The Big Picture

MC, MCMC and the Rest of the Universe

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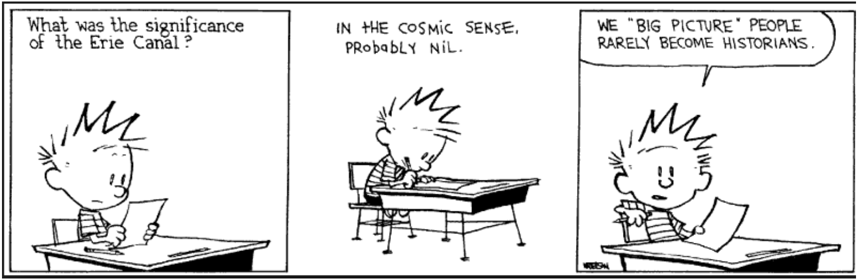
The Big Picture



credit: Bill Watterson

In this lecture, I will reveal a conceptual map to tie some things together.

Preface

In 2002-2003, I was a graduate student working on 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 $g_j > 0$, $\tau_j > 0$.

It turns out to be a particularly tricky problem to get right.

I eventually began using a MCMC optimization technique called simulated annealing.

Preface

While I was researching the technique, I found out that one of my buddies in the CS department, was using a variant of the same technique to solve a "floor-planning" problem.

Apple A5 chip. credit: chipworks

Preface

graphicriver.net

Fitting chips on a substrate is closely related to a problem that newspapers have to solve everyday.

Laying out "panels" of news stories.

> *It's amazing that the amount of news that happens in the world every day always just exactly fits the newspaper. - Sienfeld*

Motivation

Monte Carlo means different things to different disciplines.

People often use similar techniques to solve problems, which seem unique (to the people solving the problems).

The history of MC methods is littered with nearly identical methods being “rediscovered” in each disciplinary silo.

We will meet some of these methods in this class. Often, they will have multiple aliases.

A big-picture understanding allows us to look beyond 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 very core MC/MCMC can be thought of as a sampling technique.

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

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

Everything else flows from this simple fact.

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Sampling, by itself, is a fundamental problem.

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

Three important sub-classes of problems are:

- Integration

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

or, as happens quite frequently in practice,

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

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

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- Optimization

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

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

- Simulation

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

Kinetic or dynamic Monte Carlo can be used to study such problems.

Ex: traffic modeling

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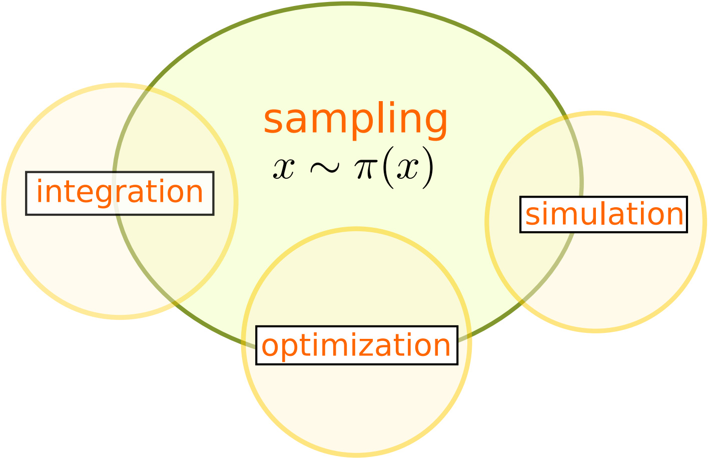

MC $\equiv$ sampling

Interpretation

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

Examples of non-MC methods the three sub-classes 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.