atchade, ...)
- Still, the theoretical underpinning of Adaptive MCMC is (even) weaker and (even) less operational than that of standard MCMC
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AirMCMC - Adapting increasingly rarely [CLR18b]

- $P_\gamma, \gamma \in \Gamma$ - a parametric family of π-invariant kernels;
  Adaptive MCMC steps:
  (1) Sample X_{n+1} from $P_{\gamma^n}(X_n, \cdot)$.
  (2) Given $\{X_0, .., X_{n+1}, \gamma^0, .., \gamma^n\}$ update γ^{n+1} according to some adaptation rule.
- How tweak the strategy to make theory easier?
- Do we need to adapt in every step?
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- **AirMCMC Sampler** [CLR18b]
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- Will such a strategy be efficient? With say $n_k = ck^\beta$
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AirMCMC - a simulation study

- $\pi(x) = \frac{l(|x|)}{|x|^{1+r}},\ x \in \mathbb{R},$
- Air version of RWM adaptive scaling
- The example is polynomially ergodic (not easy for the sampler)
- **AirRWM**
  Initiate $X_0 \in \mathbb{R}$, $\overline{\gamma} \in [q_1, q_2]$. $k := 1$, $n := 0$, a sequence $\{c_k\}_{k \geq 1}$.
  (1) For $i = 1, .., n_k$
    (1.1.) sample $Y \sim N(X_{n+i-1}, \overline{\gamma})$, $a_{\overline{\gamma}} := \frac{\phi(Y)}{\phi(X_{n+i-1})}$;
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    (1.3.) $a := a + a_{\overline{\gamma}}$.
    If $i = n_k$ then
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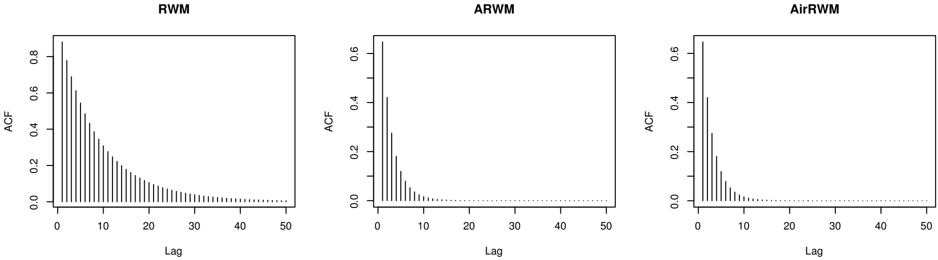


Figure: Autocorrelations (ACF)

AirMCMC - a simulation study

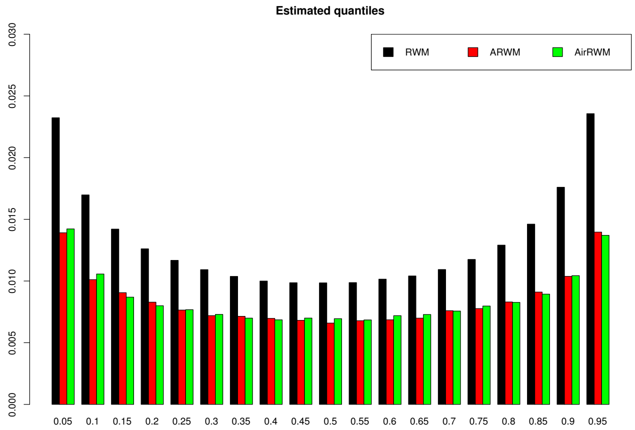
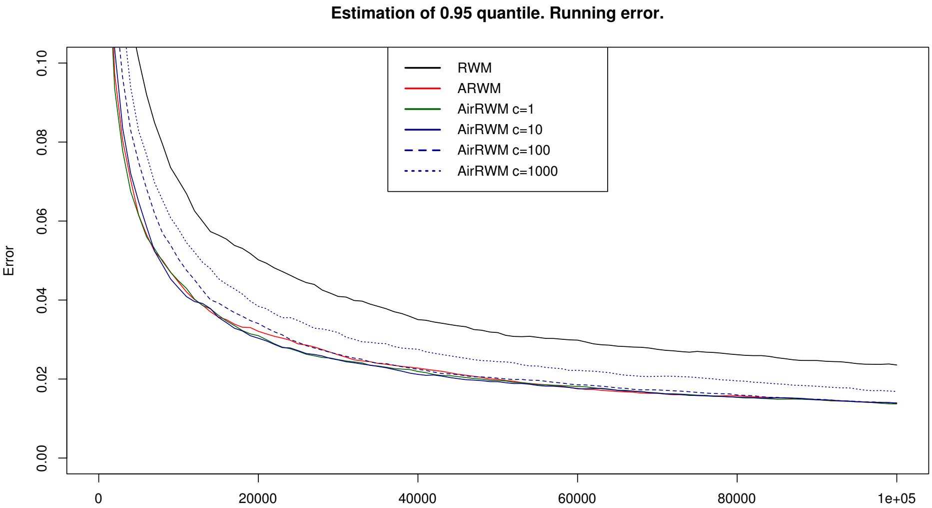
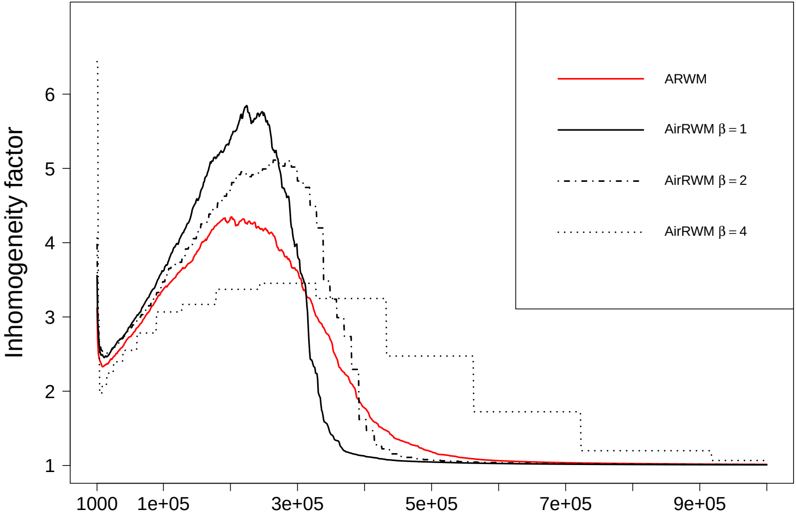


Figure: Error in quantile levels estimation. X-axis – quantile levels. Y-axis – error in

AirMCMC - a simulation study



AirMCMC - inhomogeneity factor, d=100



AirMCMC - simulation effort, d=100

Table 1: Time to obtain 1 million samples

	ARWM	AirRWM $\beta = 1$	AirRWM $\beta = 2$	AirRWM $\beta = 4$
Time (seconds)	507.6	90.5	86.9	80.2

AirMCMC theory

- **Theorem 1**
  - Kernels Simultaneously Geometrically Ergodic (SGE)
  - $n_k \geq ck^{\beta}, \quad \beta > 0$
  - $\sup \frac{|f(x)|}{V^{1/2}(x)} < \infty$

  Then
  - WLLN
  - if $\beta > 0$, also SLLN
  - if $\beta \geq 1$, also $MSE = \mathcal{O}(1/n)$
  - if $\beta > 1$ and a bit more regularity, also CLT holds!
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- Counterparts of this theorem also for
  - Kernels locally SGE
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