Lecture 15: Markov chain Monte Carlo

STAT 545: Introduction to computational statistics

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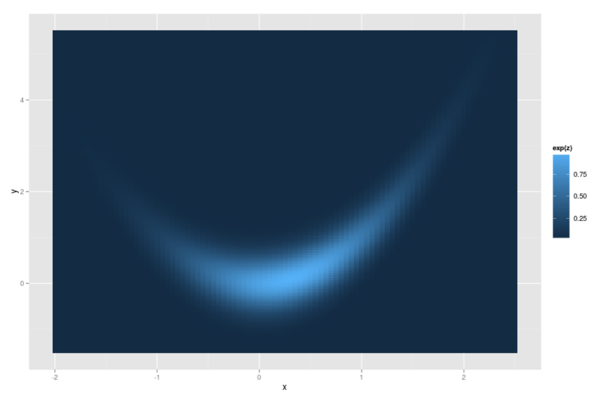
Simplest case: use current proposal to make a new proposal

The resulting algorithm: Markov chain Monte Carlo.

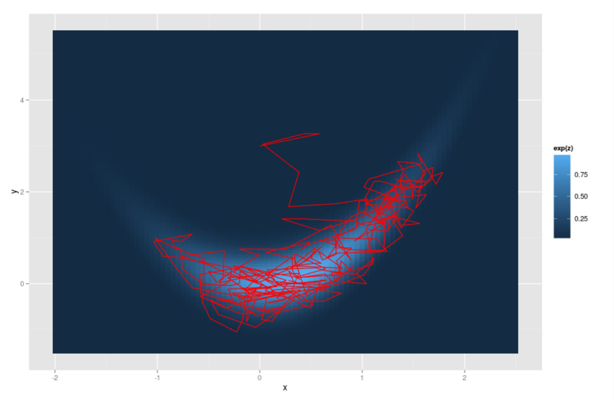
(A Markov chain: future independent of past given present)



The Rosenbrock density (a.k.a. the banana density)

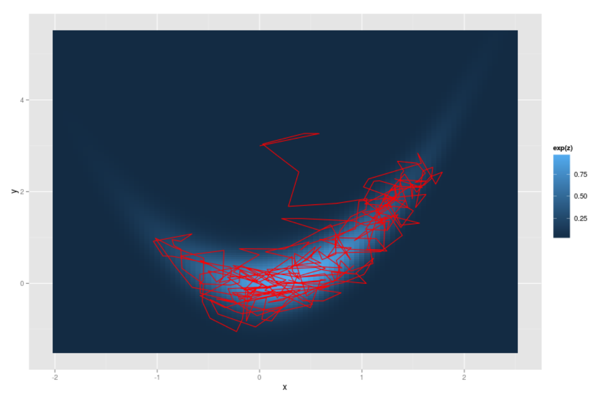
$$p(x,y) \propto \exp\left(-(a-x)^2 - b(y-x^2)^2\right) \quad (\text{here } a = .3, b = 3)$$

Markov chain Monte Carlo



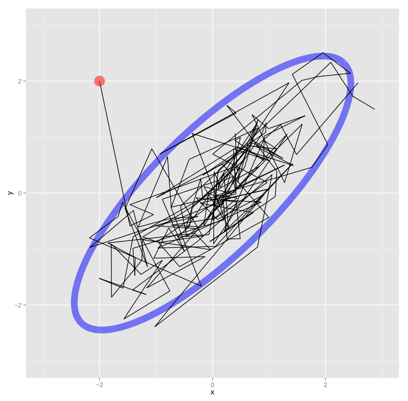
A random walk:

- start somewhere arbitrary
- make local moves



- Discard initial 'burn-in' samples
- Use remaining to obtain Monte Carlo estimates:

$$\frac{1}{N}\sum_{i=1}^{N} f(x_i) \approx \mathbb{E}_p[g]$$



A random walk over a 2-d Gaussian

Markov chain Monte Carlo

The algorithm at a high level:

- Initialize x_0 from some distribution π_0.
- Run your Markov chain for $(B + N)$ iterations.
- Discard the first B 'burn-in' samples.
- Calculate average using the remaining N samples.

Need a transition kernel $T(x_{old} \to x_{new})$ that is:

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Correct: The goal of MCMC is to find a set of local moves that produce samples (asymtotically) from the correct distribution

Efficient: The art of MCMC is to find inexpensive local moves than coverge rapidly (a chain that 'mixes rapidly')

Ergodicity

What do we mean by correctness?

- For any function h, as $N \to \infty$,

$$\frac{1}{N} \sum_{i=1}^{N} h(x_i) \to \mathbb{E}_\pi[h] \qquad \text{(Ergodicity)}$$

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What are conditions for ergodicity?

Ergodicity requires:

Stationarity If x_i is distributed according to π, then so is x_{i+1}

$$\pi(x_{i+1}) = \int_{\mathcal{X}} \pi(x_i) T(x_i \rightarrow x_{i+1}) \mathrm{d}\theta_i$$

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Aperiodicity A final technical condition (overcome by allowing self-transitions)

(Also **positive recurrence** sometimes, but we won't worry too much about this, see slide 14).

If $x_0 \sim \pi$, then $X_N \sim \pi$ for all N.

$$\mathbb{E}_\pi \left[\frac{1}{N} \sum_{i=1}^{N} g(x_i) \right] = \mathbb{E}_\pi[g]$$

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MCMC estimate has larger variance (N dependent samples usually has a smaller effective sample size (ESS)).

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Does a stationary distribution always exist?

For a finite-state chain, yes (Perron-Frobenius theorem).

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We need our Markov chain to be irreducible:

For each (x_{old}, x_{new}), there exists an n such that

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Still not sufficient: we need aperiodicity. Example?

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Still not sufficient: we need aperiodicity. Example?
Usually ensure aperiodicity by defining a 'lazy' Markov chain that can have self-transitions.

Ergodicity

A finite-state irreducible aperiodic Markov chain has a unique stationary distribution. For any starting distribution π_0,

$$\pi^N \to \pi \textit{ as } N \to \infty$$

$$\frac{1}{N}\sum_{i=1}^{N} g(x_i) \to \mathbb{E}_\pi[g] \qquad \text{(Ergodicity)}$$

Usually $\mathcal{X}$ is infinite-valued space (e.g. the real line).

Now ergodicity also needs ‘positive recurrence’.
Informally, the Markov chain should return to any neighborhood infinitely often.
Harder to establish, but often the case.

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Reversible Markov chains

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A reversible Markov chain satisfies:

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Also called **detailed balance**.

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Easy way to verify stationarity or construct T.
Note: converse is not true.

MCMC: A FIRST LOOK

Find a transition function $T(\cdot \to \cdot)$ with stationary distrib. p

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Markov chain Monte Carlo to sample from p