Monte Carlo

— Monte Carlo basics and Motivation
— Rejection sampling
— Importance sampling
— Next time: Markov chain Monte Carlo

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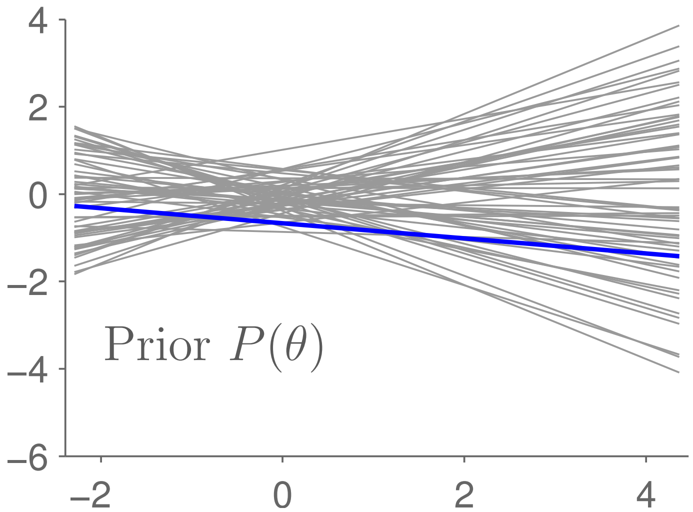
Monte Carlo and Insomnia

Enrico Fermi (1901–1954) took great delight in astonishing his colleagues with his remakably accurate predictions of experimental results. . . he revealed that his "guesses" were really derived from the statistical sampling techniques that he used to calculate with whenever insomnia struck in the wee morning hours!

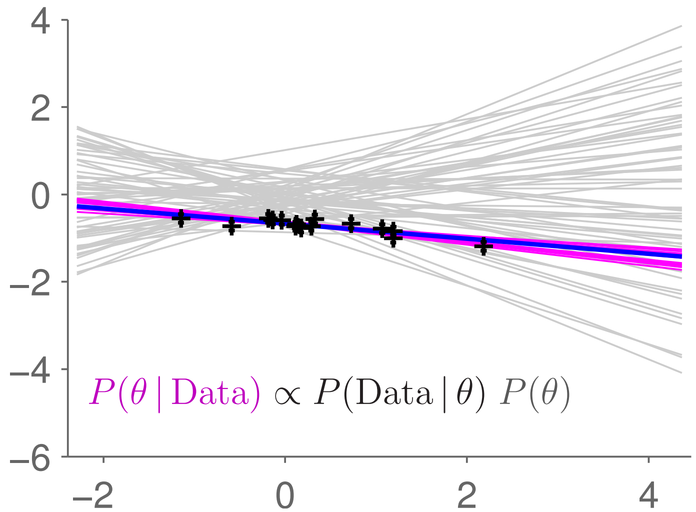
—*The beginning of the Monte Carlo method,*
N. Metropolis

Linear Regression: Prior



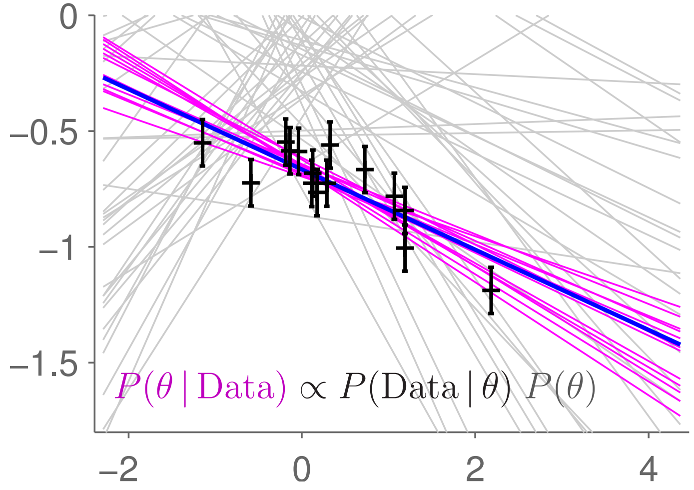
Input → output mappings considered plausible before seeing data.

Linear Regression: Posterior



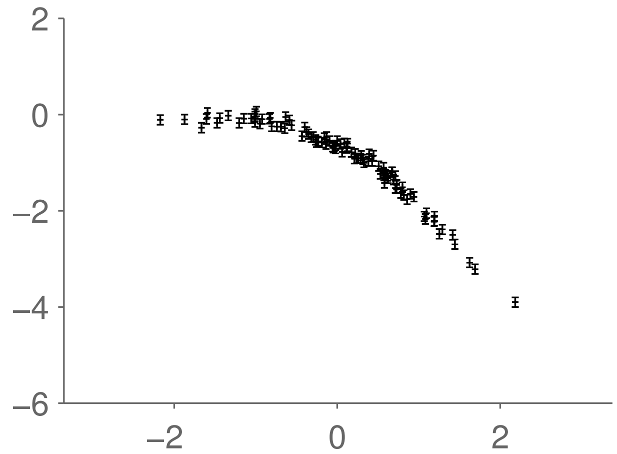
Posterior much more compact than prior.

Linear Regression: Posterior



Draws from posterior. Non-linear error envelope. Possible explanations linear.

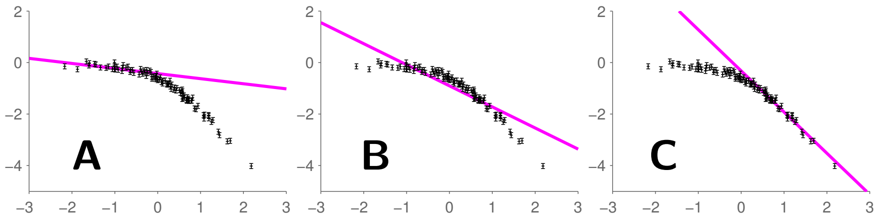
Model mismatch



What will Bayesian linear regression do?

Quiz

Given a (wrong) linear assumption, which explanations are typical of the posterior distribution?

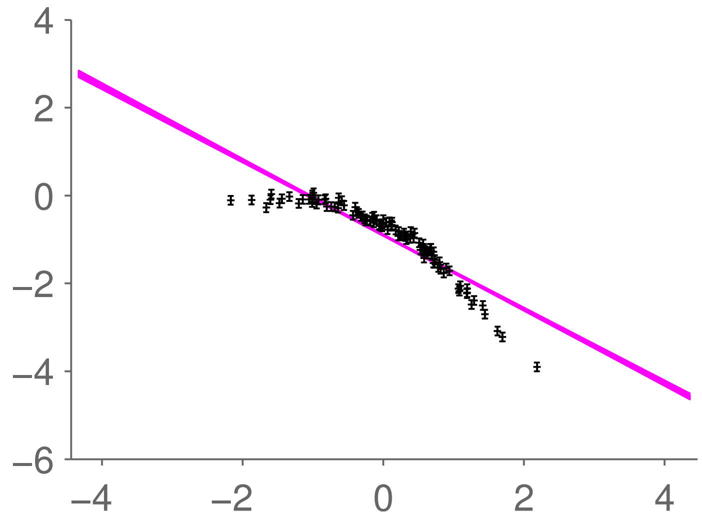


D All of the above

E None of the above

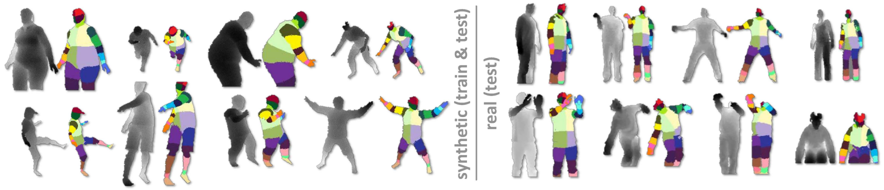
Z Not sure

'Underfitting'



Posterior *very* certain despite blatant misfit. Prior ruled out truth.

Microsoft Kinect (Shotton et al., 2011)



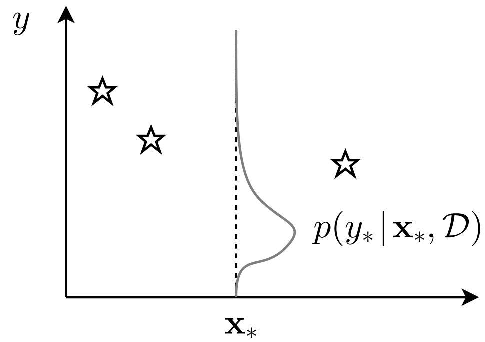
Eyeball modelling assumptions

Generate training data

Random forest applied to fantasies

The need for integrals

$$p(y_*\,|\,\mathbf{x}_*, \mathcal{D}) = \int \mathrm{d}\theta\; p(y_*, \theta\,|\,\mathbf{x}_*, \mathcal{D})$$
$$= \int \mathrm{d}\theta\; p(y_*\,|\,\theta, \cancel{\mathcal{D}})\, p(\theta\,|\,\cancel{\mathbf{x}_*}, \mathcal{D})$$



A statistical problem

What is the average height of the people in this room?
Method: measure our heights, add them up and divide by N.

What is the average height f of people p in Edinburgh $\mathcal{E}$?

$$E_{p\in\mathcal{E}}[f(p)] \equiv \frac{1}{|\mathcal{E}|}\sum_{p\in\mathcal{E}} f(p), \quad \text{“intractable”?}$$

$$\approx \frac{1}{S}\sum_{s=1}^{S} f\big(p^{(s)}\big), \quad \text{for random survey of } S \text{ people } \{p^{(s)}\} \in \mathcal{E}$$

Surveying works for large and notionally infinite populations.

Simple Monte Carlo

In general:

$$\int f(x) P(x)\,\mathrm{d}x \;\approx\; \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)$$

Example: making predictions

$$P(x\,|\,\mathcal{D}) \;=\; \int P(x\,|\,\theta)\, p(\theta\,|\,\mathcal{D})\,\mathrm{d}\theta$$
$$\approx \frac{1}{S}\sum_{s=1}^{S} P(x\,|\,\theta^{(s)}), \quad \theta^{(s)} \sim p(\theta\,|\,\mathcal{D})$$

Many other integrals appear throughout statistical machine learning

Properties of Monte Carlo

Estimator: $\int f(x)\,P(x)\,\mathrm{d}x \;\approx\; \hat{f} \;\equiv\; \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)$

Estimator is unbiased:

$$\mathbb{E}_{P(\{x^{(s)}\})}\left[\hat{f}\right] \;=\; \frac{1}{S}\sum_{s=1}^{S}\mathbb{E}_{P(x)}[f(x)] \;=\; \mathbb{E}_{P(x)}[f(x)]$$

Variance shrinks $\propto 1/S$:

$$\mathrm{var}_{P(\{x^{(s)}\})}\left[\hat{f}\right] \;=\; \frac{1}{S^2}\sum_{s=1}^{S}\mathrm{var}_{P(x)}[f(x)] \;=\; \mathrm{var}_{P(x)}[f(x)]\,/S$$

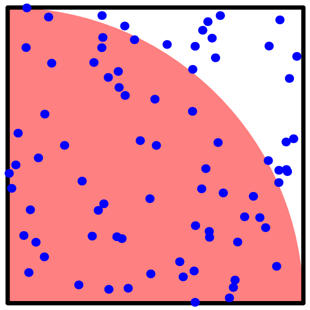
"Error bars" shrink like $\sqrt{S}$

Aside: don't always sample!

"Monte Carlo is an extremely bad method; it should be used only when all alternative methods are worse."

— Alan Sokal, 1996

A dumb approximation of π



$$P(x,y) = \begin{cases} 1 & 0<x<1 \text{ and } 0<y<1 \\ 0 & \text{otherwise} \end{cases}$$

$$\pi = 4\iint \mathbb{I}\left((x^2+y^2)<1\right) P(x,y)\,\mathrm{d}x\,\mathrm{d}y$$

```
octave:1> S=12; a=rand(S,2); 4*mean(sum(a.*a,2)<1)
ans = 3.3333
octave:2> S=1e7; a=rand(S,2); 4*mean(sum(a.*a,2)<1)
ans = 3.1418
```

Alternatives to Monte Carlo

There are other methods of numerical integration!

Example: (nice) 1D integrals are easy:

```
octave:1> 4 * quadl(@(x) sqrt(1-x.^2), 0, 1, tolerance)
```

Gives π to 6 dp's in 108 evaluations, machine precision in 2598.
(NB Matlab's `quadl` fails at `tolerance=0`, but Octave works.)

In higher dimensions sometimes determinstic approximations work: Variational Bayes, Laplace, . . . (covered later)

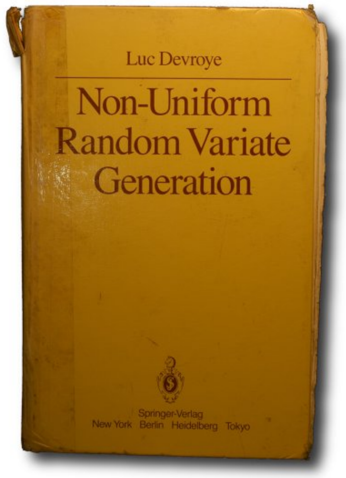
Reminder

Want to sample to approximate expectations:

$$\int f(x)P(x)\,\mathrm{d}x \;\approx\; \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)$$

How do we get the samples?

Sampling simple distributions

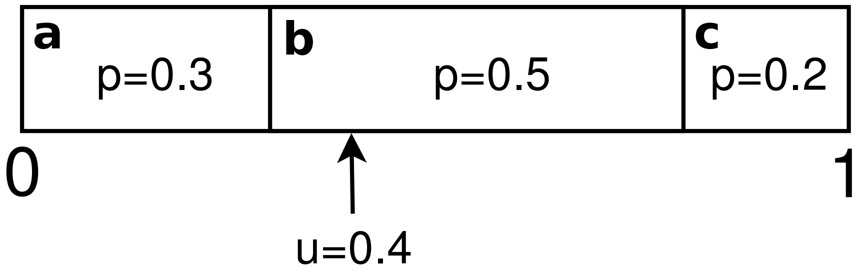


Use library routines for univariate distributions
(and some other special cases)

This book (free online) explains how some of them work

http://cg.scs.carleton.ca/~luc/rnbookindex.html

Sampling discrete values



$$u \sim \mathrm{Uniform}[0,1]$$

$$u = 0.4 \quad \Rightarrow \quad x = \mathsf{b}$$

There are more efficient ways for large numbers of values and samples. See Devroye book.

Sampling from densities

How to convert samples from a Uniform[0,1] generator:

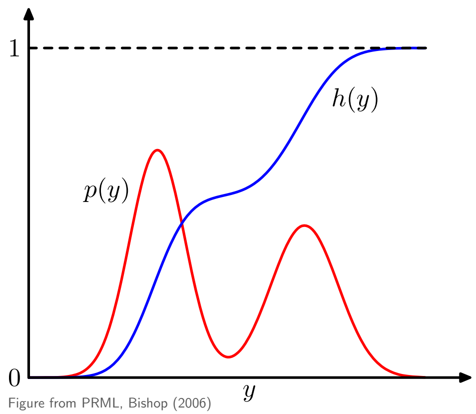


Figure from PRML, Bishop (2006)

$h(y) = \int_{-\infty}^{y} p(y')\,\mathrm{d}y'$

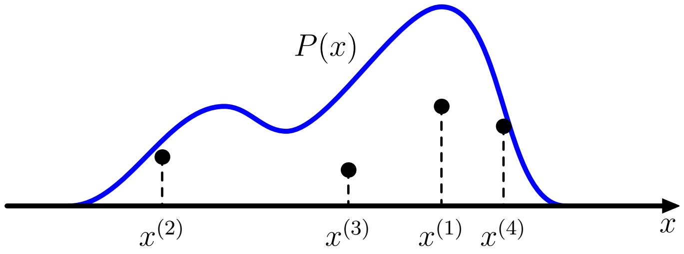
$u \sim$ Uniform[0,1]

Sample, $y(u) = h^{-1}(u)$

Although we can't always compute and invert $h(y)$

Sampling from densities

Draw points uniformly under the curve:



Probability mass to left of point $\sim$ Uniform[0,1]

Rejection sampling

Sampling from $\pi(x)$ using tractable $q(x)$:

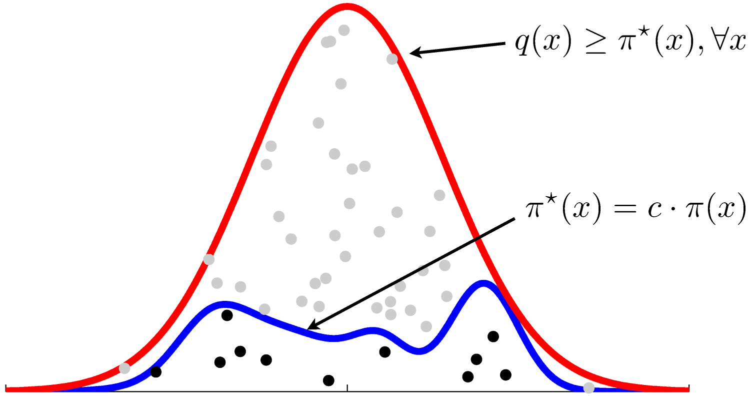


Figure credit: Ryan P. Adams

Importance sampling

Rewrite integral: expectation under simple distribution Q:

$$\int f(x)\, P(x)\, \mathrm{d}x \;=\; \int f(x) \frac{P(x)}{Q(x)} Q(x)\, \mathrm{d}x,$$

$$\approx \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)}) \frac{P(x^{(s)})}{Q(x^{(s)})}, \qquad x^{(s)} \sim Q(x)$$

Simple Monte Carlo applied to any integral.
Unbiased and independent of dimension?

Importance sampling (2)

If only know $P(x) = P^*(x)/\mathcal{Z}_P$ up to constant:

$$\int f(x)\, P(x)\, \mathrm{d}x \;\approx\; \frac{\mathcal{Z}_Q}{\mathcal{Z}_P} \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)}) \underbrace{\frac{P^*(x^{(s)})}{Q^*(x^{(s)})}}_{w^{*(s)}}, \quad x^{(s)} \sim Q(x)$$

$$\approx \cancel{\frac{1}{S}} \sum_{s=1}^{S} f(x^{(s)}) \frac{w^{*(s)}}{\cancel{\frac{1}{S}} \sum_{s'} w^{*(s')}}$$

This estimator is **consistent** but **biased**

Exercise: Prove that $\mathcal{Z}_P/\mathcal{Z}_Q \approx \frac{1}{S}\sum_s w^{*(s)}$

Application to large problems

Approximations scale badly with dimensionality

Example: $P(x) = \mathcal{N}(0, \mathbb{I}), \quad Q(x) = \mathcal{N}(0, \sigma^2\mathbb{I})$

Rejection sampling:

Requires $\sigma \geq 1$. Fraction of proposals accepted $= \sigma^{-D}$

Importance sampling:

$\text{Var}[P(x)/Q(x)] \;=\; \left(\frac{\sigma^2}{2-1/\sigma^2}\right)^{D/2} - 1$

Infinite / undefined variance if $\sigma \leq 1/\sqrt{2}$

Summary so far

- **Monte Carlo**
  approximate expectations with a sample average
- **Rejection sampling**
  draw samples from complex distributions
- **Importance sampling**
  apply Monte Carlo to 'any' sum/integral

Next: High dimensional problems: MCMC