Monte Carlo methods,

in Physics: Theoretical Physics
Experimental Physics
Computational Physics: main tool is a Computer.
Operates on models like Theo. P.
analyses "experiments" like Exp. P.

Large part of CP is Monte Carlo
Computers, Moore's Law

Principle of meas.	Algorithm
Apparatus	Program
Calibration	Debugging
Measurement	Run

Example: Ising model, in the Canonical Ensemble

$S_{\vec{n}} \in \{1, -1\}$ spins

$\vec{n} \in \Omega$ d dimensional lattice

configuration:

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+ + + - +
+ - - - +
- - + + -
+ - + - +
- + - - +
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e.g. $\hat{\nu} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ unit vector in dir. ν

$|\Omega| = L^d = V$ number of lattice points

2^V configurations

$$H[S] = -J \sum_{\vec{n}} \sum_{\nu=1}^{d} S_{\vec{n}} \cdot S_{\vec{n}+\hat{\nu}} - \mu h \cdot \sum_{\vec{n}} S_{\vec{n}}$$

Hamilton function

Observable: e.g. Magnetisation $M[S] = \frac{1}{V} \cdot \sum_{\vec{n}} S_{\vec{n}}$

Canonical Ensemble

System coupled at heat reservoir with Temperature T
Thermal equilibrium

Probability of a conf. $P[S] = \frac{1}{Z} e^{-\beta H[S]}$

$\beta = \frac{1}{k_B T}$

$$Z = \sum_{\{S\}} e^{-\beta H[S]}$$

$\leftarrow$ sum over all 2^V configs.

$k_B = 1.38 \cdot 10^{-23} \, J/K$
Boltzmann constant

Expectation value for observable $F[s]$

$$\langle F \rangle = \sum_{\{s\}} F[s]\, P[s] = \frac{1}{Z} \sum_{\{s\}} F[s]\, e^{-\beta H[s]}$$

Sum e.g. $L = 100$ $d = 3$ $V = 10^6$

\# of configs: $2^{10^6} = (2^{10})^{10^5} \approx (1000)^{10^5} = 10^{3\cdot 10^5}$

No hope to calculate exactly numerically.

Fundamental theories

Quantum field theory (e.g. QCD 6 quarks 8 gluons
Nuclear physics)

$\lambda \phi^4$ Theory: Scalar field $\phi(x) \in \mathbb{R}$ $x = (\vec{x}, t)$

Defined by action

$$S(\phi(x)) = \cancel{S} = \int d^4x\, \mathcal{L}(\phi(x)) = \int d^4x\, -\frac{1}{2}(\partial_\mu \phi(x))(\partial^\mu \phi(x)) + \frac{m^2}{2}\phi^2(x) + \frac{\lambda}{24}\phi^4(x)$$

Self interaction

Quantum mechanical expectation value can be calculated by Feynmann Path Integral

$$\langle F \rangle = \frac{1}{Z}\int D\phi\, e^{-\hbar^{-1} S[\phi]} F[\phi] \qquad Z = \int D\phi\, e^{-S[\phi]/\hbar}$$

$D\phi$: Path integral : integration over field configs.

Can be defined on a lattice in a rigorous way.

$$\phi(x) \to \phi(\vec{n}) \qquad \vec{n} \in \Omega \quad \text{4d lattice}$$

$$\partial_\mu \phi(x) \to \frac{1}{2a}\left(\phi(\vec{n}+\hat{\mu}) - \phi(\vec{n}-\hat{\mu}) \right) \qquad a = \text{lattice spacing}$$

$$S[\phi] = \sum_{n \in \Omega}\left[-\frac{1}{2}\left(\frac{\phi(\vec{n}+\hat{\mu}) - \phi(\vec{n}-\hat{\mu})}{2a}\right)^2 + \frac{1}{2}m^2\phi^2(\vec{n}) + \cancel{g}\frac{\lambda}{24}\phi^4(\vec{n}) \right]$$

$$D\phi \to \prod_{n \in \Omega} d\phi(\vec{n})$$

$$\langle F \rangle = \frac{1}{Z}\int \prod_{n \in \Omega} d\phi(\vec{n})\, e^{-S[\phi]/\hbar}\, F[\phi]$$

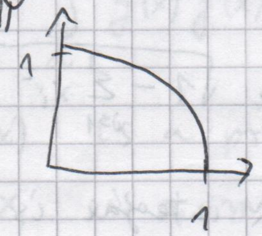
high dim. integral

Many areas: Stat. Phys. (Particle Phys., Condensed matter, ...)
Engineering, Climate change, weather predict.
Finance, Statistical tests (e.g. bootstrap)
Biology
Computer graphics, optimization,
etc.

Monte Carlo Integration

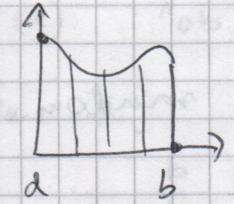
$\Theta(x) = 0 \quad x < 0$
$\Theta(x) = 1 \quad x \geq 0$

"measuring" π



$$\int_0^1 \sqrt{1-x^2}\, dx = \frac{\pi}{4} = \int_0^1 dx \int_0^1 dy\, \Theta(1-x^2-y^2)$$

Method 1



Trapezoid Rule:

$$\int_a^b f(x)\, dx \approx \sum_{i=0}^{N-1} \left[f\left(a + i\frac{b-a}{N}\right) + f\left(a+(i+1)\frac{b-a}{N}\right)\right] \frac{N}{2(b-a)}$$

$$\frac{N}{2(b-a)}$$

Method 2

Take random numbers $r_i \in [0,1]$ $i = 1 \dots 2N$
with uniform distribution

$$x_i = r_i \qquad y_i = r_{i+N}$$

$n_{in} = \#$ of indices for which $\sqrt{x_i^2 + y_i^2} < 1$

$$\frac{\pi}{4} \approx \frac{n_{in}}{N}$$

results eg:

N	π
100	3,244
1000	3,141
10000	3,1402
100000	3,1409

Results get better with more points

Can we say more?

each point has $p = \frac{\pi}{4}$ chance to be inside $q = 1 - \frac{\pi}{4}$ to be out

n_{in} has a binomial distribution $\langle \Delta n_{in}^2 \rangle = N \cdot p \cdot q$

$$\left\langle \Delta \left(\frac{n_{in}}{N}\right)^2 \right\rangle = \frac{1}{N} \cdot p\, q$$

Variance

Error: $\sqrt{\text{variance}} \sim \frac{1}{\sqrt{N}}$ 4 times the data
1/2 the error

Trapezoid rule Error $\sim \frac{1}{N^2}$ much better

Lookat 10-sphere

$V = r^{10} \cdot \frac{\pi^5}{120}$ Measure/Calculate π from this

Method 1: Trapezoid rule: $\int_0^1 \prod_{i=1}^{9} dx_i \; \sqrt{1 - \sum_{i=1}^{9} x_i^2}$

Error is still $\sim \frac{1}{N^2}$ if each integral is split to N

Method 2: Monte Carlo $x_i \in [0,1]$ random

$n_{in} = \#$ of i with $\sum x_i^2 < 1$

Take e.g. Trapezoid with $N = \cancel{100} = 10$

10^9 evaluations are needed.

Takes $O(1)$ seconds on a generic comp.

Monte Carlo with $N = 10^9$

$\text{Error}_{\text{Trapezoid}} \sim \frac{1}{100}$ $\text{Error}_{MC} \sim \frac{1}{\sqrt{10^9}} = \frac{1}{10^{4,5}}$

Monte Carlo much better

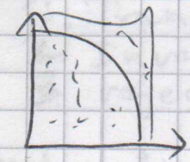
For high dim integals, Trapezoid is quickly intractable

Error $\sim \frac{1}{N^2}$ $M = N^d$ evaluations Error $\sim \frac{1}{M^{2/d}}$

Monte Carlo error independent of dim

Error $\sim \frac{1}{\sqrt{M}}$ for M evaluations

Sampling



We calculated a 2d integral $\int_0^1 dx \int_0^1 dy \; \Theta(1-x^2-y^2)$

Can also do 1d integral $\int_0^1 \sqrt{1-x^2}\, dx = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \sqrt{1-x_i^2}$

$x_i \in [0,1]$ uniform.

Generally $\int_a^b g(x) f(x)\, dx$

$f(x)$ is a probability dist. $f(x) \geq 0$ $\int f(x) = 1$

x is a random variable (can be a vector in many d)

$g(x)$ "observable"

Take x_i $i = 1 \dots N$ random

$$\int_a^b g(x) f(x)\, dx \approx \frac{1}{N} \sum_{i=1}^{N} g(x_i) = g_{Est} \quad \text{MC estimator.}$$

Variance assuming independent x_i

$$\sigma^2_{g_{Est}} = \frac{1}{N^2} \cdot \sum_{i=1}^{N} \sigma^2_{g(x_i)} = \frac{\sigma_g^2}{N} \Rightarrow \text{Error} \sim \frac{1}{\sqrt{N}}$$

We have some freedom, e.g. $\boxed{\text{but } f(x) \geq 0, \int f(x) = 1}$

$$\int_0^1 \sqrt{1-x^2}\, dx = \int_0^1 \sqrt{(1+x)(1-x)}\, dx = \int_0^1 \frac{1}{2} \sqrt{\frac{1+x}{1-x}}\, 2(1-x)\, dx$$

$g(x) = \sqrt{1-x^2}$ or $g(x) = 1$ $\qquad g(x) = \frac{1}{2}\sqrt{\frac{1+x}{1-x}}$ $f(x) = 2(1-x)$

$f(x) = 1$ $\qquad f(x) = \sqrt{1-x^2}$

$f(x) = 1$ simple sampling

$f(x) \neq 1$ biased sampling, importance sampling

in Physics usually $f(x) = \text{Boltzmann factor} = e^{-\beta H}$