Adaptive Increasingly Rarely Markov Chain Monte Carlo (AirMCMC)

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Adaptive MCMC

Air MCMC

Markov chain Monte Carlo

- let π be a target probability distribution on $\mathcal{X}$, e.g. to evaluate

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

- direct sampling from π is not possible or impractical
- 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 θ.
- it is **easy** to design an **ergodic** transition kernel P, e.g. using generic Metropolis or Gibbs recipes
- it is **difficult** to design a transition kernel P with **good convergence properties**, especially if $\mathcal{X}$ is high dimesional
- Trying to find an optimal P would be a disaster problem

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Optimal Scaling of Metropolis-Hastings P

- for Metropolis chains there is a "prescription" of how to scale proposals as dimension $d \to \infty$.
- If $\sigma_d^2 = l^2 d^{-1}$ then based on an elegant mathematical result (Roberts 1997)
- Consider

$$Z_t^{(d)} := X_{\lfloor td \rfloor}^{(d,1)}, \qquad \text{then as } d \to \infty,$$

- $Z_t^{(d)}$ converges to the solution Z of the SDE

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

- so maximise $h(l)$ to optimise Metropolis-Hastings.
- one-to-one correspondence between l_{opt} and mean acceptance rate of 0.234.

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Adaptive MCMC

- Use scale γ of the proposal such that mean acceptance rate of M-H is 0.234
- one needs to learn π to apply this
- Trial run? High dimensions? Metropolis within Gibbs?
- Adaptive MCMC: update the scale **on the fly**.
- For adaptive scaling Metropolis-Hastings one may use

$$\log(\gamma_n) = \log(\gamma_{n-1}) + n^{.7}(\alpha(X_{n-1}, Y_n) - 0.234)$$

- so P_n used for obtaining $X_n|X_{n-1}$ may depend on $\{X_0, \ldots, X_{n-1}\}$
- however now the process is **not** Markovian, so the possible benefit comes at the price of more involving theoretical analysis

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Success story of Adaptive Metropolis-Hastings

- 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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- Adaptive scaling beyond Metropolis-Hastings?
- **YES.** Similar optimal scaling results are available for MALA, HMC, etc. Each yields an adaptive version of the algorithm!
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- What can you optimise beyond scale?
- E.g. **covariance matrix of the proposal.**

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The fly in the ointment

- $P_\gamma, \gamma \in \Gamma$ - 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.
- Adaptive MCMC is not Markovian
- The standard MCMC theory does not apply
- 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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Post-mortem of the fly

- Standard assumptions to validate Adaptive MCMC are e.g. as follows:
- **(DA) Diminishing Adaptation**:
  $\lim_{n\to\infty} D_n = 0$, in probability, where
  $D_n = \sup_{x\in\mathcal{X}} \|P_{\gamma_{n+1}}(x,\cdot) - P_{\gamma_n}(x,\cdot)\|_{TV}$.
- **(C) Containment**:
  The sequence $\{M_\varepsilon(X_n,\gamma_n)\}_{n=0}^{\infty}$ is bounded in probability, where
  $M_\varepsilon : \mathcal{X}\times\Gamma \to \mathbb{N}$ is defined as
  $M_\varepsilon(x,\gamma) := \inf\{n \geq 1 : \|P_\gamma^n(x,\cdot) - \pi(\cdot)\|_{TV} \leq \varepsilon\}$.
- DA + C guarantee ergodicity, i.e. convergence in distribution (Roberts + Rosenthal 2007)
- and also nondeterioration (KL + Rosenthal 2014)
- but for SLLN, you **need additional conditions**! (Roberts + Rosenthal 2007; Fort + Moulines + Priouret 2011; Atchade + Fort 2010)

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- **Two setting to verify containment**:
- **(SGE) Simultaneous Geometric Ergodicity**:
  $P_\gamma V(x) \leq \lambda V(x) + bI_C(x)$,
  $P_\gamma(x, \cdot) \geq \delta\nu(\cdot)$ for all $x \in C$,
  same $\lambda,\ b,\ C,\ \delta,\ \nu$ for all $\gamma \in \Gamma$
- **(SPE) Simultaneous Polynomial Ergodicity**:
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Adaptive Gibbs Sampler - a generic algorithm

- AdapRSG
  1. Set $p_n := R_n(p_{n-1}, X_{n-1}, \dots, X_0) \in \mathcal{Y} \subset [0,1]^d$
  2. Choose coordinate $i \in \{1, \dots, d\}$ according to selection probabilities p_n
  3. Draw $Y \sim \pi(\cdot|X_{n-1,-i})$
  4. Set $X_n := (X_{n-1,1}, \dots, X_{n-1,i-1}, Y, X_{n-1,i+1}, \dots, X_{n-1,d})$
- Given the target distribution π, what are the optimal selection probabilities p?
- Pretend π is a Gaussian - optimal p is known for Gaussians - and it works outside the Gaussian class.
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AirMCMC - Adapting increasingly rarely

- $P_\gamma, \gamma \in \Gamma$ - 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 - 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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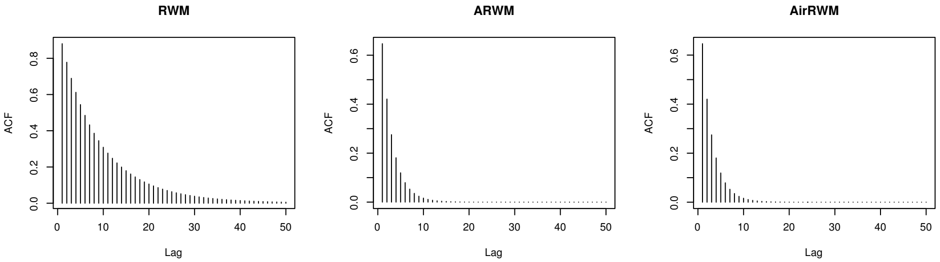

Figure: Autocorrelations (ACF)

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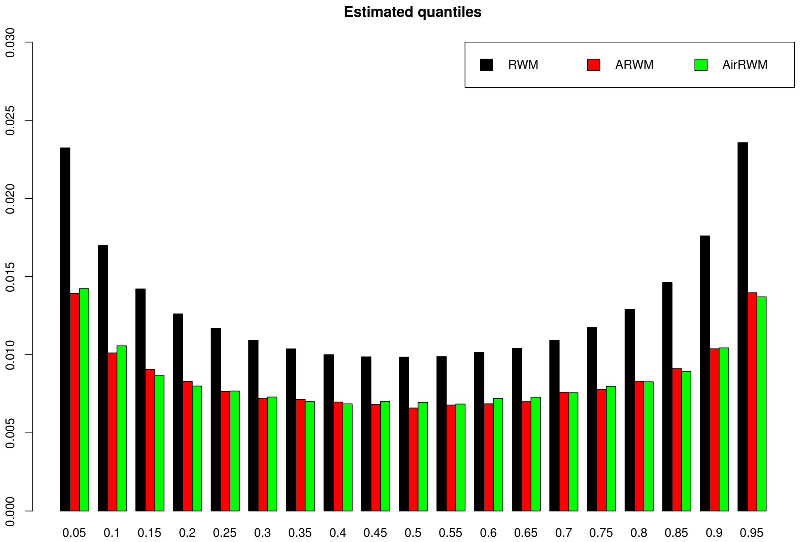

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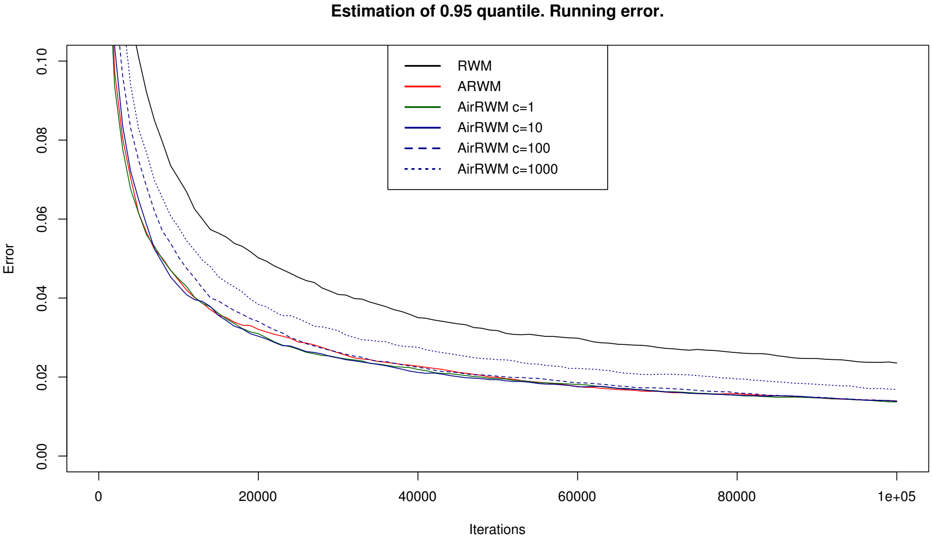

AirMCMC - theory - the SGE case

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

  Then WLLN holds, and also for any $\delta \in (0, 2)$

  $\lim_{N\to\infty} \mathbf{E}\left|\frac{1}{N}\sum_{i=0}^{N-1} f(X_i) - \phi(f)\right|^{2-\delta} = 0,$
- **Theorem 2**
  - Kernels SGE and reversible
  - $\frac{d\nu}{d\pi} \in L_2(\mathcal{X}, \pi)$
  - $n_k \geq ck^{\beta}, \quad \beta > 0$
  - $\sup \frac{|f(x)|}{V^{\frac{\beta}{2(\beta+1)}-\delta}(x)} < \infty$, for some $\delta > 0$,

  Then SLLN holds.
- Note that diminishing adaptation is not needed!

AirMCMC - theory - the SGE case

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  - $\sup \frac{|f(x)|}{V^{\frac{\beta}{2(\beta+1}-\delta}(x)} < \infty$, for some $\delta > 0$,

  Then SLLN holds.
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AirMCMC - theory - the local SGE case

- **Theorem 3**
  - Γ is compact
  - Kernels are locally SGE
  - $n_k \geq ck^\beta, \quad \beta > 0$, and adaptation takes place if in a compact set B
  - $\sup \frac{|f(x)|}{V_i^{1/2}(x)} < \infty$

  Then WLLN holds, and also for any $\delta \in (0, 2)$

  $\lim_{N\to\infty} \mathbf{E}\left|\frac{1}{N}\sum_{i=0}^{N-1} f(X_i) - \phi(f)\right|^{2-\delta} = 0,$

- **Theorem 4**
  - Γ is compact
  - Kernels are locally SGE and reversible
  - $\frac{d\nu}{d\pi} \in L_2(\mathcal{X}, \pi)$
  - $n_k \geq ck^\beta, \quad \beta > 0$, and adaptation takes place if in a compact set B
  - $\sup \frac{|f(x)|}{V_i^{\frac{\beta}{2(\beta+1)}-\delta}(x)} < \infty$, for some $\delta > 0$,

  Then SLLN holds.

AirMCMC - theory - the local SGE case

- **Theorem 3**
  - Γ is compact
  - Kernels are locally SGE
  - $n_k \geq ck^{\beta}, \quad \beta > 0$, and adaptation takes place if in a compact set B
  - $\sup \frac{|f(x)|}{V_i^{1/2}(x)} < \infty$

  Then WLLN holds, and also for any $\delta \in (0,2)$

  $$\lim_{N\to\infty} \mathbf{E}\left|\frac{1}{N}\sum_{i=0}^{N-1} f(X_i) - \phi(f)\right|^{2-\delta} = 0,$$

- **Theorem 4**
  - Γ is compact
  - Kernels are locally SGE and reversible
  - $\frac{d\nu}{d\pi} \in L_2(\mathcal{X}, \pi)$
  - $n_k \geq ck^{\beta}, \quad \beta > 0$, and adaptation takes place if in a compact set B
  - $\sup \frac{|f(x)|}{V_i^{\frac{\beta}{2(\beta+1}-\delta}(x)} < \infty$, for some $\delta > 0$,

  Then SLLN holds.

AirMCMC - theory - the SPE case

- **Theorem 5**
  - Kernels SPE with $\alpha > 2/3$
  - $\beta > \frac{2\alpha(1-\alpha)}{2\alpha-1}$ *if* $\alpha < \frac{3}{4}$
    $\beta > \frac{\alpha}{4\alpha-2}$ *if* $\alpha \geq \frac{3}{4}$.
  - $n_k \geq ck^\beta, \quad \beta > 0$
  - $\sup \frac{|f(x)|}{V^{3/2\alpha-1}(x)} < \infty$

  Then WLLN holds.