Markov Chain Monte Carlo: design and optimisation

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Prior-posterior: the usual MCMC setting

- let π be a target probability distribution on Θ, typically arising as a posterior distribution in Bayesian inference,
- in Bayesian Statistics we typically consider a model $\mathcal{M}(\theta)$, parametrised by $\theta \in \Theta$
- there is a prior distribution $p(\theta)$ on Θ. It can be chosen to:
- 1. convey prior information or belief about values of θ
  2. be uninformative
  3. facilitate computations and consequently enable inference
- there is data y that has likellihood $l(\theta) = l(\theta|y)$ under model $\mathcal{M}(\theta)$
- the posterior distribution $\pi(\theta)$ arises from the Bayes formula as

$$\pi(\theta) = \pi(\theta|y) := \frac{p(\theta)l(\theta|y)}{\int_\Theta p(\theta)l(\theta|y)d\theta} \propto p(\theta)l(\theta)$$

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Example: a diffusion model

- Consider a diffusion model $\mathcal{M}(\theta)$ where $\theta = (\mu, \sigma)$:

$$dX_t = \mu dt + \sigma dB_t$$

  observed at discrete time points $(t_0, t_1, \dots, t_N)$ as $(x_{t_0}, x_{t_1}, \dots, x_{t_N})$
- The likelihood function is

$$l(\theta|x_{t_0}, x_{t_1}, \dots, x_{t_N}) = \prod_{i=1}^{N} l(\theta|x_{t_i}, x_{t_{i-1}}) = \prod_{i=1}^{N} \phi_{N(\mu(t_i - t_{i-1}), \sigma^2(t_i - t_{i-1}))}(x_{t_i} - x_{t_{i-1}}).$$

- This posterior $\pi(\theta)$ summarises uncertainty about the parameter $\theta \in \Theta$ and is used for all inferential questions like credible sets, decision making, prediction, model choice, etc.
- In the diffusion example predicting the value of the diffusion at time $t > t_N$ would amount to repeating the following steps:
  1. sample from the posterior $\theta = (\mu, \sigma) \sim \pi(\theta)$
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the MAP estimator

- One of the classical estimation tasks is to compute the Maximum a Posteriori Estimator (MAP), say θ_{MAP}.
- $$\theta_{MAP} := \text{argmax}_\theta \pi(\theta) = \text{argmax}_\theta \left\{ p(\theta) l(\theta | y_1, \dots, y_n) \right\}$$
- Computing θ_{MAP} may be nontrivial, especially if $\pi(\theta)$ is multimodal.
- There are specialised algorithms for doing this.
- Some non-bayesian statistical inference approaches can be rewritten as bayesian MAP estimators (for example the LASSO).

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the Bayesian estimator

- Bayesian estimator is an estimator that minimizes the posterior expected value of a loss function.
- The loss function
$$L(\cdot,\cdot) : \Theta \times \Theta \to \mathbb{R}$$
- After seeing data $(y_1, \ldots, y_n)$ we choose an estimator $\hat{\theta}(y_1, \ldots, y_n)$
- Its expected loss is
$$\begin{aligned}\mathbb{E}L(\theta, \hat{\theta}(y_1, \ldots, y_n)) &= \int_{\mathbb{Y}^n \times \Theta} L(\theta, \hat{\theta}(y_1, \ldots, y_n)) m(y_1, \ldots, y_n|\theta) p(\theta) \\ &= \int_{\mathbb{Y}^n \times \Theta} L(\theta, \hat{\theta}(y_1, \ldots, y_n)) \pi(\theta) p(dy)\end{aligned}$$
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- $\hat{\theta}(y_1,\ldots,y_n)$ is a Bayesian estimator if it minimizes the above expected loss.

the Bayesian estimator and computing integrals

- The most common choice is the quadratic loss function

$$L(\theta_1, \theta_2) = (\theta_1 - \theta_2)^2$$

- in which case

$$\hat{\theta}(y_1, \dots, y_n) = \mathbb{E}_\pi \theta$$

  so it is the posterior mean.
- So computing the Bayesian estimator is computing the integral wrt the posterior

$$\int_\Theta \theta \pi(\theta)$$

- Similarly answering other inferential questions like credible sets, posterior variance etc involve computing integrals of the form

$$\int_\Theta f(\theta)\pi(\theta).$$

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The MCMC estimator

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

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Asymptotic validity

- $$\hat{I} := \frac{1}{n}\sum_{k=t}^{t+n} f(X_k) \qquad I := \int_{\mathcal{X}} f(x)\pi(dx).$$
- **SLLN** for Markov chains holds under very mild conditions
- **CLT** for Markov chains holds under some additional assumptions:
  - a mixing condition on P
  - an integrability condition for f

  and is verifiable in many situations of interest
- **CLT**
  $$n^{1/2}(\hat{I} - I) \to N\big(0, \sigma_{\text{as}}(f, P)\big)$$
- Usually $\sigma_{\text{as}}(f, P) >> Var_{\pi}(f)$

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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 $\mathcal{X} \times \mathcal{X}$
- **Lemma.** If P is reversible with respect to π then $\pi P = \pi$, so it is also stationary.

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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
- For the **Random Walk Metropolis** $Y_{n+1} \sim Q(X_n, \cdot) = N(X_n, \Sigma)$ often $\Sigma = \sigma I$

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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 $X_{n+1} = X_n$
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The Gibbs Sampler - exploits conditional distributions

- For $\Theta = \Theta_1 \times \Theta_2 \times \cdots \times \Theta_d$
- denote the marginals of π as
$$\pi(\theta_k|\theta_{-k})$$
where
$$\theta_{-k} = (\theta_1, \dots, \theta_{k-1}, \theta_{k+1}, \dots, \theta_d)$$
- The Gibbs sampler algorithms iterates between updates of
$$\theta_i|\theta_{-i} \sim \pi(\theta_i|\theta_{-i})$$
- There are two basic coordinate selection strategies:
- (1) in each step pick a coordinate at random (Random Scan Gibbs Sampler)
- (2) Update systematically one after another (Systematic Scan Gibbs Sampler)
- If sampling directly from $\sim \pi(\theta_i|\theta_{-i})$ is not possible or not practical, one can design P_i that admits $\sim \pi(\theta_i|\theta_{-i})$ as its invariant distribution. This is called Metropolis within Gibbs

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The MALA Algorithm

- Is based on the $\pi-$limiting Langevin diffusion

$$dX_t = \frac{1}{2}\nabla \log \pi(X_t)dt + dB_t$$

- Euler discretisation of this diffusion suggests the Metropolis-Hastings proposal

$$q(\cdot|X_{(n-1)}) := X_{(n-1)} + \frac{h}{2}\nabla \log \pi(X_{(n-1)}) + h^{1/2}N(0, I_{d\times d})$$

  with the usual accept-reject formula
- MALA works well for "nice" examples, but is unstable for light-tailed π.
- Manifold MALA is based on

$$\begin{aligned} dX_t &= \left(\frac{\sigma(X_t)}{2}\nabla \log \pi(X_t) + \frac{\gamma(X_t)}{2}\right)dt + \sqrt{\sigma}(X_t)dB_t \\ \gamma_i(\theta_t) &= \sum_j \frac{\partial \sigma_{ij}(\theta_t)}{\partial \theta_j}, \end{aligned}$$

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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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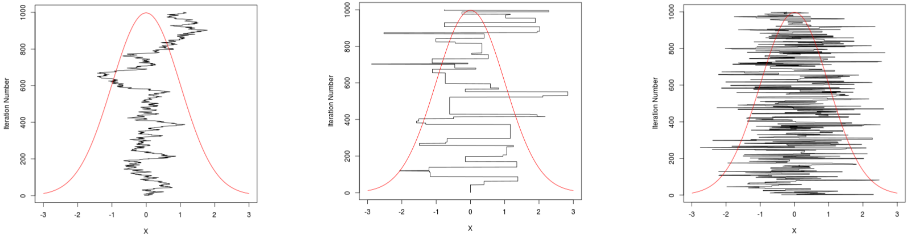
Adaptive MCMC in 3 minutes (3 examples)

- 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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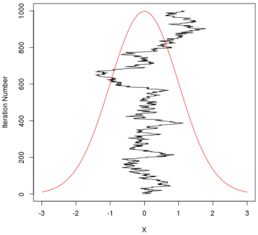

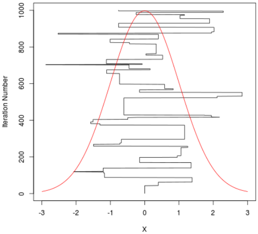

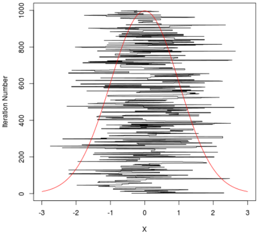

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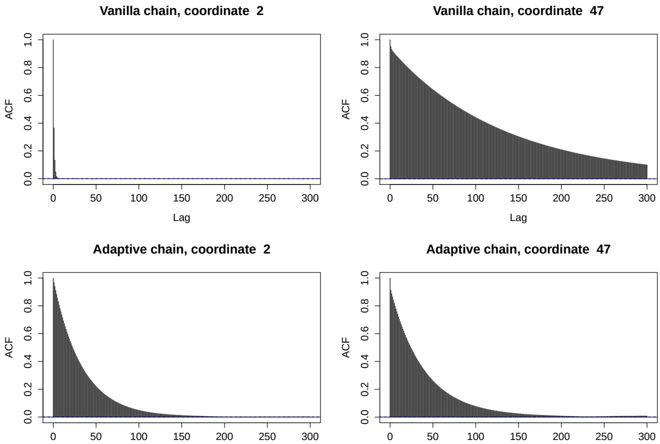
- Random Scan Gibbs Sampler for 50d Truncated Multivariate Normals
  Are uniform $1/d$ selection probabilities optimal?



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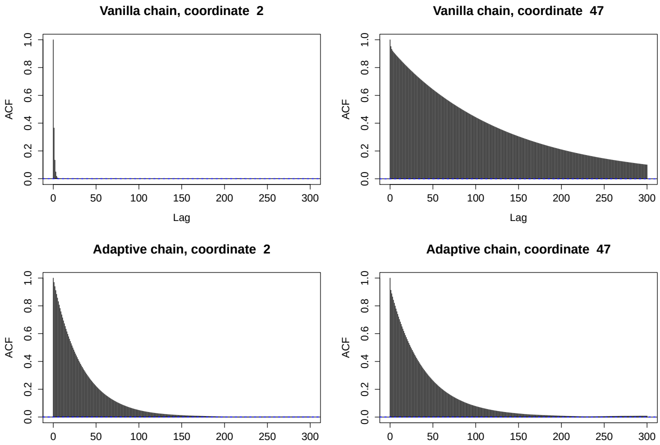
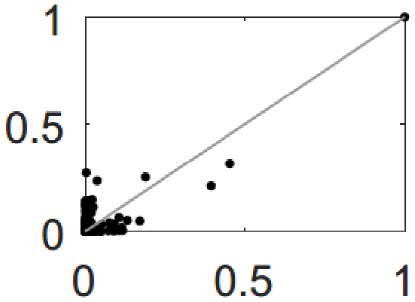
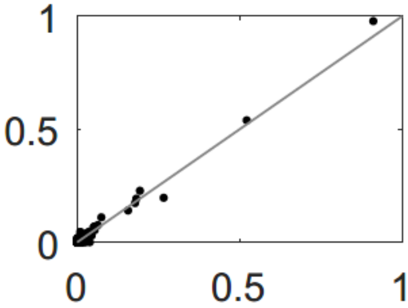


Adaptive MCMC in 3 minutes (3 examples)

- 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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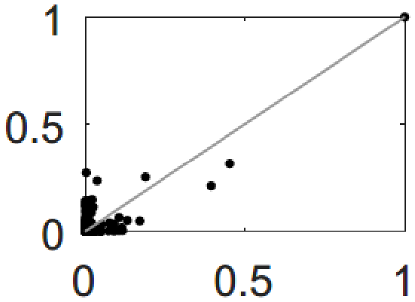

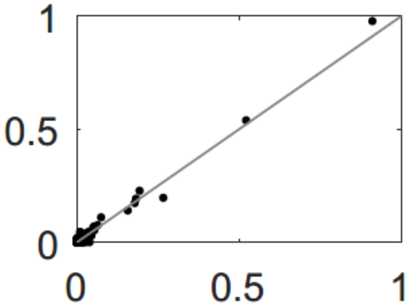

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Adaptive MCMC in 5 minutes (ingredients that we need)

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

- **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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- 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

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 $\mathcal{X} \times \mathcal{X}$

- **Lemma.** If P is reversible with respect to π then $\pi P = \pi$, so it is also stationary.

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

- Under mild assumptions on Q the algorithm is ergodic.
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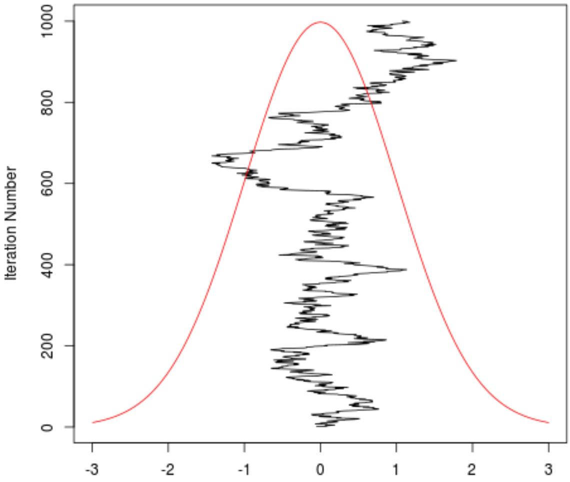

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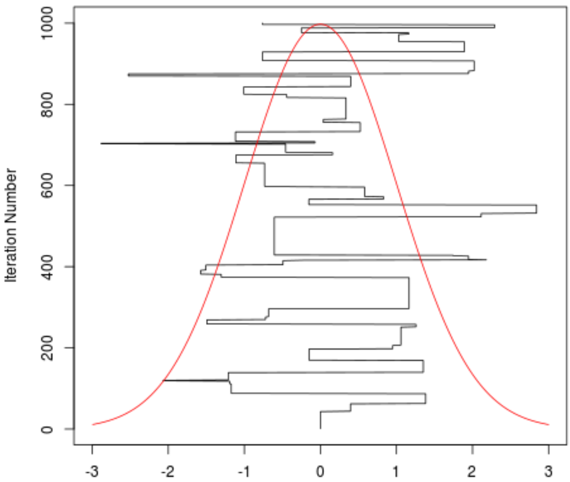

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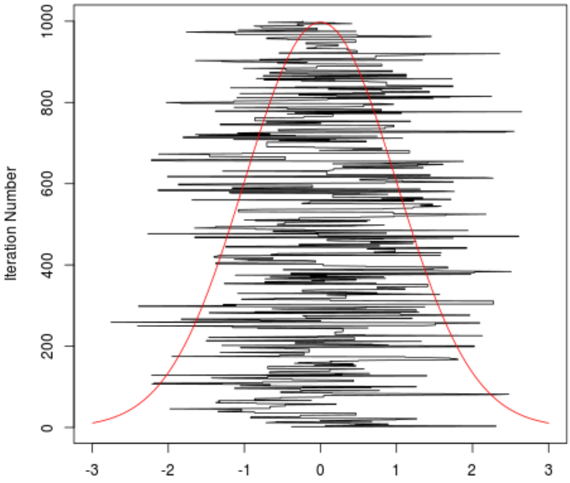

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- maximising the speed $h(l)$ yields the optimal acceptance rate

$$A(l) = 0.234$$

  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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- take Random Walk Metropolis with proposal increments
- $$Y_{n+1} \sim q_\sigma(X_n, \cdot) = X_n + \sigma N(0, Id).$$
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$$\bar{\alpha} := \int \int \alpha(x,y) q_\sigma(x, dy)\pi(dx)$$
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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- 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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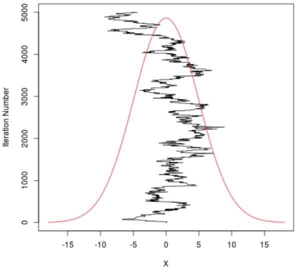
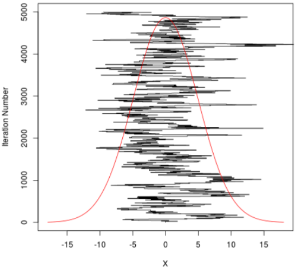
- Every optimal scaling result can be used to design an adaptive version of the algorithm!

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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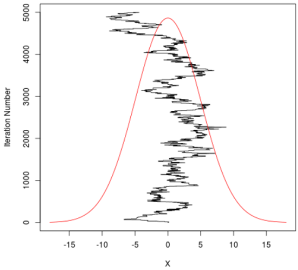

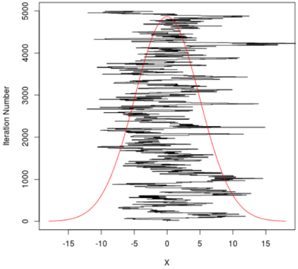

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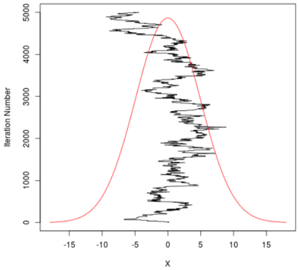

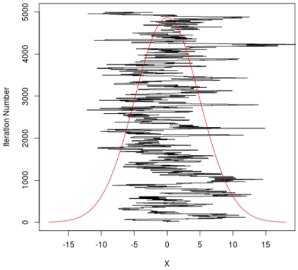

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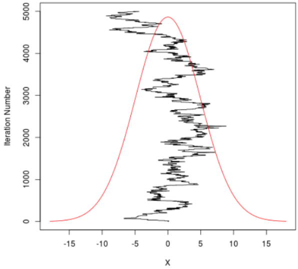

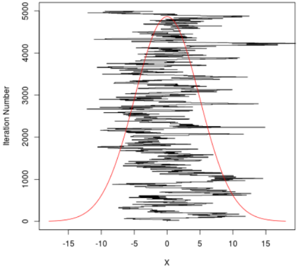

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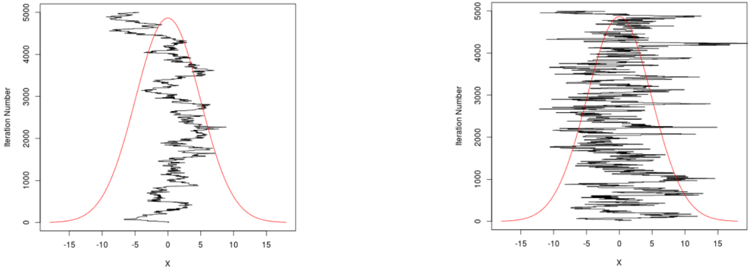

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- And if $\pi = N(0, \Sigma)$, is a $d-$dimensional Gaussian, then [RR01]

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

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

$$q_\theta = \sigma N(0, \tilde{\Sigma})$$

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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  $$q_\theta = \theta N(0, Id)$$
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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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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),

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

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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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$$\nabla G(p) = F(\Sigma, p, x),$$
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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
$$\mathrm{argmax}_p \Big(G(p) \Big)$$
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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Toy Example 1 - a difficult pair

- $$\mathrm{Corr} = \begin{pmatrix} 1 & -\rho_1 & 0 & 0 & \cdots & 0 \\ -\rho_1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & -\rho_2 & \cdots & 0 \\ 0 & 0 & -\rho_2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & 1 & -\rho_k \\ 0 & \cdots & \cdots & 0 & -\rho_k & 1 \end{pmatrix}$$
- 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

$$\max_i \sigma^2_{as}(h_i)$$

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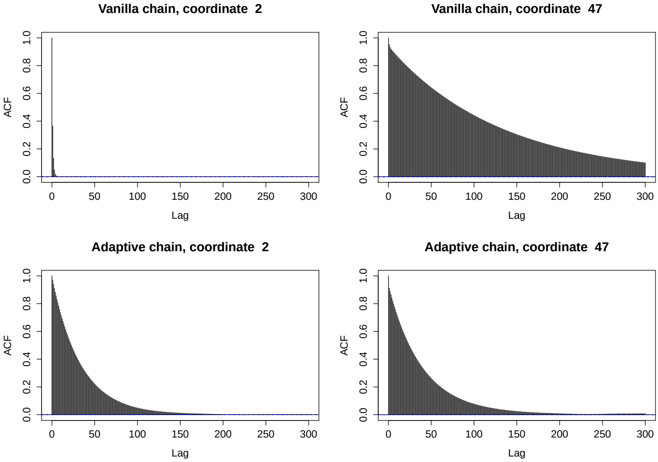
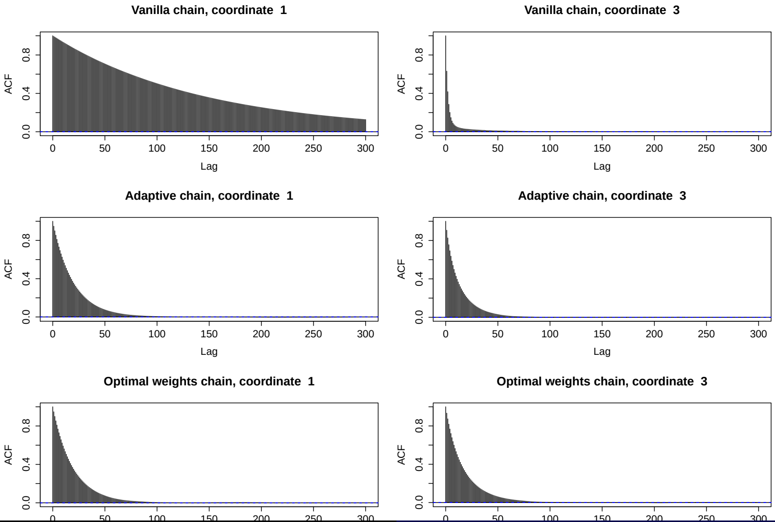
Truncated Multivariate Normals, d=50



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

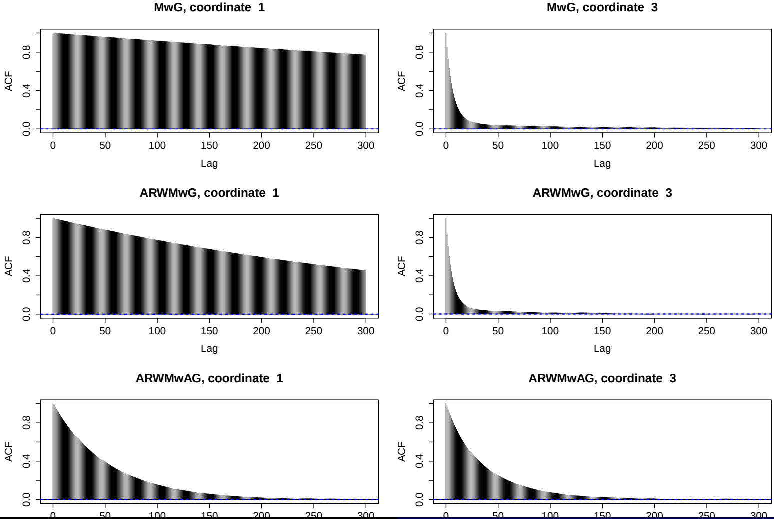
Poisson Hierarchical Model, d=50, Gibbs Sampler



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

	$\max_i \sigma^2_{as}(h_i)$	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].
- Briefly talk about [GLS17]

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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 $\eta = (A, D) = (A_1, \ldots, A_p, D_1, \ldots, D_p)$,
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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
	ASI	29.9	126.9	2053.1	2271.3	53.5	353.3	12319.5	7612.3
(1000, 500)	IA	5.9	16.3	7.7	4.2	1.6	80.7	4.4	1.8
	ASI	41.9	2.1	16.9	12.0	32.8	34.0	27.9	14.4
(1000, 5000)	IA	2.2	2.2	9167.2	11.3	5.6	2.5	15960.7	199.8
	ASI	15.4	37.0	4423.1	30.8	54.9	53.4	11558.2	736.4

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	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
	ASI	29.9	126.9	2053.1	2271.3	53.5	353.3	12319.5	7612.3
(1000, 500)	IA	5.9	16.3	7.7	4.2	1.6	80.7	4.4	1.8
	ASI	41.9	2.1	16.9	12.0	32.8	34.0	27.9	14.4
(1000, 5000)	IA	2.2	2.2	9167.2	11.3	5.6	2.5	15960.7	199.8
	ASI	15.4	37.0	4423.1	30.8	54.9	53.4	11558.2	736.4

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
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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
  - (ii) The random scan Gibbs sampler with fixed selection probabilities α induces an ergodic Markov chain with stationary distribution π.
- The above theorem is simple, neat and wrong.

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a cautionary example that disproves [LC06]

- Let $\mathcal{X} = \{(i,j) \in \mathbb{N} \times \mathbb{N} : i = j \text{ or } i = j+1\}$,
- with target distribution given by $\pi(i,j) \propto j^{-2}$
- consider a class of adaptive random scan Gibbs samplers with update rule given by:

$$R_n\Big(\alpha_{n-1}, X_{n-1} = (i,j)\Big) = \begin{cases} \left\{\frac{1}{2} + \frac{4}{a_n}, \frac{1}{2} - \frac{4}{a_n}\right\} & \text{if} \quad i = j, \\ \left\{\frac{1}{2} - \frac{4}{a_n}, \frac{1}{2} + \frac{4}{a_n}\right\} & \text{if} \quad i = j+1, \end{cases}$$

  for some choice of the sequence $(a_n)_{n=0}^{\infty}$ satisfying $8 < a_n \nearrow \infty$
- if $a_n \to \infty$ slowly enough, then X_n is **transient** with positive probability, i.e. $\mathbb{P}(X_{1,n} \to \infty) > 0$.

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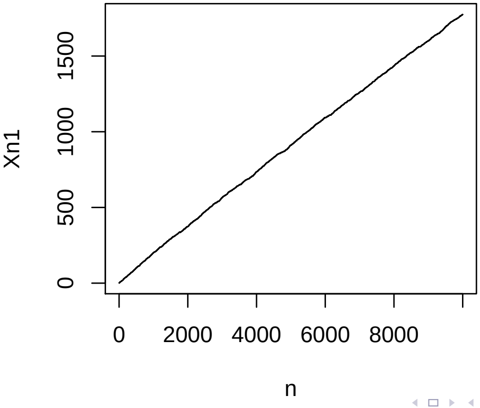

Ergodicity of an adaptive algorithm - framework

- $\mathcal{X}$ 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

$$\lim_{n\to\infty} T(x, \theta, n) = 0 \qquad \text{for all } x \in \mathcal{X} \quad \text{and } \theta \in \Theta.$$

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Tools for establishing ergodicity

- **(Diminishing Adaptation)** Let $D_n = \sup_{x\in\mathcal{X}} \|P_{\Gamma_{n+1}}(x,\cdot) - P_{\Gamma_n}(x,\cdot)\|$ and assume $\lim_{n\to\infty} D_n = 0$ in probability
- **(Simultaneous uniform ergodicity)** For all $\varepsilon > 0$, there exists $N = N(\varepsilon)$ s.t. $\|P^N_\gamma(x,\cdot) - \pi(\cdot)\| \leq \varepsilon$ for all $x \in \mathcal{X}$ and $\gamma \in \mathcal{Y}$
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Tools for establishing ergodicity

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- **(Simultaneous uniform ergodicity)** For all $\varepsilon > 0$, there exists $N = N(\varepsilon)$ s.t. $\|P_\gamma^N(x,\cdot) - \pi(\cdot)\| \leq \varepsilon$ for all $x \in \mathcal{X}$ and $\gamma \in \mathcal{Y}$
- **(Containment condition)** Let $M_\varepsilon(x,\gamma) = \inf\{n \geq 1 : \|P_\gamma^n(x,\cdot) - \pi(\cdot)\| \leq \varepsilon\}$ and assume $\{M_\varepsilon(X_n,\gamma_n)\}_{n=0}^\infty$ is bounded in probability, i.e. given $X_0 = x_*$ and $\Gamma_0 = \gamma_*$, for all $\delta > 0$, there exists N s.t. $\mathbb{P}[M_\varepsilon(X_n,\Gamma_n) \leq N | X_0 = x_*, \Gamma_0 = \gamma_*] \geq 1-\delta$ for all $n \in \mathbb{N}$.

Theorem (Roberts Rosenthal 2007)

(diminishing adaptation) $+$ *(simultaneous uniform ergodicity)* $\Rightarrow$ *ergodicity.*

Theorem (Roberts Rosenthal 2007)

(diminishing adaptation) $+$ *(containment)* $\Rightarrow$ *ergodicity.*

Containment: a closer look

- **(Containment condition)** $M_\varepsilon(x,\gamma) = \inf\{n \geq 1 : \|P^n_\gamma(x,\cdot) - \pi(\cdot)\| \leq \varepsilon\}$
  given $X_0 = x_*$ and $\Gamma_0 = \gamma_*$, for all $\delta > 0$,
  there exists N s.t. $\mathbb{P}[M_\varepsilon(X_n,\Gamma_n) \leq N | X_0 = x_*, \Gamma_0 = \gamma_*] \geq 1 - \delta$ for all $n \in \mathbb{N}$.
- Containment can be verified using simultaneous geometrical ergodicity or simultaneous polynomial ergodicity. (details in [BRR10])
- The family $\{P_\gamma : \gamma \in \mathcal{Y}\}$ is Simultaneously Geometrically Ergodic if
  - there exist a uniform ν_m-small set C i.e.
    for each γ $\quad P^m_\gamma(x,\cdot) \geq \delta\nu_\gamma(\cdot) \quad$ for all $x \in C$.
  - $P_\gamma V \leq \lambda V + b\mathbb{I}_C \quad$ for all γ.
- S.G.E. implies containment

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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

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

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

`AdapRSadapMwG`

1. Set $\alpha_n := R_n(\alpha_{n-1}, X_{n-1}, \dots, X_0, \gamma_{n-1}, \dots, \gamma_0) \in \mathcal{Y}$
2. Set $\gamma_n := R'_n(\alpha_{n-1}, X_{n-1}, \dots, X_0, \gamma_{n-1}, \dots, \gamma_0) \in \Gamma_1 \times \dots \times \Gamma_n$
3. Choose coordinate $i \in \{1, \dots, d\}$ 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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Ergodicity Adaptive Random Scan Gibbs [ŁRR13]

- Assuming that `RSG(`β`)` is uniformly ergodic and $|\alpha_n - \alpha_{n-1}| \to 0$, we can prove ergodicity of
  - `AdapRSG`
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  by establishing diminishing adaptation and simultaneous uniform ergodicity
- Assuming that $|\alpha_n - \alpha_{n-1}| \to 0$ and regularity conditions for the target and proposal distributions (in the spirit of Roberts Rosenthal 98, Fort et al 03) ergodicity of
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Adaptive Metropolis - versions and stability

- 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

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

  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`.

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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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- Is it possible to modify other challenging adaptive algorithms to make them easier to analyze without destroying their empirical properties?

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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?
- How about adapting increasingly rarely?
- **AirMCMC Sampler** [CLR18b]
  Initiate $X_0 \in \mathcal{X}$, $\gamma^0 \in \Gamma$. $\overline{\gamma} := \gamma^0$ $k := 1$, $n := 0$.
  (1) For $i = 1, .., n_k$
    1.1. sample $X_{n+i} \sim P_{\overline{\gamma}}(X_{n+i-1}, \cdot)$;
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  (2) Set $n := n + n_k$, $k := k + 1$. $\overline{\gamma} := \gamma_n$.
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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 $Y \sim N(X_{n+i-1}, \overline{\gamma})$, $a_{\overline{\gamma}} := \frac{\phi(Y)}{\phi(X_{n+i-1})}$;
    (1.2.) $X_{n+i} := \begin{cases} Y & \text{with probability} \quad a_{\overline{\gamma}}, \\ X_{n+i-1} & \text{with probability} \quad 1 - a_{\overline{\gamma}}; \end{cases}$
    (1.3.) $a := a + a_{\overline{\gamma}}$.
    If $i = n_k$ then
    $\overline{\gamma} := \exp\left(\log(\overline{\gamma}) + c_n\left(\frac{a}{n_k} - 0.44\right)\right)$.
  (2) Set $n := n + n_k$, $k := k + 1$, $a := 0$.

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    (1.2.) $X_{n+i} := \begin{cases} Y & \text{with probability} \quad a_{\overline{\gamma}}, \\ X_{n+i-1} & \text{with probability} \quad 1 - a_{\overline{\gamma}}; \end{cases}$
    (1.3.) $a := a + a_{\overline{\gamma}}$.
    If $i = n_k$ then
    $\overline{\gamma} := \exp\left(\log(\overline{\gamma}) + c_n \left(\frac{a}{n_k} - 0.44\right)\right)$.
  (2) Set $n := n + n_k$, $k := k + 1$, $a := 0$.

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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AirMCMC - a simulation study

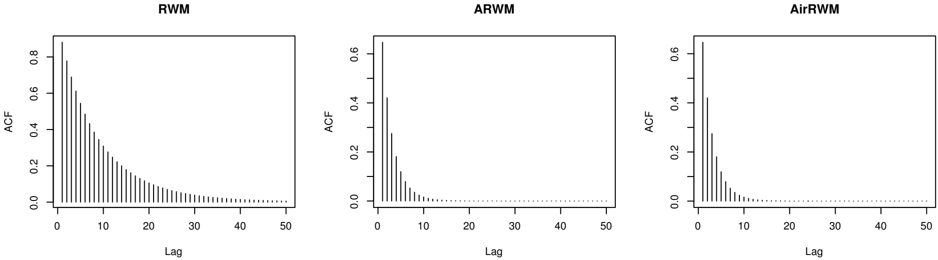
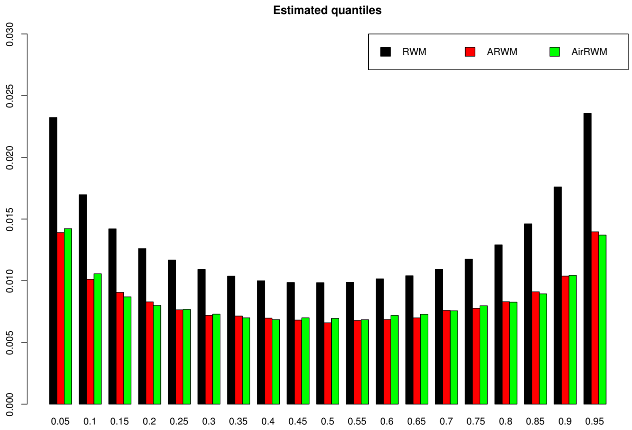
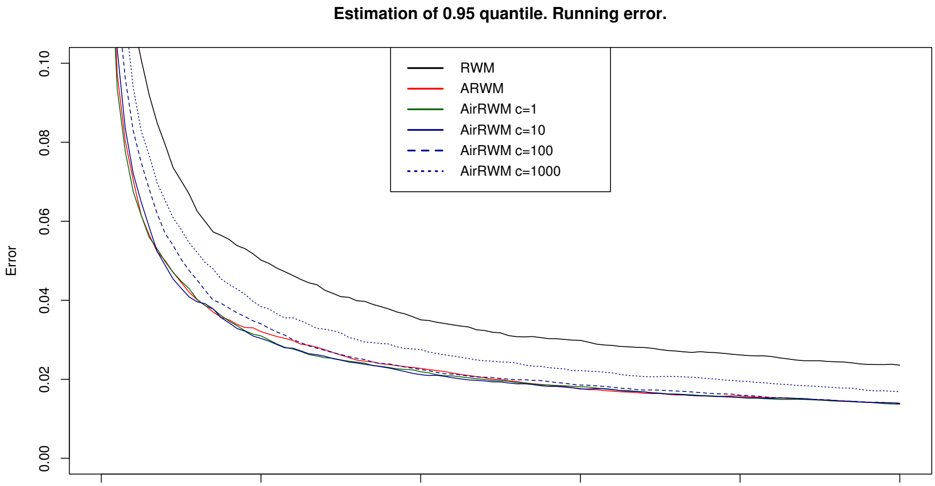


Figure: Autocorrelations (ACF)

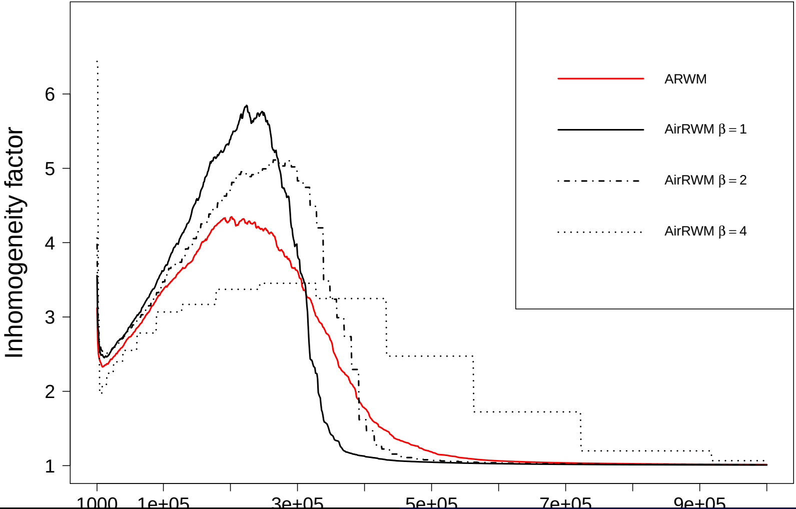
AirMCMC - a simulation study



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!
-
- Counterparts of this theorem also for
  - Kernels locally SGE
  - Kernels Polynomially Simultaneously Ergodic
- Note that diminishing adaptation is not needed!

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