Optimal Scaling of MCMC Algorithms

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Outline

- What is Optimal Scaling?
  - Gareth Roberts’ work: Random walk Metropolis and Langevin Algorithm
  - Hybrid Monte Carlo Algorithm
  - Optimal Scaling in Infinite Dimensions
  - Conclusion
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Seminal paper: Roberts, Gelman and Gilks, 1997. (1000 citations)

Target density: i.i.d components

$$\pi^N(x) = \prod_{i=1}^{N} f_i(x_i) \propto \prod_{i=1}^{N} e^{-g_i(x_i)}$$

Simple Random walk Proposal:

$$y = x + \sqrt{\ell} \delta Z_N$$

- $$Z_N \sim \text{No}(0, I_N)$$.
- $$\ell$$ - “optimisation” parameter.
- $$\delta = \delta(N)$$ is the SCALE.
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Metropolis Algorithm: RGG97

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Traditionally, ....

- Study of **Mixing times**
- Time to attain **Stationarity**
- ‘Burn in time’
- Spectral gap

Hard problems ...

For practical MCMC arguably **optimisation questions** (find the best algorithm from a class) are more important
The new perspective in Roberts, Gelman and Gilks, 1997

- Study the Markov chain **AFTER** Stationarity
  - thus complementing work on convergence, robustness to starting values etc..

- **Scale** the proposal as a function of the dimension.

- **Goldilocks Principle** (attributed to Rosenthal, J.)
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Acceptance Probability

- Acceptance Probability = \( \min(1, \frac{\pi(y)}{\pi(x)}) \).
- If \( y \approx x \), \( \pi(y) \approx \pi(x) \), and thus acceptance probability is equal is very high.
- If \( y \) is far away from \( x \), then \( \frac{\pi(y)}{\pi(x)} \ll 1! \)
Goldilock’s Principle; Figure courtesy: Roberts and Rosenthal, 2001.

**Fig. 2.** Simple Metropolis algorithm with (a) too-large variance (left plots), (b) too-small variance (middle) and (c) appropriate variance (right). Trace plots (top) and autocorrelation plots (below) are shown for each case.
Choose the scale such that

\[ \mathbb{E}(\text{acc prob}) = \mathcal{O}(1) \]

For large \( N \),

\[ \mathbb{E}(\text{acc prob}) = a(N) \approx a \]

Optimise \( a \), to obtain “best” acceptance probability.
Theorem: (for distributions with exponential moments + mild conditions)

- $\delta = \delta(N) = \frac{1}{N}$.
- A SINGLE component (rescaled): $x^k \Rightarrow X_t$
  
  $$dX_t = -h(\ell) \nabla g(X_t) dt + \sqrt{2h(\ell)} \, dW_t$$

- $\mathbb{E}(\text{acc prob}) \to 2\Phi(-\frac{\ell}{\sqrt{2}})$
- Expected Squared Jumping Distance:
  
  $$h(\ell) = \mathbb{E}(x^{k+1} - x^k)^2 \to 2\ell^2 \Phi(-\frac{\ell}{\sqrt{2}})$$

- Optimal acceptance probability: Maximizes the expected squared jumping distance:
  
  $\hat{a} = 0.234$
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Fig. 5. Convergence times for Metropolis algorithms as a function of their acceptance rates. The plotting symbol indicates the dimension of the simulation.
**Diffusion limit: Insights**

- **Why maximize** $\mathbb{E}(x^{k+1} - x^k)^2$?

  At stationarity

  $\mathbb{E}(x^{k+1} - x^k)^2 = \mathbb{E}(x^{k+1})^2 + \mathbb{E}(x^k)^2 - 2\text{Cov}(x^{k+1}, x^k) = 2M - 2\text{Cov}(x^{k+1}, x^k)$

- **Why only lag-1 correlation? Higher orders?**

- The quantity $h(\ell)$ is the **Speed** of the diffusion.

- Thus, because of the **diffusion limit**, maximizing $h(\ell)$ leads to minimizing the asymptotic variance.
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Diffusion limit: Insights

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Practical Conclusion of Diffusion Limit

Suppose we want to estimate \( \int f(u) \pi(du) \).

- Given the precision \( \epsilon \), find \( T \) and compute

\[
\hat{f} = \frac{1}{T} \int f(X_t) dt
\]

- Diffusion Limit + Optimal Scaling implies that

\[
\hat{f}_N = \frac{1}{T} \sum_{k=1}^{\lceil T/\delta \rceil} f(X_k) \quad \delta = O(N^{-1})
\]

has the same precision as \( \hat{f} \).

- The mixing time of the RWM is \( O(N) \).
Langevin Algorithm

- Recall Langevin diffusion: \( dx_t = - \nabla g(x_t) dt + \sqrt{2} dW_t. \)
- Langevin Proposal:
  \[
  y = x - \nabla g(x) \ell \delta + \sqrt{2\ell} \delta Z_N
  \]
- Need a Metropolis Accept/Reject mechanism.
- \( x^k \) is the Langevin Markov chain on \( \mathbb{R}^N \) for iid target.
- Theorem (Roberts + Rosenthal 1998): The scale is \( \delta(N) = N^{-1/3} \) and after rescaling the first component of the Markov chain \( \{x^k\} \) converges in distribution to \( X_t \):
  \[
  dX_t = -h_1(\ell) \nabla g(X_t) dt + \sqrt{2h_1(\ell)} dW_t.
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- Optimal Acceptance Probability = 0.574.
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Comparing RWM vs. Langevin

- Recall RWM had complexity of $O(N)$
- Langevin has complexity of $O(N^{1/3})$.
- Thus optimal scaling gives a nice way to compare algorithms.
So far:

Summary:
- optimal scaling: tuning proposals.
- Diffusion limits for RWM and Langevin
- Hybrid Monte Carlo Algorithm
- Infinite Dimensional Result
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Hybrid Monte Carlo Algorithm

Infinite Dimensional Result
Hybrid Monte Carlo

- Algorithm from Physics, (Duane et. al. (1987))
- Based on Hamiltonian Dynamics, conservation of energy.
Hamiltonian Dynamics

- Location $x$, velocity $v$; total energy,

$$H(x, v) = g(x) + \frac{1}{2} v^2$$

- Hamiltonian equations

$$\frac{dx}{dt} = v; \quad \frac{dv}{dt} = -\nabla g(x)$$

- They give rise to solution operator

$$\phi^T : (x_0, v_0) \mapsto (x_T, v_T)$$

that preserves total energy.

- Equivalently the joint density

$$\exp\{-H(x, v)\} = \exp\{-g(x) - \frac{1}{2} v^2\}$$

is preserved.
**Hamiltonian Dynamics**

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‘Exact’ Hamiltonian Dynamics
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\[ v \]

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‘Exact’ Hamiltonian Dynamics
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Leapfrog Discretisation

- In practice, dynamics are approximated:
  \[ \phi^T \approx \phi^{T,h} \].

- For initial state \((x_0, v_0)\): Leapfrog Discretisation,
  \[ v_{h/2} = v_0 - \frac{h}{2} \nabla g(x_0) \]
  \[ x_h = x_0 + h v_{h/2} \]
  \[ v_h = v_0 - \frac{h}{2} \nabla g(x_h) \]

- \(\phi^{T,h}\) is obtained by composing \(\frac{T}{h}\) leapfrog steps.
- The crucial properties of this approach are that it is volume preserving and reversible.
Acceptance probability

- \((x_0, v_0)\): Initial position
- \((x_T, v_T)\): Final position
- Accept with probability

\[
1 \land \exp\{H(x_0, v_0) - H(x_T, v_T)\}
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- Acceptance probability = 1, if Hamilton’s Differential Equations can be solved explicitly.
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"Although HMC has been found useful for Bayesian computations, many important issues remain open. For example, how to choose tuning parameters in HMC, e.g., the step-size and the number of the leapfrog iterations, is still a difficult problem. A rule of thumb is to maintain an acceptance rate of nearly 70%. But there seems to be no clear theoretical basis for this rule."
Main result

- Target density

\[ \pi^N(x) = \prod_{i=1}^{N} e^{-g_i(x_i)} \]

- Theorem: For any fixed integration length \( T \), the step size which maximizes the expected squared distance:

\[ h = h(N) = \frac{1}{N^{1/4}}. \]

- For any fixed integration length \( T \), optimal scaling leads to a complexity of \( O(N^{1/4}) \).
- For any volume preserving, time reversible second order numerical integrator, the optimal acceptance probability is 0.651.
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HMC, the optimal behavior is not Diffusive!

The complexity of HMC is $O(N^{\frac{1}{4}})$. 
HMC, the optimal behavior is not Diffusive!
The complexity of HMC is \( O(N^{\frac{1}{4}}) \).
Universality: How general?

- This first result was proved for IID targets only.
- Empirically seen to be robust well beyond IID case!
- What are the challenges for the Non-Product case?
  - progress made by Roberts, Rosenthal, Sherlock, Neal, Bedard and others ...
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Infinite Dimensional Distribution

- Let $\mathcal{H}$ be an infinite dimensional Hilbert space, $\pi_0 \sim \text{N}(0, C)$.
- Our target measure:

$$\pi(f) \propto \exp\{-\psi(f)\}\pi_0(f)$$

- For $N$ large, we take $N$ dimensional projection:

$$\pi^N \approx \pi$$

- $\pi$ is NOT a product measure.
Target Measure: Radon Nikodym Derivative w.r.t to Gaussian

- $\mathcal{H}$ Hilbert space, $\pi_0 \sim \mathcal{N}(0, C)$.
- Target:

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- Diffusion bridges. (Girsanov)
- Constructive Quantum Field Theory, $P(\phi^4_2)$ model.
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Infinite Dimensional Result

- Recall $f$ is a function, target $\pi$ measure on $\mathcal{H}$.

  $$\pi(f) \propto \exp\{-\Psi(f)\} \pi_0(f), \quad \pi_0(f) \sim \text{No}(0, C)$$

- Proposal $y = x + Z_N, \quad Z_N \sim \text{No}(0, C^N)$.


- $\{x^k\}$ is the Random Walk Metropolis Markov chain on $\mathbb{R}^N$.

- Theorem: For the scaling $\delta(N) = \frac{1}{N}$ the (rescaled) Markov chain $\{x^k\}$ converges in distribution to an infinite dimensional diffusion (SPDE) $X_t$

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- Weak Convergence in $C([0, T], \mathcal{H})$.

- Optimal Acceptance Probability $= 0.234$. 

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Weak Convergence to SPDE: Proof Sketch

- Decompose the Markov Chain into Drift + Noise

\[ x^{k+1} = x^k + \mathbb{E}(x^{k+1} - x^k | x^k) + \sqrt{2\ell \delta} \Gamma^k. \]

- Obtain Drift and Diffusion Estimates

\[ \mathbb{E}(x^{k+1} - x^k | x^k) \approx -\nabla \psi(x^k) \delta \]

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- Recall that, at stationarity, the scaling for Langevin is $N^{-1/3}$.
- For RWM, Langevin, before reaching stationarity, the scaling is $N^{-1}$ (O.F. Christensen, G.O. Roberts, and J.S. Rosenthal, 2003.)
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Optimal scaling is an important idea, with deep practical implications.

Lots more to do!

“Dimension” can be different things.
Thank you!

Thanks to:

- Gareth O. Roberts
- Jeffrey S. Rosenthal
- Organizers + Applied Probability Society
References
