Probabilistic Inference and Learning
Lecture 21
Markov Chain Monte Carlo

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14 January 2019

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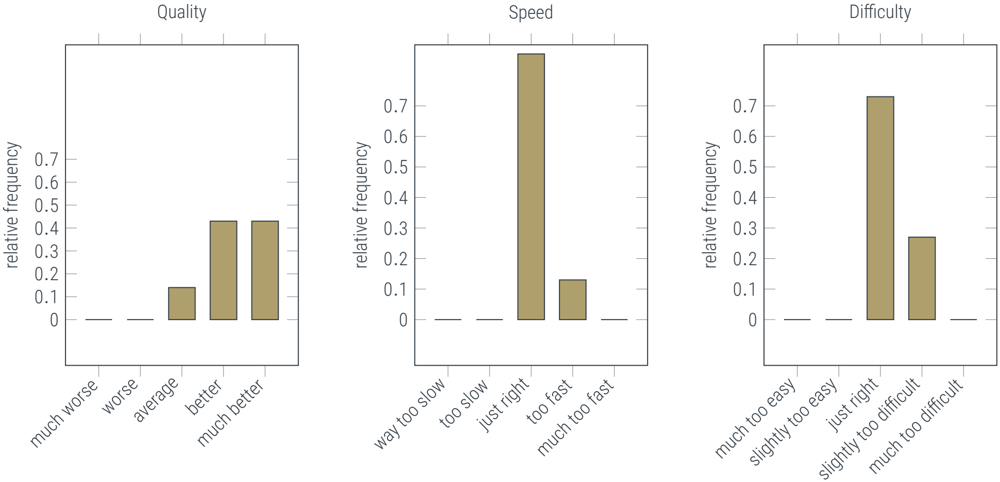
Chair for the Methods of Machine Learning

Last Lecture: Debrief

Feedback dashboard



Last Lecture: Debrief

Detailed Feedback

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Things you did not like:

-

Things you did not understand:

- Why would you want to use a **biased** estimator at all?
- slide 12: Why is it $\mathbb{E}[\frac{1}{S}\sum_{s=1}^{S}(f(x)-\phi)]^2$, shouldn't it be $\mathbb{E}[\frac{1}{S}(\sum_{s=1}^{S} f(x)) - \phi]^2$

Things you enjoyed:

- **discussion of randomness**
- **historical aside**
- discussion of biasedness
- figures
- π-example
- inefficiency of rejection sampling
- "erwartungstreu"
- repetitions from earlier lectures

Ein Hinweis in Eigener Sache …

http://sciencenotes.de

- 17.01.2019, Schlachthaus Tübingen
- Einlass: 19:30 Uhr, Beginn: 20:00 Uhr

1. Wie sehen Maschinen unsere Welt?,
   Dr. Wieland Brendel
2. tbd ,
   Dr. Caterina deBacco
3. Präzise Unsicherheit – Rechenalgorithmen für lernende Maschinen, Prof. Dr. Philipp Hennig
4. Understanding Self-Organization of the Brain,
   Dr. Anna Levina
5. Open Mic: Künstliche Intelligenz und Wir

LIVE-SET: STRÖME

Sampling (Monte Carlo) Methods

Recap from Monday

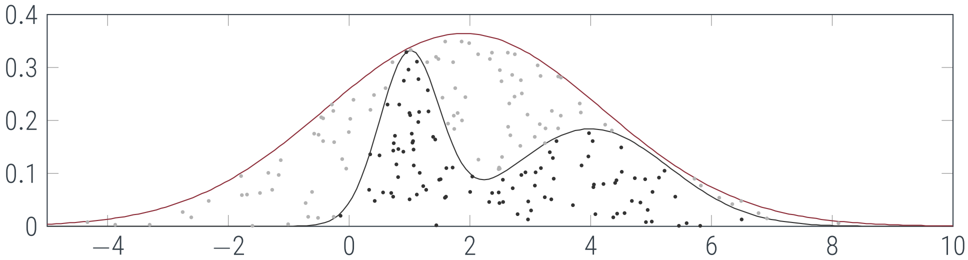
$$\mathbb{E}_p(f) = \int f(x)p(x)\,dx \approx \frac{1}{S}\sum_{s=1}^{S} f(x_s) := \hat{f} \quad \text{if} \quad x_s \sim p \quad \mathbb{E}[\hat{f}] = \mathbb{E}[f], \quad \operatorname{var}[\hat{f}] = \frac{\operatorname{var}(f)}{S}$$

Sampling is a way of performing rough probabilistic computations, in particular for **expectations** (including **marginalization**).

- samples from a probability distribution can be used to estimate expectations, roughly
- 'random numbers' don't need to be **unpredictable**, but rather **unstructured**
- uniformly distributed random numbers can be **transformed** into other distributions. This can be done numerically efficiently in some cases, and it is worth thinking about doing so
- Rejection sampling is a primitive but **exact** method that works with **intractable** models

Rejection Sampling

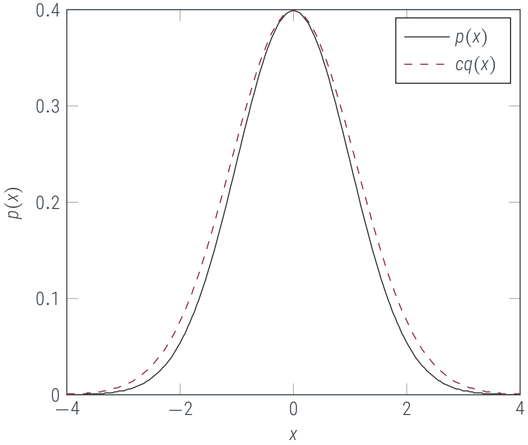
a simple method [Georges-Louis Leclerc, Comte de Buffon, 1707–1788]



- for any $p(x) = \tilde{p}(x)/Z$ (normalizer Z not required)
- choose $q(x)$ s.t. $cq(x) \geq \tilde{p}(x)$
- draw $s \sim q(x)$, $u \sim \text{Uniform}[0, cq(s)]$
- reject if $u > \tilde{p}(s)$

The Problem with Rejection Sampling

the curse of dimensionality [MacKay, §29.3]



Example:

- $p(x) = \mathcal{N}(x; 0, \sigma_p^2)$
- $q(x) = \mathcal{N}(x; 0, \sigma_q^2)$
- $\sigma_q > \sigma_p$
- optimal c is given by

$$c = \frac{(2\pi\sigma_q^2)^{D/2}}{(2\pi\sigma_p^2)^{D/2}} = \left(\frac{\sigma_q}{\sigma_p}\right)^D \exp\left(D \ln \frac{\sigma_q}{\sigma_p}\right)$$

- acceptance rate is ratio of volumes: $1/c$
- rejection rate rises **exponentially** in D
- for $\sigma_q/\sigma_p = 1.1$, $D = 100$, $1/c < 10^{-4}$

Importance Sampling

a slightly less simple method

- computing $\tilde{p}(x), q(x)$, then throwing them away seems wasteful
- instead, rewrite (assume $q(x) > 0$ if $p(x) > 0$)

$$\begin{aligned}\phi = \int f(x)p(x)\,\mathrm{d}x &= \int f(x)\frac{p(x)}{q(x)}q(x)\,\mathrm{d}x \\ &\approx \frac{1}{S}\sum_s f(x_s)\frac{p(x_s)}{q(x_s)} =: \frac{1}{S}\sum_s f(x_s)w_s \qquad \text{if } x_s \sim q(x)\end{aligned}$$

- this is just using a new function $g(x) = f(x)p(x)/q(x)$, so it is an unbiased estimator
- w_s is known as the **importance (weight)** of sample s
- if normalization unknown, can also use $\tilde{p}(x) = Zp(x)$

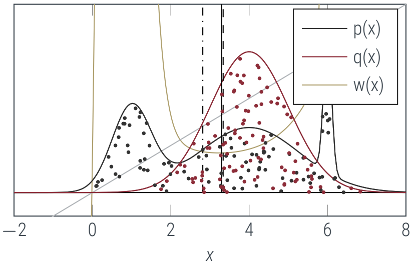
$$\begin{aligned}\int f(x)p(x) &= \frac{1}{Z}\frac{1}{S}\sum_s f(x_s)\frac{\tilde{p}(x_s)}{q(x_s)}\,\mathrm{d}x \\ &= \frac{1}{S}\sum_s f(x_s)\frac{\tilde{p}(x_s)/q(x_s)}{\frac{1}{S}\sum_{s'} 1\tilde{p}(x_s)/q(x_s)} =: \sum_s f(x_s)\tilde{w}_s\end{aligned}$$

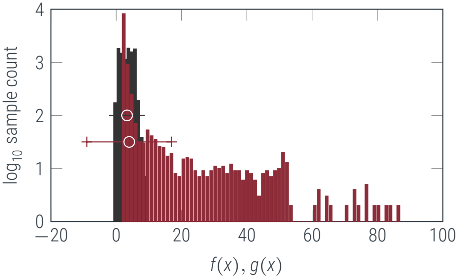
- this is consistent, but biased

What's wrong with Importance Sampling?

the curse of dimensionality, revisited

- recall that $\operatorname{var}\hat{\phi} = \operatorname{var}(f)/S$ – importance sampling replaces $\operatorname{var}(f)$ with $\operatorname{var}(g) = \operatorname{var}\left(f\frac{p}{q}\right)$
- $\operatorname{var}\left(f\frac{p}{q}\right)$ can be very large if $q \ll p$ somewhere. In many dimensions, usually all but everywhere!
- if p has "undiscovered islands", some samples have $p(x)/q(x) \to \infty$





Markov-Chain Monte Carlo

random walks drawing random numbers

- problem of importance sampling: samples generated independently, requires q good approximation to p everywhere.
- instead: generate samples **iteratively**, approximation q only needs to be good *locally*

Definition (Reminder: Markov Chains)

A joint distribution $p(X)$ over a sequence of random variabels $X := [x_0, \dots, x_N]$ is said to have **the Markov property** if

$$p(x_i \mid x_0, x_1, \dots, x_{i-1}) = p(x_t \mid x_{i-1}).$$

The sequence is then called a **Markov chain**.

An analogy

optimization

assume we wanted to find the maximum of $\tilde{p}(x)$

- given current estimate x_t
- draw proposal $x' \sim q(x' \mid x_t)$
- evaluate

$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)}$$

- if $a \geq 1$, accept: $x_{t+1} \leftarrow x'$
- else stay: $x_{t+1} \leftarrow x_t$

Usually, throw away estimates at the end, only keep "best guess". But the estimates do contain information about the shape of $\tilde{p}$!

The Metropolis-Hastings* Method

* Authorship controversial. Likely inventors: M. Rosenbluth, A. Rosenbluth & E. Teller, 1953

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we want to find representers (**samples**) of $\tilde{p}(x)$

- given current sample x_t
- **draw proposal** $x' \sim q(x' \mid x_t)$ (for example, $q(x' \mid x_t) = \mathcal{N}(x'; x_t, \sigma^2)$)
- **evaluate**

$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)}$$

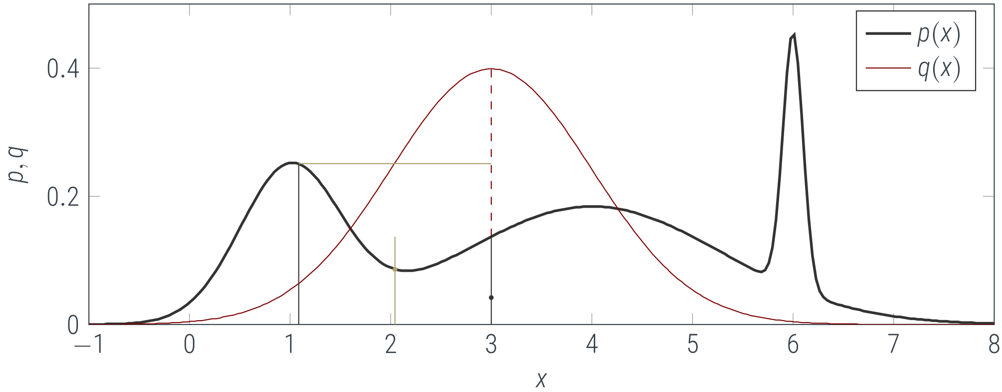
- if $a \geq 1$, **accept**: $x_{t+1} \leftarrow x'$
- else
  - **accept** with probability a: $x_{t+1} \leftarrow x'$
  - **stay** with probability $1 - a$: $x_{t+1} \leftarrow x_t$

Usually, assume symmetry $q(x_t \mid x') = q(x' \mid x_t)$ (the Metropolis method)

- no rejection. Every sample counts!
- like optimization, but with a chance to move downhill

Metropolis-Hastings in pictures

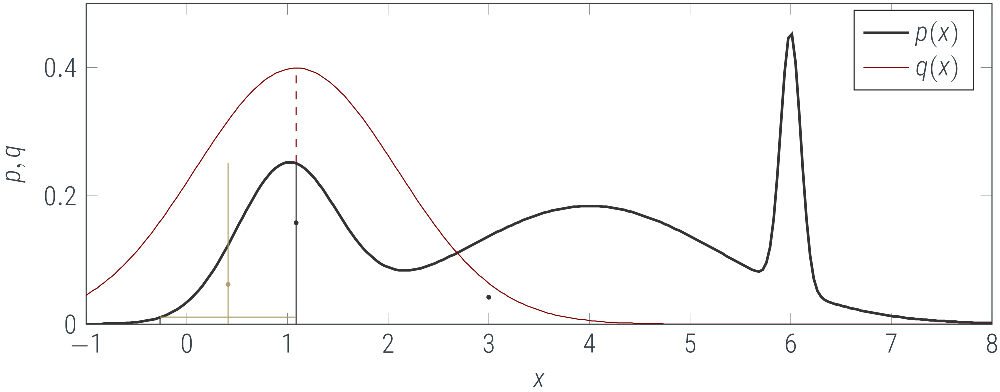
$t = 1$



$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)} \qquad \text{accept with } p = \min(1, a)$$

Metropolis-Hastings in pictures

$t = 2$

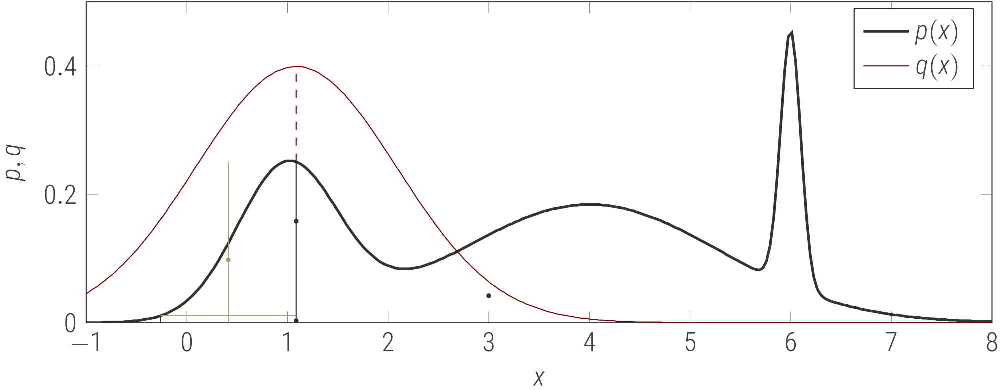


$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)}$$

accept with $p = \min(1, a)$

Metropolis-Hastings in pictures

$t = 3$

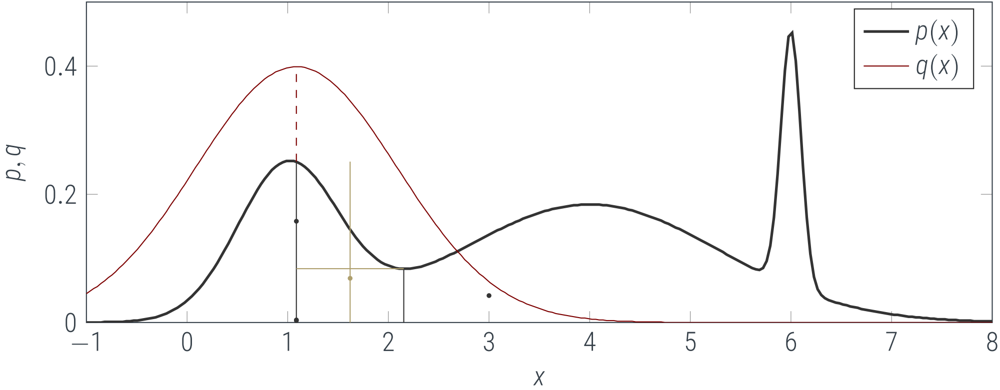


$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)}$$

accept with $p = \min(1, a)$

Metropolis-Hastings in pictures

$t = 4$

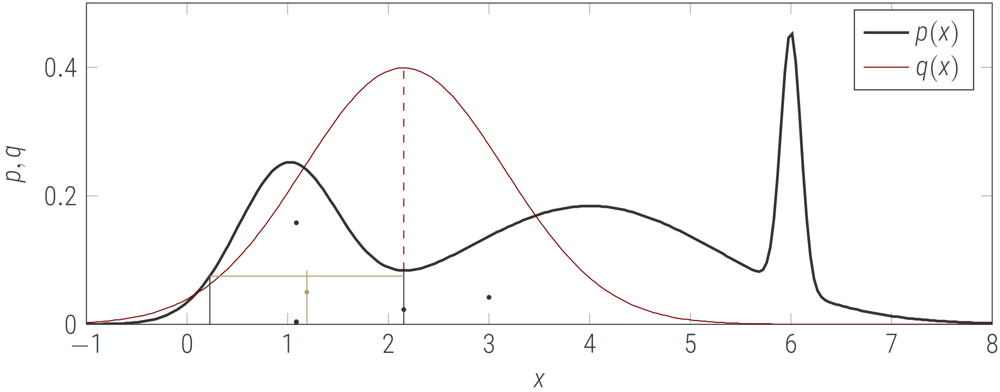


$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)}$$

accept with $p = \min(1, a)$

Metropolis-Hastings in pictures

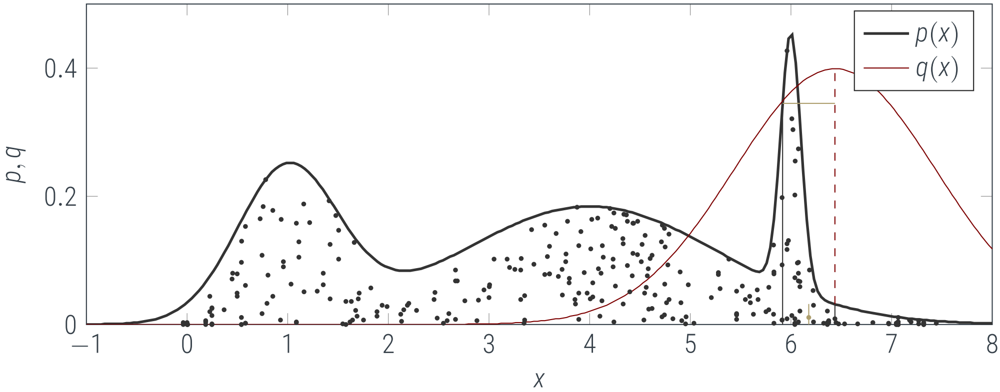
$t = 5$



$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)} \qquad \text{accept with } p = \min(1, a)$$

Metropolis-Hastings in pictures

$t = 300$



$$a = \frac{\tilde{p}(x')}{\tilde{p}(x_t)} \frac{q(x_t \mid x')}{q(x' \mid x_t)} \qquad \text{accept with } p = \min(1, a)$$

Why is this a Monte Carlo Method?

MH draws from $p(x)$ in the limit of ∞ samples

proof (sketch) existence of stationary distribution: detailed balance

- MH satisfies detailed balance

$$
\begin{aligned}
p(x)T(x \to x') &= p(x) \cdot q(x' \mid x) \min\left[1, \frac{p(x')q(x \mid x')}{p(x)q(x' \mid x)}\right] \\
&= \min[p(x)q(x' \mid x), p(x')q(x \mid x')] \\
&= p(x') \cdot q(x \mid x') \min\left[\frac{p(x)q(x' \mid x)}{p(x')q(x \mid x')}, 1\right] \\
&= p(x')T(x' \to x)
\end{aligned}
$$

- Markov Chains satisfying detailed balance have **at least one *stationary distribution***

$$
\int p(x)T(x \to x')\,\mathrm{d}x = \int p(x')T(x' \to x)\,\mathrm{d}x = p(x') \int T(x' \to x)\,\mathrm{d}x = p(x')
$$

Why is this a Monte Carlo Method?

MH draws from $p(x)$ in the limit of ∞ samples

proof (sketch) uniqueness of stationary distribution:

Definition

Ergodicity A sequence $\{x_t\}_{t\in\mathbb{N}}$ is called **ergodic** if it

1. is *a-periodic* (contains no recurring sequence)
2. has *positive recurrence*: $x_t = x_*$ implies there is a $t' > t$ such that $p(x_{t'} = x_*) > 0$

→ $\{x_t\}_{t\in\mathbb{N}}$ is ergodic (by definition)

- ergodic Markov Chains have **at most one stationary distribution**

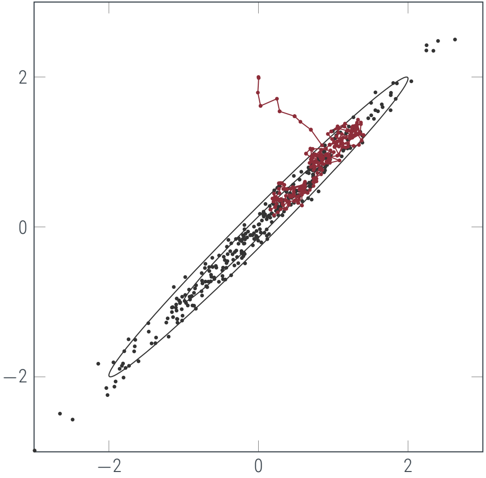
Theorem (convergence of Metropolis-Hastings, simplified)

If $q(x' \mid x_t) > 0 \ \forall (x', x_t)$, then, for any x_0, the density of $\{x_t\}_{t\in\mathbb{N}}$ approaches $p(x)$ as $t \to \infty$.

- this is not a statement about convergence rate!

Metropolis-Hastings performs a (biased) random walk

hence diffuses $\mathcal{O}(s^{1/2})$



Rule of Thumb: [MacKay, (29.32)]

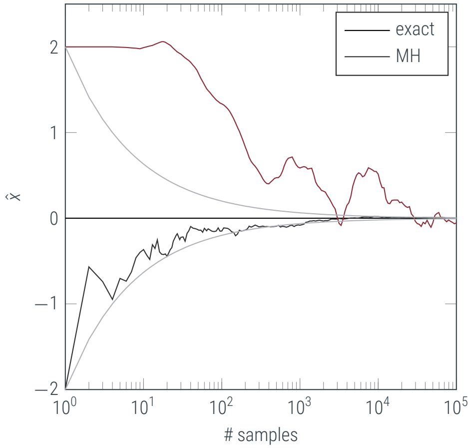
- typical use-case: high-dimensional D problem of largest length-scale L, smallest ε, isotropic proposal distribution
- have to set width of q to $\approx \varepsilon$, otherwise acceptance rate r will be very low.
- then Metropolis-Hastings does a **random walk** in D dimensions, moving a distance of $\sqrt{\mathbb{E}[\|x_t - x_0\|^2]} \sim \epsilon\sqrt{rt}$
- so, to create **one** independent draw at distance L, MCMC has to run for **at least**

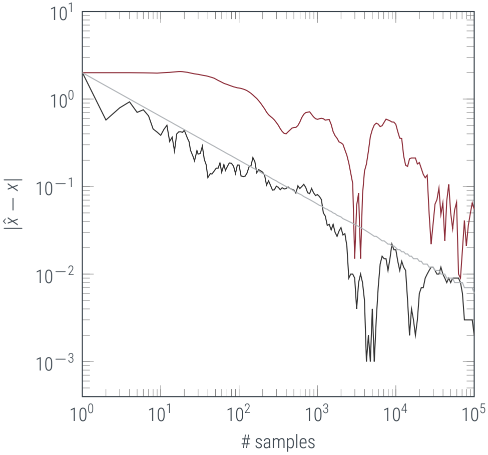
$$t \sim r\left(\frac{L}{\epsilon}\right)^2$$

iterations. In practice (e.g. if the distribution has *islands*), the situation can be **much** worse.

Metropolis-Hastings performs a (biased) random walk

estimating the mean of a correlated Gaussian





Gibbs Sampling

MCMC with optimal proposal distribution

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[D. & S. Geman, 1984]

- $x_t \leftarrow x_{t-1}; x_{ti} \sim p(x_{ti} \mid x_{t1}, x_{t2}, \dots, x_{t(i-1)}, x_{t(i+1)}, \dots)$
- a special case of Metropolis-Hastings:
  - $q(x' \mid x_t) = \delta(x'_{\setminus i} - x_{t,\setminus i}) p(x'_i \mid x_{t,\setminus i})$
  - $p(x') = p(x'_i \mid x'_{\setminus i}) p(x'_{\setminus i}) = p(x'_i \mid x_{t,\setminus i}) p(x_{t,\setminus i})$
  - acceptance rate:

$$a = \frac{p(x')}{p(x_t)} \cdot \frac{q(x_t \mid x')}{q(x' \mid x_t)} \qquad = \frac{p(x'_i \mid x_{t,\setminus i}) p(x_{t,\setminus i})}{p(x_{ti} \mid x_{t,\setminus i}) p(x_{t,\setminus i})} \cdot \frac{q(x_t \mid x')}{\delta(x'_{\setminus i} - x_{t,\setminus i}) p(x'_i \mid x_{t,\setminus i})}$$

$$= \frac{q(x_t \mid x')}{p(x_{ti} \mid x_{t,\setminus i}) \delta(x'_{\setminus i} - x_{t,\setminus i})} \qquad = 1$$

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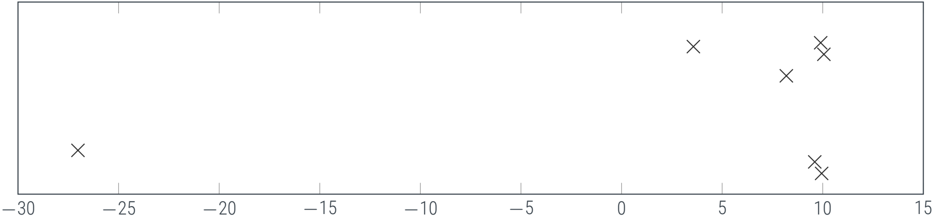
a simple example (DJC MacKay, Information Theory, Inference and Learning Algorithms, Ex. 22.15)



Scientist	A	B	C	D	E	F	G
x_n	-27.020	3.570	8.191	9.898	9.603	9.945	10.056

- likelihood: choose Gaussian, typical noise model

$$p(\boldsymbol{x} \mid \mu, \boldsymbol{\sigma}) = \prod_i^7 \mathcal{N}(x_i; \mu, \sigma_i^2) = \prod_i \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(x_i - \mu)^2}{2\sigma_i^2}\right)$$

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setting up the model

- likelihood: choose Gaussian, typical noise model

$$p(\boldsymbol{x} \mid \mu, \boldsymbol{\sigma}) = \prod_i^7 \mathcal{N}(x_i; \mu, \sigma_i^2) = \prod_i \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(x_i - \mu)^2}{2\sigma_i^2}\right)$$

- priors: **exponential families**
  - vague Gaussian prior on μ (e.g. $m = 0, s = 100$)

$$p(\mu) = \mathcal{N}(\mu; m, s^2) = \frac{1}{\sqrt{2\pi}s} \exp\left(-\frac{(\mu - m)^2}{2s^2}\right)$$

  - vague Gamma priors on σ_i^{-2} (e.g. $k = 1, \theta = 10$)

$$p(\sigma_i) = \mathcal{G}(\sigma_i^{-2}; k, \theta) = \frac{1}{\Gamma(k)\theta^k} (\sigma_i^{-2})^{k-1} \exp\left(-\frac{\sigma_i^{-2}}{\theta}\right)$$

(there are good algorithms for sampling from $\mathcal{G}(k, \theta)$).

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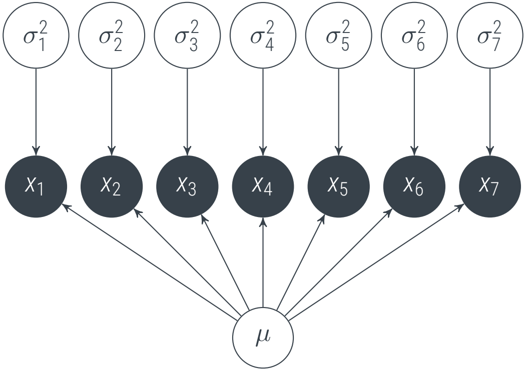
graphical model



$$p(\boldsymbol{x}, \boldsymbol{\sigma}, \mu) = \mathcal{N}(\mu; m, v^2) \prod_i \mathcal{N}(x_i; \mu, \sigma_i^2) \mathcal{G}(\sigma_i^{-2}; a, b)$$

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how about maximum likelihood?

- Can we get away without priors? Maximum likelihood inference

$$\log p(\boldsymbol{x} \mid \mu, \boldsymbol{\sigma}) = \sum_i -\frac{(x_i - \mu)^2}{2\sigma_i^2} - \frac{1}{2}\log \sigma_i^2 - \frac{1}{2}\log 2\pi$$

$$\frac{\partial p(\boldsymbol{x} \mid \mu, \boldsymbol{\sigma})}{\partial \mu} = \sum_i \frac{(x_i - \mu)}{\sigma_i^2} = 0 \quad \Rightarrow \quad \mu_* = \frac{\sum_i x_i/\sigma_i^2}{\sum_i 1/\sigma_i^2}$$

$$\frac{\partial p(\boldsymbol{x} \mid \mu, \boldsymbol{\sigma})}{\partial \sigma_i} = \frac{(x_i - \mu)^2}{\sigma_i^3} - \frac{1}{\sigma_i} = 0 \quad \Rightarrow \quad \sigma_i \rightarrow 0$$

- maximum likelihood solution: choose arbitrary i, set $\sigma_i \rightarrow 0$, $\mu \rightarrow x_i$

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conditional independences

- if $\boldsymbol{\sigma}$ were known, posterior on μ would be **analytical conjugate prior!** (1)

$$p(\mu \mid \mathbf{x}, \boldsymbol{\sigma}) \propto \mathcal{N}(\mu; m, s^2) \prod_i^7 \mathcal{N}(x_i; \mu, \sigma_i^2) \propto \mathcal{N}\left[\mu; \psi^2 \left(\frac{m}{s^2} + \sum_i \frac{x_i}{\sigma_i^2}\right), \psi^2 = \left(\frac{1}{s^2} + \sum_i \frac{1}{\sigma_i^2}\right)^{-1}\right]$$

- if μ were known, posterior on $\boldsymbol{\sigma}$ would be **analytical conjugate prior!** (2)

$$p(\boldsymbol{\sigma} \mid \mathbf{x}, \mu) \propto \prod_i^7 \mathcal{N}(x_i; \mu, \sigma_i^2)\mathcal{G}(\sigma_i^{-2}; k, \theta) \propto \prod_i \mathcal{G}\left[\sigma_i^{-2}; k + \frac{1}{2}, \left(\frac{1}{\theta} + \frac{(x_i - \mu)^2}{2}\right)^{-1}\right]$$

→ Gibbs sampling: fix some $\boldsymbol{\sigma}_0$ (e.g. from prior). repeat:
  - draw $\mu_t \sim p(\mu \mid \mathbf{x}, \boldsymbol{\sigma}_{t-1})$ from (1)
  - draw $\boldsymbol{\sigma}_t \sim p(\boldsymbol{\sigma} \mid \mathbf{x}, \mu_t)$ from (2)

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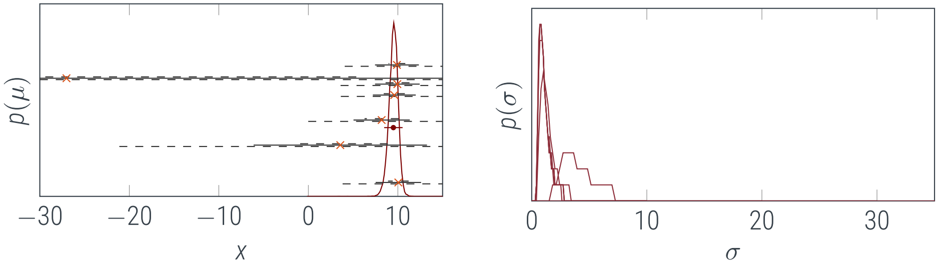
sampling posterior from $3 \cdot 10^4$ samples



Further Reading

A field of its own. [MacKay, chapters 29 & 30]

Hamiltonian Monte Carlo (aka hybrid Monte Carlo)

- introduce momentum variables to reduce diffusion (requires gradient of p)
- various adaptations, e.g. for local shape of p ("Riemannian MCMC")
- NUTS (the No U-Turn Sampler) (M. Hoffman & A. Gelman, JMLR 15, 2014): a parameter free HMC method, currently arguably the gold standard for models allowing auto-diff

Slice Sampling

- very efficient (exponentially fast) exploration in one dimension
- almost no free parameters (but problems in many dimensions)
- elliptical slice sampling [Murray et al., 2010]: Very efficient for Gaussian priors, no free parameters

But:

- in nontrivial situations no sampling method except exact sampling gives exact finite-time bounds
- diagnostic tricks exist, but are not without flaws

Summary

Markov Chain Monte Carlo (MCMC) methods

- Methods drawing $\{x_t\}_{t\in\mathbb{N}}$ from $p(x_t \mid x_{t-1})$ are called **Markov Chains**
- if the density of $\{x_t\}$ converges to $p(x)$ as $t \to \infty$, the method is called **Markov Chain Monte Carlo (MCMC)**
- **Metropolis-Hastings** is a simple MCMC method requiring **few assumptions**
- **Gibbs** sampling is MH with optimal proposal distributions, requiring analytical samples from **conditional distributions**
- improved, more elaborate methods exist
- all MCMC methods suffer from **diffusion**, which can be very difficult to detect in practice
- MCMC approach **exact** answers after an **unknown** time