Monte Carlo Methods in Physics

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Outline:

WHAT IS MONTE CARLO?

- The π game

DIRECT MONTE CARLO

- Drunkard walks
- Particle transport, *e.g.*,
  - accelerator design
  - space engineering
- Earthquakes

INDIRECT MONTE CARLO

- Designer materials?
- Phase transitions (ice → water); protein folding

- over-simplified
- GOAL: give “big picture”

WHAT IS MONTE CARLO

Monte Carlo: a class of computational methods whose essence is the invention of games of chance and whose behavior and outcome can be used to study some interesting phenomena.

A game to calculate π:

On a computer, *random numbers* play an essential role:

`rand()`: gives numbers uniformly distributed on $(0, 1)$

(x, y): `x=rand()`; `y=rand()`.

$$\pi = 4 \times \frac{\#\text{ of points inside circle}}{\#\text{ of points inside square}}$$

$\Rightarrow$ Monte Carlo can do integrals → many-dimension

Random *does not* imply inaccurate

DIRECT MONTE CARLO

Drunkard's walks

1) Drunkard on a street with 2 bars

Moves *left* or *right* by 1 with equal probability in each step.

Is trapped forever upon arrival at bar.

Q: What is probability distribution of drunkard after t steps?

Pseudo-code:

```
if rand() $\leq$ 0.5, then x=x+1;
else, x=x-1
```

Heat conduction in a metal stick: identical!

DIRECT MC: simulation of a natural stochastic process

INDIRECT MC: solution of non-probabilistic problems by probabilistic (MC) methods

Distinction between 'direct' and 'indirect' is not always clear

DIRECT MONTE CARLO

Drunkard's walks

2) Rain drop in random swirling breeze

Starts from h above ground:

	↓	↑	←	→
prob.	0.6	0.1	0.15	0.15

Q: Average time to reach ground?

Pseudo-code:

```
r=rand()
if r ≤ 0.6, then y = y - 1 ;
  else if r ≤ 0.6 + 0.1, then y = y + 1 ;
    else if r ≤ 0.6 + 0.1 + 0.15, then x = x - 1 ;
      else,  x = x + 1
```

In general, to *sample* a discrete probability density function p_i:

i) Draw $r = \texttt{rand}()$.

ii) Solve $\Sigma_{j=0}^{i-1} p_j \le r \le \Sigma_{j=0}^{i} p_j$ for i.

One way to sample a continuous P.D.F. $f(x)$: $\quad x \in (a, b)$

i) Draw $r = \texttt{rand}()$.

ii) Solve $\int_a^x f(x)dx = r$ for x.

DIRECT MONTE CARLO

Particle transport

Neutron transmission through a plate:

Neutron collides with atoms inside plate.

Distance l between collisions is distributed as:

$$f(l) = 1/\lambda \ \exp(-l/\lambda), \qquad l \in (0, \infty)$$

Upon collision,

with probability p_s — scattered [†]
with probability $p_c = 1 - p_s$ — captured

[†] Scattering is uniform in all directions

Q: What is probability for neutron to pass through plate?

Follow N neutron paths and see how many come through:

```
do while still inside plate          ← for 1 neutron
  sample distance $l$
  advance neutron by $l$ along current direction
  if rand() $\le p_c$, then
     trajectory ends   (captured)
  else
     sample random new direction   (scattered)
  end if
end do
```

Basic idea has many applications:

- accelerator design
- space engineering (radioactive effects on astronauts)
- semi-conductor (CPU chips) study and manufacturing
- crystal growth

DIRECT MONTE CARLO

Earthquakes

Q: Are earthquakes exceptional events due to special circumstances? Or are they part of a more general pattern of events that would occur *without* any specific external intervention?

Empirically, probability distribution of earthquake magnitudes:

$N(E) \propto E^{-b}$ – "Gutenberg-Richter" law

Scale-invariant: $E \to sE$ leads to *same* $N(E)$.

- No characteristic scale.
- Large events do occur.

Many objects in nature have scale-invariant (or fractal) structures.

In contrast, in the more familiar Gaussian form $e^{-(E/E_0)^2}$ — result of combining a large number of independent random events:

- Characteristic scale (E_0).
- Large events pratically do not occur.

Need models to understand scale-invariant states without parameter tuning!

DIRECT SIMULATIONS

Earthquakes

A Model (Cellular Automata):

- Square lattice $N = L \times L$.
- Block on each site, connected by springs.
- $z(i, j)$ is the force at site (i, j)
- z_{cr} (*e.g.*, $z_{cr} = 4$) is critical threshold value.

Algorithm:

1 Increase z everywhere by p, *e.g.*, $p = 0.00001$, and advance clock. ⇐ Represents increase of force from tectonic plate motion.

2 Check if $z(i, j) > z_{cr}$. If not, go to 1; else go to 3. ⇐ "no" means system is stable.

3 Let (i) $z \rightarrow z - z_{cr}$ at the appropriate position(s) and (ii) $z \rightarrow z + 1$ at the four nearest-neighbors. ⇐ (i) represents the release of force due to slippage of a block and (ii) represents force transfer.

INDIRECT MONTE CARLO

The story of high-temperature superconductors

- discovered around 1990
- normally insulators
- become superconducting below temperature T_c
- T_c remarkably high: $T_c \sim 150\,\mathrm{K}$ (compare liquid nitrogen)
- enormous potential — explosion in research effort

Q: Why? How?

INDIRECT MONTE CARLO

The story of high-temperature superconductors

Q: Why? How? — *Hubbard model?*

To answer, study interacting electrons on a 2-dim lattice:

- Must solve Schroedinger equation (quantum mechanics)
- However, to study a 10 × 10 lattice with 90 electrons requires diagonalization of a $L \times L$ matrix, where L is 3775914614554522689854057515489705090212865742534001561600
- Need new computational method — one of the most outstanding problems in computational physics
- Recently, progress has been made by exploiting the similarity between the Schroedinger equation and the diffusion equation (drunkard!).
- Now 10 × 10 lattice above can be turned into random walks in (only!) 180 dimensions with birth/death, which can then be carried out by MC simulations.

SUMMARY:

- Monte Carlo refers to methods to solve problems which utilizes games of chance in an essential way.
- Monte Carlo methods are widely applied in physics.
  - direct Monte Carlo simulation
    - particle transport
    - earthquakes
  - indirect Monte Carlo calculation
    - *e.g.*, quantum mechanics
    - often much more involved, but also much more powerful
- Monte Carlo methods are not necessarily rough
  - Individual methods can be extremely complex and elaborate.
  - Its results can be the most accurate possible; sometimes it's the *only* way to solve the problem.