“Monte Carlo” Simulations

(the real things)

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Prob 1: Random Walk Simulation

- Random walks in nature
  - Brownian motion (perfume)
  - electron transport
- Problem: $N$ collisions to travel $R$?
- Model: walk $N$ steps of $r$
  - random directions
Random Walk Theory

How far from origin after $N$ steps?

$$R^2 = (\Delta x_1 + \cdots + \Delta x_N)^2 + (x \to y)$$  \hspace{1cm} (1)

$$= \Delta x_1^2 + \cdots + \Delta x_N^2 + 2\Delta x_1\Delta x_2 + \cdots + (x \to y)$$ \hspace{1cm} (2)

Random: all directions, average for large numbers

$$R^2 \approx \Delta x_1^2 + \cdots + \Delta x_N^2 + \Delta y_1^2 + \cdots + \Delta y_N^2$$ \hspace{1cm} (3)

$$= N \langle r^2 \rangle,$$  \hspace{1cm} (4)

$$\Rightarrow R \approx \sqrt{N} r_{\text{rms}}$$ \hspace{1cm} (5)

Each step with root-mean-square length $r$
Virtual Lab

- Use computer to “simulate” a random walk
- Computer = “virtual” lab
Random Walk Simulation

1. Is $R_{rms} = \sqrt{\langle R^2 \rangle} \propto \sqrt{N}$?
2. Need ensure much randomness
3. Both random $\Delta x$ & $\Delta y$
4. Range $[-1, 1]$
5. Normalize each step $r = 1$:

\[ \Delta x = \frac{1}{L} \Delta x', \quad \Delta y = \frac{1}{L} \Delta y', \quad (1) \]

\[ L = \sqrt{\Delta x'^2 + \Delta y'^2} \quad (2) \]

6. Plot several independent
   1000-steps walks
7. Do these look random?
Random Walk Simulation (specifics)

8. Good Statistics: \( N = \# \) steps single trial, different seeds
\( K \approx \sqrt{N} \) = number trials

9. Calculate squared-distance each \( K \) trials

\[
R_k^2(N) = \left( \sum_{i=1}^{N} \Delta x_i \right)^2 + \left( \sum_{i=1}^{N} \Delta y_i \right)^2 \quad (1)
\]

Then average trials: mean squared \( R \)

\[
\langle R^2(N) \rangle = \frac{1}{K} \sum_{k=1}^{K} R_k^2(N) \quad (2)
\]

Then, root mean squared

\[
R_{rms} = \sqrt{\langle R^2(N) \rangle} \quad (3)
\]

10. Plot \( R_{rms} \) vs \( \sqrt{N} \)

11. Large \( N \) for theory OK

12. \( N \) for 2-3 place agreement?
Problem 2: Spontaneous Decay

Facts of Nature

1. Natural process (we describe)
2. Atomic & nuclear decays
3. “Spontaneous” process
   a. no external stimulate
4. Transmutation (in nucleus)
   a. $U \rightarrow Th + \alpha$
5. $t$ when decays: random
6. Independent of:
   a. how long exist
   b. number others around

Theory:

$P(t) = \text{prob decay/t/particle}$

$= -\lambda$  \hspace{1cm} (1)

$\Rightarrow N(t), \frac{dN}{dt} \downarrow \text{with time}$
Simulation Problem

- Simulate various number decays
- Ever look exponential $N(t) \propto e^{-\lambda t}$?
- When look “stochastic”?
- Simulation or $e^{-\lambda t}$ more accurate?

**Law of Nature:** Number decay/t/# = $-\lambda$

\[
\frac{\Delta N(t)}{N(t)\Delta t} = -\lambda
\]  \hspace{2cm} (1)

\[
\frac{\Delta N(t)}{\Delta t} = -\lambda N(t) \quad \text{def} \quad \text{activity}
\]  \hspace{2cm} (2)
Method: Decay Simulation

Algorithm:
Loop through remaining nuclei
\[ r_i < \lambda? \Rightarrow \text{decays (} \lambda \propto \text{rate} \uparrow \Rightarrow \text{more decay)} \]
\[ t = t + \Delta t \]
Repeat loop

while \( N > 0 \)
\[ \Delta N = 0 \]
for \( i = 1 \ldots N \)
\[ \text{if (} r_i < \lambda \text{)} \Delta N = \Delta N + 1 \]
\[ t = t + 1 \]
\[ N = N - \Delta N \]
Output \( t, \Delta N, N \)
Model: Continuous Decay

If \( N \rightarrow \infty, \) & \( \Delta N \rightarrow 0, \) & \( \Delta t \rightarrow 0 \)

\[
\frac{\Delta N(t)}{\Delta t} \rightarrow \frac{dN(t)}{dt} = -\lambda N(t)
\]  

(1)

Can integrate differential equation

\[
N(t) = N(0)e^{-\lambda t} = N(0)e^{-t/\tau}
\]  

(2)

\[
\Rightarrow \lambda = \frac{1}{\tau}
\]  

(3)

\[
\frac{dN}{dt}(t) = -\lambda N(0)e^{-\lambda t} = \frac{dN}{dt}(0)e^{-\lambda t}
\]  

(4)

Exponential decay = approx to simulation

Nature: small N & stochastic