Optimising and Adapting the Metropolis Algorithm

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Motivation

Given some complicated, high-dimensional density function $\pi : \mathcal{X} \to [0, \infty)$, for some $\mathcal{X} \subseteq \mathbf{R}^d$ with d large.

(e.g. Bayesian posterior distribution)

Want to compute probabilities like :

$$\Pi(A) \ := \ \int_A \pi(x)\, dx \,,$$

and/or expected values of functionals like :

$$\mathbf{E}_\pi(h) \ := \ \int_{\mathcal{X}} h(x)\, \pi(x)\, dx \,.$$

Calculus ? Numerical integration ?

Impossible ! Typical π is something like . . .

Typical π : Variance Components Model

$$
\begin{aligned}
&\pi(V, W, \mu, \theta_1, \ldots, \theta_K) \\
&\quad = C\, e^{-b_1/V} V^{-a_1-1} e^{-b_2/W} W^{-a_2-1} \\
&\qquad \times e^{-(\mu-a_3)^2/2b_3} V^{-K/2} W^{-\frac{1}{2}\sum_{i=1}^{K} J_i} \\
&\qquad \times \exp\left[-\sum_{i=1}^{K}(\theta_i-\mu)^2/2V \right. \\
&\qquad\qquad \left. -\sum_{i=1}^{K}\sum_{j=1}^{J_i}(Y_{ij}-\theta_i)^2/2W\right],
\end{aligned}
$$

with, say, $K = 19$, $d = 22$.

High-dimensional! Complicated! What to do?

Estimation from sampling : Monte Carlo

Can try to sample from π, i.e. generate i.i.d.

$$X_1, X_2, \ldots, X_M \sim \pi$$

(meaning that $\mathbf{P}(X_i \in A) = \int_A \pi(x)\,dx$).

Then can estimate by e.g.

$$\mathbf{E}_\pi(h) \;\approx\; \frac{1}{M}\sum_{i=1}^{M} h(X_i)\,.$$

Good. But how to sample? Often infeasible!

Instead ...

Markov chain Monte Carlo (MCMC)

Define a Markov chain $X_0, X_1, X_2, \ldots$, such that for large n, $\mathbf{P}(X_n \in A) \approx \int_A \pi(x)\,dx$.

(Just approximate ... and not i.i.d.)

Still, hopefully for $M \gg B \gg 1$,

$$\mathbf{E}_\pi(h) \;\approx\; \frac{1}{M-B} \sum_{i=B+1}^{M} h(X_i)\,.$$

But how to define a simple Markov chain such that

$$\mathbf{P}(X_n \in A) \;\rightarrow\; \int_A \pi(x)\,dx$$

The Metropolis Algorithm

π = target density (important! complicated! high-dim!)

Goal : obtain samples from π.

The algorithm : for $n = 1, 2, 3, \ldots$,

- $Y_n := X_{n-1} + Z_n$, where $Z_n \sim Q$ (i.i.d., symmetric)
- $\alpha := \min\left(1, \frac{\pi(Y_n)}{\pi(X_{n-1})}\right)$
- with probability α, $X_n := Y_n$ ("accept")
- else, with probability $1 - \alpha$, $X_n := X_{n-1}$ ("reject")

Assuming "irreducibility", have $\mathbf{P}(X_n \in A) \to \pi(A)$.

Good!

Example #1 : Java applet

$\pi(\cdot)$ simple distribution on $\mathcal{X} = \{1, 2, 3, 4, 5, 6\}$.
[Take $\pi(x) = 0$ for $x \notin \mathcal{X}$.]

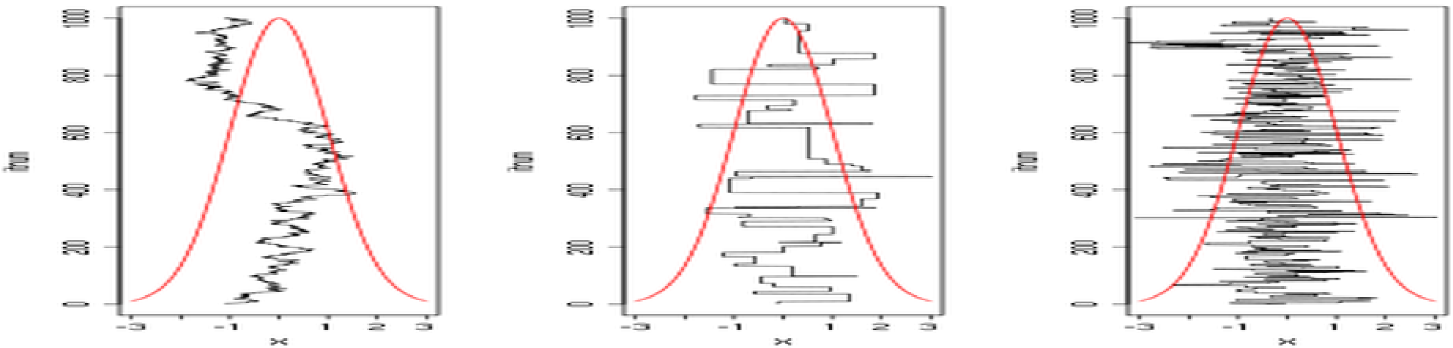
$Q(\cdot) = \text{Uniform}\{-1, 1\}$. [APPLET]

Works.
But what if $Q(\cdot) = \text{Uniform}\{-2, -1, 1, 2\}$.
Or, $Q(\cdot) = \text{Uniform}\{-\gamma, -\gamma + 1, \ldots, -1, 1, 2, \ldots, \gamma\}$.
Which γ is best ? ? ("optimise")

Good γ is <u>between</u> the two extremes, i.e. acceptance rate should be far from 0 <u>and</u> far from 1.
("Goldilocks Principle")

Example #2 : N(0,1)

Target $\pi(\cdot) = N(0,1)$. Proposal $Q(\cdot) = N(0,\sigma^2)$. Which σ ? ?



$\sigma = 0.1$? too small !	$\sigma = 25$? too big !	$\sigma = 2.38$? (better !)
A.R. = 0.962	A.R. = 0.052	A.R. = 0.441

What about higher dimensions ? (need smaller σ ...)

How to make theoretical progress ?

Consider diffusion limits !

Analogy : if $\{X_n\}$ is simple random walk, and $Z_t = d^{-1/2} X_{dt}$ (i.e., we speed up time, and shrink space), then as $d \to \infty$, the process $\{Z_t\}$ converges to Brownian motion.

Theorem [Roberts, Gelman, Gilks, AAP 1994] :

If $\{X_n\}$ is a Metropolis algorithm in high dimension d, with $Q(\cdot) = N(0, \frac{\ell^2}{d} I_d)$, and $Z_t = d^{-1/2} X_{dt}^{(1)}$, then under "certain conditions" on $\pi(\cdot)$, the process $\{Z_t\}$ converges to a diffusion.

More precisely, as $d \to \infty$, $Z_t = d^{-1/2} X^{(1)}_{dt}$ converges to a Langevin diffusion which satisfies :

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

where

$$\text{speed} = h(\ell) \;=\; 2\,\ell^2\,\Phi(-C_\pi \ell/2)$$

and

$$\text{acceptance rate} \;\equiv\; A(\ell) \;=\; 2\,\Phi(-C_\pi \ell/2)\,.$$

(Here C_π depends on $\pi(\cdot)$, and $\Phi(x) = \int_{-\infty}^{x} \frac{e^{-u^2/2}}{\sqrt{2\pi}} du$.)

<u>Key point</u> : algorithm's speed $h(\ell)$ is <u>explicitly</u> related to its asymptotic acceptance rate $A(\ell)$.

Lots of information here!

- The speed $h(\ell)$ is related to the acceptance rate $A(\ell)$.
- To optimise the algorithm, we should maximize $h(\ell)$.
- The maximization is easy : $\ell_{opt} \doteq 2.38/C_\pi$.
- Then we can compute that : $A(\ell_{opt}) \doteq 0.234$.

So, for $Q(\cdot) = N(0, \sigma^2 I_d)$, it is optimal to choose

$$\sigma^2 = \frac{\ell_{opt}^2}{d} = \frac{(2.38)^2}{(C_\pi)^2 d},$$

which leads to an acceptance rate of 0.234.

Clear, simple rule – good!

(Also shows algorithm's running time is $O(d)$.)

What are these "conditions" on π ?

Original result : $\pi(\mathbf{x}) = \prod_{i=1}^{d} f(x_i)$ for fixed f (i.i.d.). Very restrictive, artificial condition.

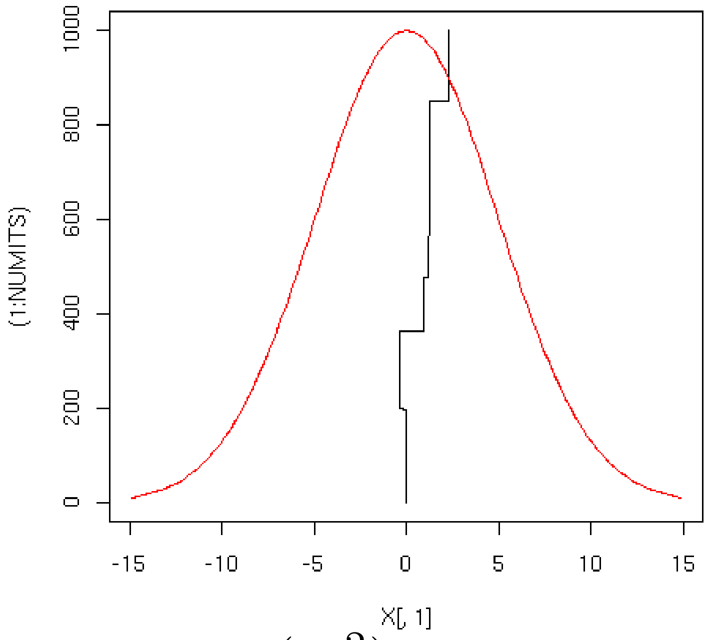
Some generalizations (Bédard, AAP 2007) : $\pi(\mathbf{x}) = \prod_{i=1}^{d} \theta_i(d)\, f(\theta_i(d)\, x_i)$, where certain $\{\theta_i(d)\}$ repeat more and more as $d \to \infty$. More flexible! (Also, for certain <u>other</u> cases, 0.234 is no longer optimal : Bédard, SPA 2008.)

Anyway, 0.234 is often <u>nearly</u> optimal, even if the theorem conditions are not satisfied. ("robust")

But does acceptance rate tell us everything?

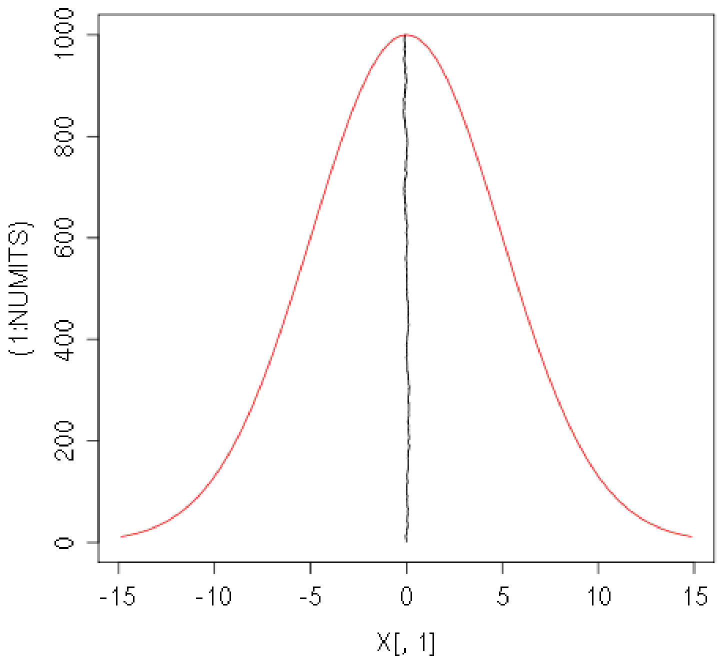
Example #3 : $\pi = N(0, \Sigma)$ in dimension 20

First try : $Q(\cdot) = N(0, I_{20})$ (acc rate = 0.006)



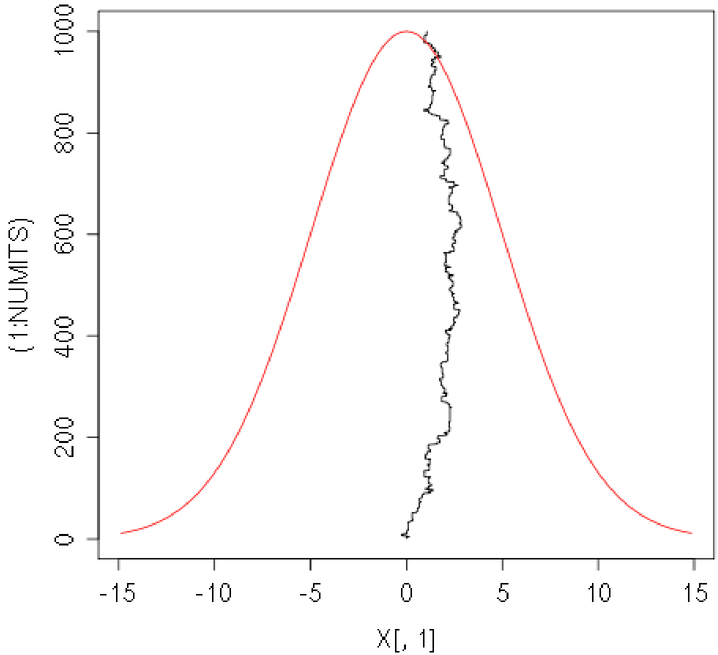
Horrible : $\Sigma_{11} = 24.54$, $E(X_1^2) = 1.50$.

Second try : $Q(\cdot) = N\left(0, (0.0001)^2 I_{20}\right)$ (acc=0.892)



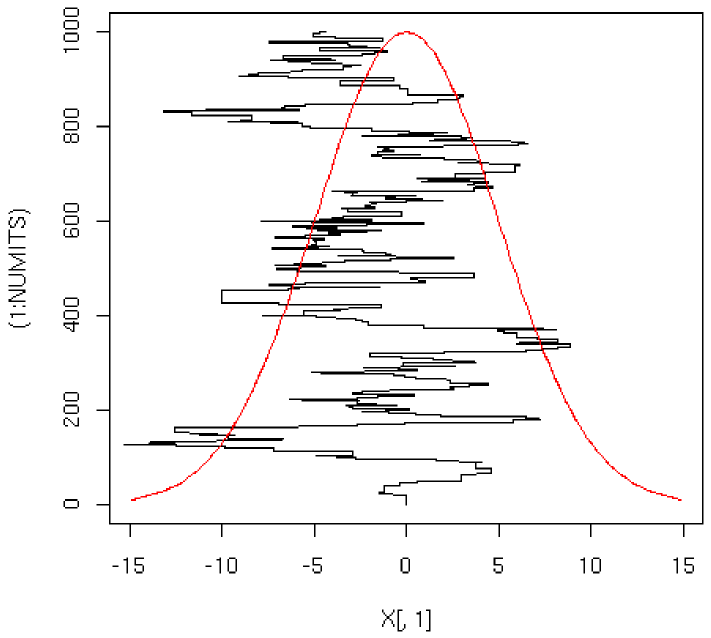
Also horrible : $\Sigma_{11} = 24.54$, $E(X_1^2) = 0.0053$.

Third try : $Q(\cdot) = N\left(0, (0.02)^2 I_{20}\right)$ (acc=0.234)



Still poor : $\Sigma_{11} = 24.54$, $E(X_1^2) = 3.63$.

Fourth try : $Q(\cdot) = N\Big(0, [(2.38)^2/20]\,\Sigma\Big)$ (acc=0.263)



Much better : $\Sigma_{11} = 24.54$, $E(X_1^2) = 25.82$.

Optimal Proposal Covariance

Theorem [Roberts and R., Stat Sci 2001] :

Under certain conditions on $\pi(\cdot)$, the optimal Metropolis algorithm Gaussian proposal distribution as $d \to \infty$ is

$$Q(\cdot) \;=\; N\Big(0,\ ((2.38)^2/d)\,\Sigma\Big)\,.$$

(Not $N(0,\, \sigma^2 I_d)$ ...) Furthermore, with this choice, the asymptotic acceptance rate is again 0.234.

And, optimal / nearly optimal for many other high-dimensional densities, too.

But this only helps if Σ is known !

What if it isn't ? ?

How to use this result if Σ is unknown ?

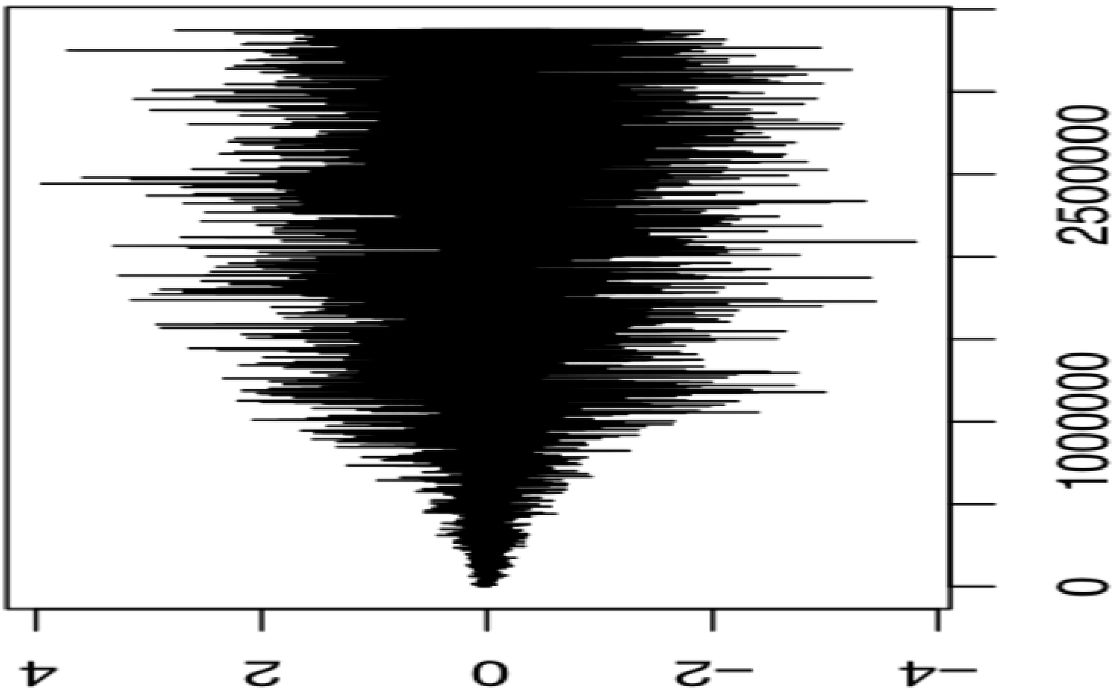
Use adaptive MCMC ! (Haario et al., Bernoulli 2001)

- Replace Σ by the empirical estimator Σ_n.
- Hope that for large n, we have $\Sigma_n \approx \Sigma$.
- Then $N\Big(0,\ ((2.38)^2/d)\Sigma_n\Big) \approx N\Big(0,\ ((2.38)^2/d)\Sigma\Big)$.
- So, use this proposal instead !

Are we allowed to do this ? ? (Subtle, because the process is no longer Markovian.)

- In examples, it usually works well . . . (next page)
- But not always . . . [APPLET]

Good adaptation in dimension 200 . . .



Is Adaptive MCMC Valid ? ?

Theorem [Roberts and R., J Appl Prob 2007] : Yes, any adaptive MCMC converges asymptotically to $\pi(\cdot)$, assuming :

1. "Diminishing Adaptation" : Adaption chosen so that

$$\lim_{n\to\infty} \sup_{x\in\mathcal{X}} \sup_{A\subseteq\mathcal{X}} |P_{\Gamma_{n+1}}(x,A) - P_{\Gamma_n}(x,A)| = 0 \quad \text{(in prob.)}$$

2. "Containment" : Times to stationary from X_n, if we fix $\gamma = \Gamma_n$, remain bounded in probability as $n \to \infty$. [Technical condition. Satisfied e.g. under compactness and continuity.]

Meanwhile, in applications, adaption often leads to significant speed-ups, even in hundreds of dimensions (Roberts and R., JCGS 2009 ; Richardson, Bottolo, R., Valencia 2010).

Another application : Simulated Tempering

Simulated Tempering : replace π by a family $\{\pi^{\beta_i}\}_{i=1}^m$, with $0 \leq \beta_m < \beta_{m-1} < \ldots < \beta_0 = 1$.

Here π^{β_m} is the "hot" distribution (easily sampled).

And $\pi^{\beta_0} = \pi$ is the "cold" distribution (the distribution of interest, but hard to sample).

Hope the algorithm can move efficiently between the different π^{β_i}, so it can "benefit" from π^{β_m} to efficiently explore π^{β_0}.

Question : how to choose the values β_i ?

Often chosen to be "geometric" : $\beta_i = a^i$ for $0 < a < 1$.

Theorem [Atchadé, Roberts, R., Stat & Comput 2010] : optimal to choose $\{\beta_i\}$ so that the asymptotic acceptance rate for moves $\beta_i \mapsto \beta_{i\pm 1}$ is 0.234. (Not necessarily geometric !)

Langevin Algorithms

If possible, it's more efficient to use a non-symmetric proposal distribution, inspired by Langevin diffusions :

$$Y_n = X_{n-1} + \sigma\, Z_n + \frac{\sigma^2}{2} \nabla \log \pi(X_{n-1})\,.$$

Theorem [Roberts and R., JRSSB 1997] :

Optimal choice is now $\sigma = \ell\, d^{-1/6}$ (not $\sigma = \ell\, d^{-1/2}$), and $A(\ell_{opt}) \doteq 0.574$ (not $A(\ell_{opt}) \doteq 0.234$).

In this case, the algorithm's running time is $O(d^{1/3})$, not $O(d)$, with optimal acceptance rate 0.574, not 0.234.

Summary

- The Metropolis algorithm is very important.
- The optimisation of the algorithm can be crucial.
- Want acceptance rate far from 0, far from 1.
- Various theorems tell us how to optimise under certain conditions : 0.234, $N\left(0,\ (2.38)^2\Sigma\,/\,d\right)$, etc.
- Even if some information is unknown (e.g., Σ), can still adapt towards the optimal choice ; valid if the adaption satisfies "Diminishing Adaptation" and "Containment".
- Can lead to tremendous speed-up in high dimensions.
- Application to computing rare tail probabilities of $\pi(\cdot)$? ?

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