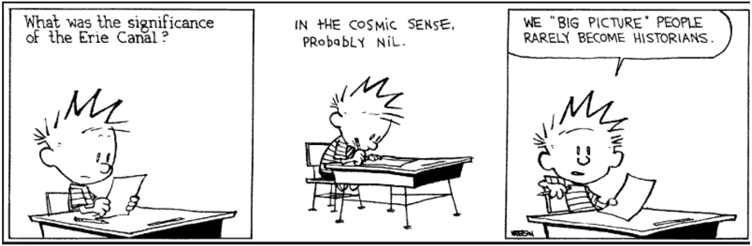
The Big Picture

MC, MCMC and the Rest of the Universe



credit: Bill Watterson

The Big Picture

Goal: a conceptual map to tie some things together.

Monte Carlo means different things to different disciplines.

Similar techniques, different terminology.

Rediscovery is a recurring pattern.

A big-picture understanding allows us to look at broad themes, beyond these domain-specific boundaries.

Motivation

What is the connection between:

- Monte Carlo
- Markov Chain Monte Carlo
- Other numerical methods like finite elements, steepest descent, Gauss quadrature etc.?

At its core MC/MCMC is a sampling technique.

It draws or samples x from any desired distribution $\pi(x)$.

Everything else flows from this simple fact.

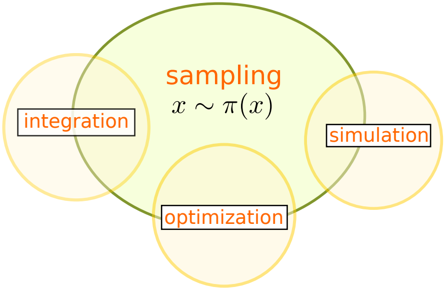
x is usually multidimensional; but in class, we will start with 1D

The Big Picture

Sampling, by itself, is a fundamental problem.

$$x \sim \pi(x).$$

Three important sub-classes of problems are:



Integration

We have seen a little bit of this already;

$$I = \int g(x)dx.$$

Often, we encounter integrals like,

$$I = \int f(x)\pi(x)dx.$$

The $\pi(x)$ highlights the relationship to the sampling problem.

Optimization

$$x^* = \max_x f(x),$$

where x^* is the value at which $f(x)$ is maximized.

Example: A classic fitting problem in condensed matter physics. Given a scatter of data $\{t_i, G_i\}$, fit a sum of decaying exponentials so that:

$$G(t) = \sum_{j=1}^{M} g_j \; e^{-t/\tau_j},$$

with $g_j > 0$, $\tau_j > 0$.

Problem is often approached using a MC-inspired optimization technique called simulated annealing.

Simulation

This is a general term, which defines the evolution of a system subject to particular stochastic mathematical models or rules.

In science and engineering, kinetic or dynamic Monte Carlo can be used to study such problems based on a master equation.

Sometimes used to model different scenarios to account for parametric or model uncertainty. Ex: Hurricane predictions.

Cellular automata type models for applications like traffic modeling.

Game theory simulations.

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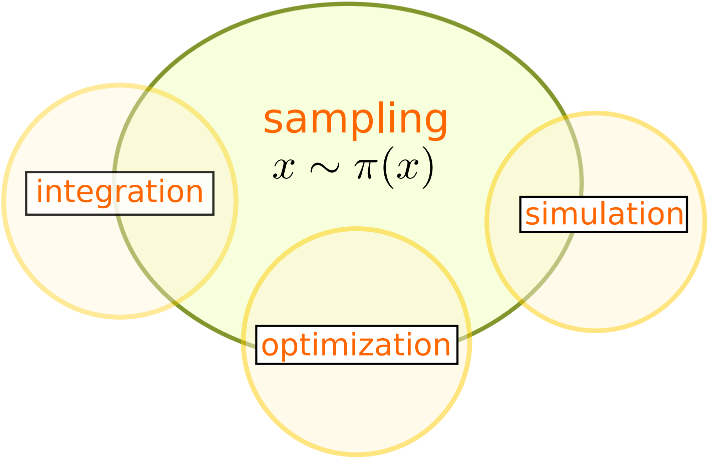

MC $\equiv$ sampling

Interpretation

A certain subclass of problems, say integration, can be attacked using MC or non-MC methods.

Examples of non-MC methods include:

- Integration
  analytical, Gauss quadrature, Newton-Cotes, Clenshaw-Curtis etc.
- Optimization
  analytical, steepest descent, conjugate-gradient, linear-programming, Levenberg-Marquardt etc.
- Simulation
  analytical, finite elements, finite differences, molecular dynamics, etc.

Sampling

Prefer direct Monte Carlo, whenever possible.

Advantage: individual samples are independent, which makes error analysis easier

But many complex problems cannot be tacked with direct MC, and MCMC becomes the method of last resort

Samples in MCMC are correlated. This complicates analysis.

Possibly helpful analogy:

analytical : numerical :: MC : MCMC

In numerical solutions, we have to worry about tolerance, stability, round-off error, convergence, choice of method etc, as the price for being able to solve a wider range of problems.