A Dirichlet Form approach to MCMC Optimal Scaling

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Warwick Statistics

Introduction

Introduction to Markov chain Monte Carlo (MCMC)

General reference: Brooks et al. (2011) MCMC Handbook.

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Conditional density → $p(x|y)$; Joint probability density → $p(x,y)$

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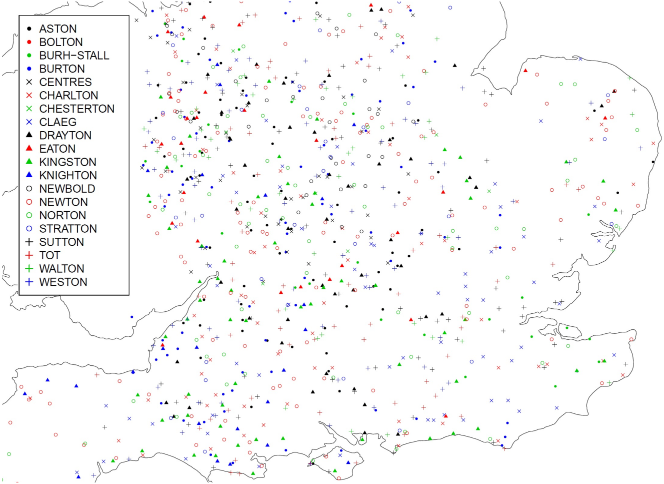
Build Markov chain with this as equilibrium (no need to know Z) ← $p(x|y)$

Norming constant Z can be hard to compute! ← Z

Simulate Markov chain till approximate equilibrium.

Example: MCMC for Anglo-Saxon statistics

Some historians conjecture, Anglo-Saxon placenames cluster by *dissimilar* names. Zanella (2015, 2016) uses MCMC: data provides some support, resulting in useful clustering.



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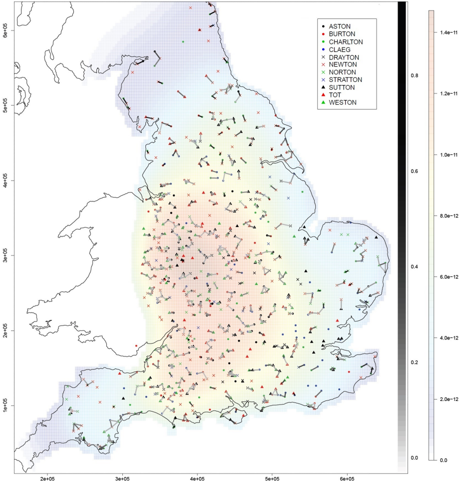

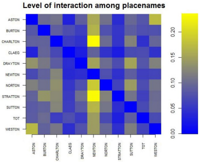

MCMC and optimal scaling

MCMC idea

Goal: estimate $E = \mathbb{E}_\pi[h(X)]$.

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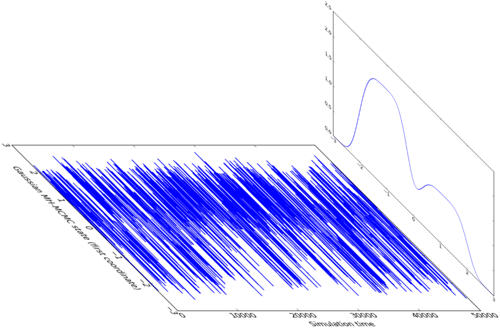
Theory: $\hat{E}_n \to E$ almost surely.



Varieties of MH-MCMC

Here is the famous Metropolis-Hastings recipe for drawing from a distribution with density f:

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Propose Y using conditional density q(y|x);
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We shall focus on RW MH-MCMC with Gaussian proposals.

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while not mcmc.stopped():
  z = normal(0, tau, size=mcmc.dim)
  if exponential() > mcmc.phi(mcmc.x + z)-mcmc.phi(mcmc.x):
    mcmc.x += z
mcmc.record_result()
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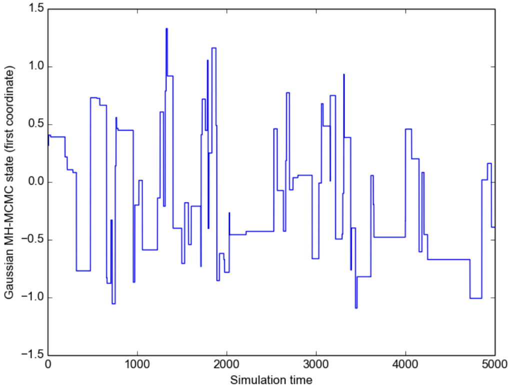
What is best choice of scale / standard deviation `tau`?

RW MH-MCMC with Gaussian proposals

(smooth target, marginal $\propto \exp(-x^4)$)

Target is given by 10 *i.i.d.* coordinates.



Scale parameter for proposal: $\tau = 1$ is too large!

Acceptance ratio 1.7%

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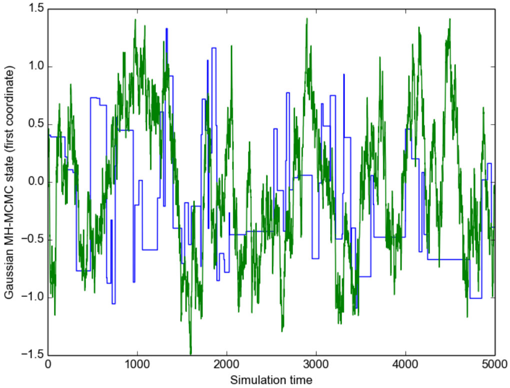

Scale parameter for proposal: $\tau = 0.1$ is better.

Acceptance ratio 76.5%

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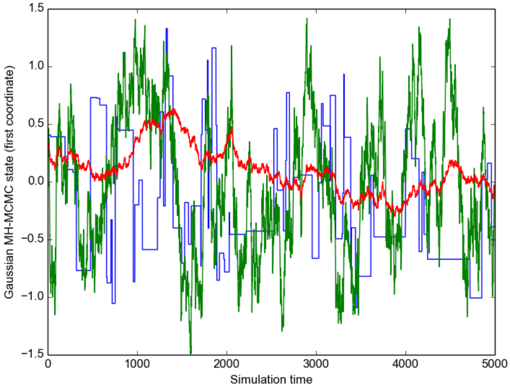

Scale parameter for proposal: $\tau = 0.01$ is too small.

Acceptance ratio 98.5%

MCMC Optimal Scaling: classic result (I)

RW MH-MCMC on $(\mathbb{R}^d, \pi^{\otimes d})$

$\pi(dx_i) = e^{-\phi(x_i)} dx_i$; MH acceptance rule $A^{(d)} = 0$ or 1.

$$\underline{X}_0^{(d)} = (\quad X_1 \quad , \ldots , \quad X_d \quad) \qquad X_i \overset{iid}{\sim} \pi$$

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Theorem (Roberts, Gelman and Gilks, 1997)

Given $\sigma_d^2 = \frac{\sigma^2}{d}$, *Lipschitz* ϕ', *and finite* $\mathbb{E}_\pi[(\phi')^8]$, $\mathbb{E}_\pi[(\phi'')^4]$

$$\{X^{(d)}_{\lfloor td \rfloor,1}\}_t \Rightarrow Z \quad \textit{where} \quad \mathrm{d}Z_t = s(\sigma)^{\frac{1}{2}} \, \mathrm{d}B_t + \tfrac{1}{2} s(\sigma) \, \phi'(Z_t) \, \mathrm{d}t \, .$$

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Answers: **(1)** mix in $O(d)$ steps; **(2)** $\sigma_{\max} = \arg\max_\sigma s(\sigma)$.

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Optimization: maximize $s(\sigma)$!

Given $\mathcal{I} = \mathbb{E}_\pi[\phi'(X)^2]$ and normal CDF Φ,

$$s(\sigma) = \sigma^2\, 2\Phi(-\frac{\sigma\sqrt{\mathcal{I}}}{2}) = \sigma^2 A(\sigma) = \frac{4}{\mathcal{I}}\,(\Phi^{-1}(\frac{A(\sigma)}{2}))^2 A(\sigma)$$

So σ_{max} maximized by choosing asymptotic acceptance rate $A(\sigma_{\text{max}}) = \arg\max_{A\in[0,1]} \left\{(\Phi^{-1}(\frac{A}{2}))^2 A\right\} \approx 0.234$

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Some weaknesses that we will address: (there are others)

- Convergence of marginal rather than joint distribution
- Strong regularity assumptions: Lipschitz g', finite $\mathbb{E}\left[(g')^8\right]$, $\mathbb{E}\left[(g'')^4\right]$.

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All these build on the s.d.e. approach of Roberts, Gelman and Gilks (1997); hence regularity conditions tend to be severe (but see Durmus et al., 2016).

Dirichlet forms and optimal scaling

Dirichlet forms and MCMC 1

Definition of Dirichlet form

A (symmetric) Dirichlet form $\mathcal{E}$ on a Hilbert space H is a closed bilinear function $\mathcal{E}(u, v)$, defined / finite for any $u, v \in \mathcal{D} \subseteq H$, which satisfies:

1. $\mathcal{D}$ is a dense linear subspace of H;
2. $\mathcal{E}(u, v) = \mathcal{E}(v, u)$ for $u, v \in \mathcal{D}$, so $\mathcal{E}$ is symmetric;
3. $\mathcal{E}(u) = \mathcal{E}(u, u) \geq 0$ for $u \in \mathcal{D}$;
4. $\mathcal{D}$ is a Hilbert space under the ("Sobolev") inner product $\langle u, v \rangle + \mathcal{E}(u, v)$;
5. If $u \in \mathcal{D}$ then $u_* = (u \wedge 1) \vee 0 \in \mathcal{D}$, moreover $\mathcal{E}(u_*, u_*) \leq \mathcal{E}(u, u)$.

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Relate to Markov process if (quasi)-regular.
Regular Dirichlet form for locally compact Polish E:
$\mathcal{D} \cap C_0(E)$ is $\mathcal{E}^{\frac{1}{2}}$-dense in $\mathcal{D}$, uniformly dense in $C_0(E)$.

Dirichlet forms and MCMC 2

Two examples

1. Dirichlet form obtained from (re-scaled) RW MH-MCMC:

$$\mathcal{E}_d(h) \quad = \quad \frac{d}{2}\,\mathbb{E}\left[\left(h(\underline{X}_1^{(d)}) - h(\underline{X}_0^{(d)})\right)^2\right].$$

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   Can we deduce that the RW MH-MCMC scales to look like the "infinite-dimensional diffusion",
   by showing that $\mathcal{E}_d$ "converges" to $\mathcal{E}_\infty$?

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2. Mosco (1994) introduces stronger conditions;

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   - (Γ1) $\mathcal{E}_\infty(h) \leq \liminf_n \mathcal{E}_n(h_n)$ whenever $h_n \to h \in H$;
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4. Sun (1998) gives further conditions which imply weak convergence of the associated processes: these conditions are implied by existence of a finite constant C such that $\mathcal{E}_n(h) \le C(|h|^2 + \mathcal{E}(h))$ for all $h \in H$.

Results and methods of proofs

Results

Theorem (Zanella, Bédard and WSK, 2016)

Consider the Gaussian RW MH-MCMC based on proposal variance σ^2/d with target $\pi^{\otimes d}$, where $\mathrm{d}\pi = f\,\mathrm{d}x = e^{-\phi}\,\mathrm{d}x$. Suppose $\mathcal{I} = \int_\infty^\infty |\phi'|^2 f\,\mathrm{d}x < \infty$ (finite Fisher information), and $|\phi'(x+v) - \phi'(x)| < \kappa \max\{|v|^\gamma, |v|^\alpha\}$ for some $\kappa > 0$, $0 < \gamma < 1$, and $\alpha > 1$.

Let $\mathcal{E}_d$ be the corresponding Dirichlet form scaled as above. $\mathcal{E}_d$ Mosco-converges to $\mathbb{E}\left[1 \wedge \exp(\mathcal{N}(-\frac{1}{2}\sigma^2\mathcal{I}, \sigma^2\mathcal{I}))\right]\mathcal{E}_\infty$, so corresponding L^2 semigroups also converge.

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Corollary

Suppose in the above that ϕ' is globally Lipschitz. The correspondingly scaled processes exhibit weak convergence.

Methods of proof 1: a CLT result

Lemma (A conditional CLT)

Under the conditions of the Corollary, almost surely (in $\underline{x}$ with invariant measure $\pi^{\otimes\infty}$) the log Metropolis-Hastings ratio converges weakly (in $\underline{W}$) as follows as $d \to \infty$:

$$\log\left(\prod_{i=1}^{d} \frac{f(x_i + \frac{\sigma W_i}{\sqrt{d}})}{f(x_i)}\right) = \sum_{i=1}^{d}\left(\phi(x_i + \frac{\sigma W_i}{\sqrt{d}}) - \phi(x_i)\right) \Rightarrow \mathcal{N}(-\tfrac{1}{2}\sigma^2\mathcal{I}, \sigma^2\mathcal{I}).$$

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We may use this to deduce the asymptotic acceptance rate of the RW MH-MCMC sampler.

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Key idea for CLT

Use exact Taylor expansion techniques:

$$\sum_{i=1}^{d} \left(\phi(x_i + \tfrac{\sigma W_i}{\sqrt{d}}) - \phi(x_i) \right) \quad =$$

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3. Use Hoeffding's inequality then absolute expectations: $\mathbb{E}\left[\sum_{i=1}^{d} \frac{\sigma W_i}{\sqrt{d}} \int_0^1 \left(\phi'(x_i + \frac{\sigma W_i}{\sqrt{d}} u - \phi'(x_i) \right) \mathrm{d}u \right] \to -\frac{1}{2}\sigma^2 \mathcal{I}$.

Methods of proof 2: establishing condition (M2)

For every $h \in L^2(\pi^{\otimes\infty})$, find $h_n \to h$ (strongly) in $L^2(\pi^{\otimes\infty})$ such that $\mathcal{E}_\infty(h) \geq \limsup_n \mathcal{E}_n(h_n)$.

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Methods of proof 3: establishing condition (M1)

If $h_n \to h$ weakly in $L^2(\pi^{\otimes\infty})$, show $\mathcal{E}_\infty(h) \leq \liminf_n \mathcal{E}_n(h_n)$.
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3. Use integration by parts, careful analysis and conditions on ϕ'.

Doing even better

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L^p mean differentiability applies straightforwardly to the Zanella, Bédard and WSK (2016) argument *mutatis mutandis*: the regularity conditions can be weakened even more at least for vague convergence.

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commit d81469c5f14c484aa363616e3d701c6e3fbb1141
Author: Wilfrid Kendall <W.S.Kendall@warwick.ac.uk>

    Made it explicit that Lp mean differentiability still doesn't cover weak
    without extra regularity: need to beat this!
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