Markov Chain Monte Carlo

Review

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- Sampling Methods
  - Direct
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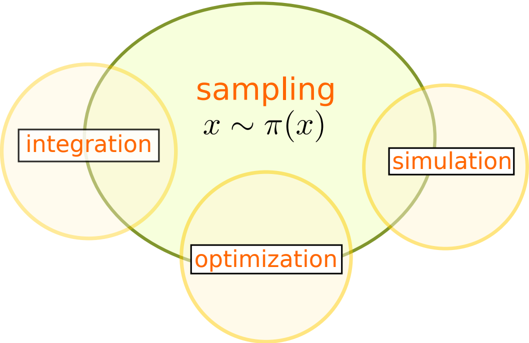
Monte Carlo: The Big Picture

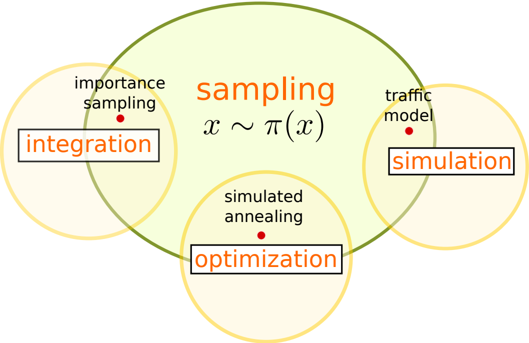


integration: high-dimensions, marginalization, normalization

optimization: global extrema, rough landscape

simulation: scenario modeling, emergent phenomena

Monte Carlo: The Big Picture



integration: high-dimensions, marginalization, normalization

optimization: global extrema, rough landscape

simulation: scenario modeling, emergent phenomena

Sampling Methods

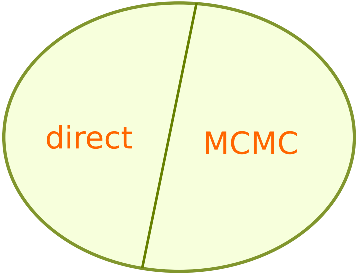
How do I sample from $x \sim \pi(x)$?

Direct Sampling

- accept-reject
- transformation

MCMC

- Metropolis
- Metropolis-Hastings
- MC^3
- Gibbs
- Slice, HMC etc



Sampling Methods

Accept-Reject

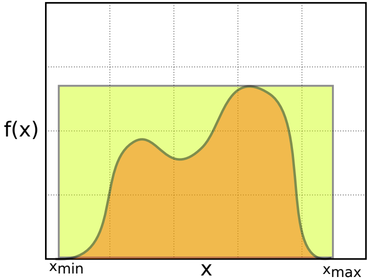
Inspiration: "integration by darts"

simple algorithm, shift burden from human to computer.

(i) pick $x \sim U[x_{min}, x_{max}]$

(ii) pick another random number $u \sim U[0, f_{max}]$

(iii) If $u \leq f(x)$, then accept x. If not, reject x and repeat.



Disadvantages:

(i) infinite domains

(ii) rejection of points: *adaptive rejection sampling*

(iii) peaked distributions, higher dimensions

Transformation Method

Efficient direct sampling method for arbitrary 1D $\pi(x)$.

Unlike accept-reject there are no rejections

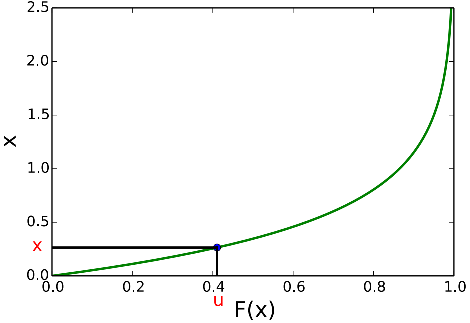
(i) Find CDF $F(x)$

$$F(x) = \int \pi(x) dx$$

(ii) Method is given by

$$u = F(x)$$

where $u \sim U[0, 1)$



Method works best when $x = F^{-1}(u)$ is explicitly available.

Transformation Method: 2D

Consider:

$$(X, Y) \sim f(x, y), \text{ and } (U, V) \sim g(u, v).$$

If $x(u, v)$ and $y(u, v)$ are known 1-1 maps, then,

$$g(u, v) = f(x, y)|\text{det}(J)|,$$

where the Jacobian J is given by,

$$J = \frac{\partial(x, y)}{\partial(u, v)} = \left[\begin{array}{cc} \partial x/\partial u & \partial x/\partial v \\ \partial y/\partial u & \partial y/\partial v \end{array} \right].$$

For multidimensional distributions,

- easy: given transformation $\rightarrow$ determine distribution
- hard: given distribution $\rightarrow$ develop transformation

Error Analysis

Integration Error in Direct Methods

Given an integral,

$$I = \int_a^b f(x)dx$$

The key results for MC integration,

$$I = (b-a)\langle f \rangle$$
$$\sigma_I = \frac{(b-a)\sigma_f}{\sqrt{n}},$$

where

$$\sigma_f^2 = \langle f^2 \rangle - \langle f \rangle^2$$

is the variance of f on the domain.

Given $f(x)$ and domain $[a, b]$, the only way to reduce error is to increase n.

Importance Sampling

Variance reduction technique: lower apparent σ_f^2.

Select suitable $\pi(x)$ so that integral:

$$I = \int_a^b \frac{f(x)}{\pi(x)} \pi(x) dx,$$

Use "Method 2":

1. Draw $x_1, x_2, ..., x_n$ from $\pi(x)$
2. Estimate $I = E(f/\pi)$ via

$$I \approx \frac{1}{n} \sum_{i=1}^{n} \frac{f(x_i)}{\pi(x_i)}.$$

For importance sampling,

$$\sigma_{I,is}^2 = \frac{\sigma_{f/\pi}^2}{n}.$$

Course Trajectory

Overview Material so Far

integrals

$\int_a^b f(x)dx = \bar{f}(b-a)$

$x \sim U[0,1]$

LCD/RNG

$x \sim \pi(x)$

non-uniform

accept/reject

transformation method

error in integrals $\bar{f} = \sum f_i / N$

propagation errors $q(x_1, x_2)$

$$\sigma_q^2 = \left(\frac{\partial q}{\partial x_1}\sigma_{x_1}\right)^2 + \left(\frac{\partial q}{\partial x_2}\sigma_{x_2}\right)^2$$

error in means

$\sigma_{\bar{f}}^2 = \sigma_f^2 / N$

mean distribution is Gaussian

central limit theorem

importance sampling

$$\int f(x)dx = \int \frac{f(x)}{\pi(x)}\pi(x)dx$$

$$\sigma_{\bar{f}}^2 = \sigma_{f/\pi}^2 / N$$

"method 2"

Quizzes

Exam Skills

- some symbolic software: sympy, Matlab, Mathematica
  - algebra, integration/differentiation
- Proficiency in plotting, histograms etc.
- Go through HWs and past exam
- Focus on multidimensional distributions and importance sampling

Exam Details

- in class: Oct 24 between 9:45am-11am
- single question: multiple parts