Lecture 9

Random Process

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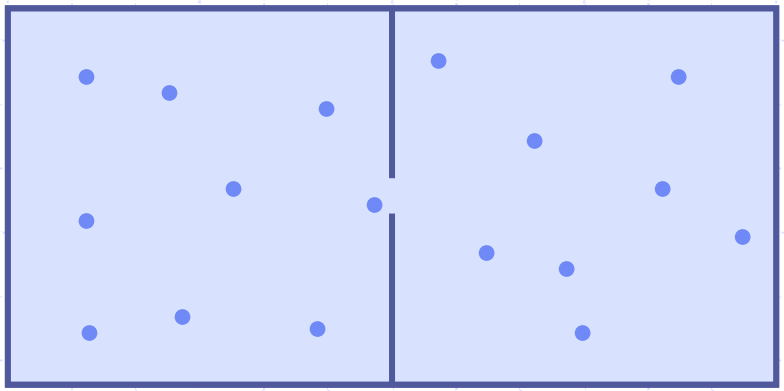
This PowerPoint Notes Is Based on the Textbook '***An Introduction to Computer Simulation Methods : Applications to Physical Systems***', 2nd Edition, Harvey Gould and Jan Tobochnik, Addison-Wesley(1996); "A First Course in Computational Physics"; "Numerical Recipes"; "Elementary Numerical Analysis"; "Computational Methods in Physics and Engineering".

Order to Disorder

- Random process is a ***non-deterministic*** process.
- The basic assumption underlying the probabilistic model is that the motion of the particles is so complex that we can assume random behaviour.
- Example: *N* identical particles in a box.



Question and Objective

- Random processes are common in nature, how do we simulate them?
- Most computer simulations use random number generator. What is it? How to use it? What are its general features?
- Random walk and its connection to physical systems.
- Data analysis, least squares (LSQ).
- More on random walks.

N Particles in a Box

- Assume the no. of particles on the left side is ***n***, then the probability per unit time that a particle moves from left to right is ***n*/*N***.
- Thus we can simulate the motion of particles according to the following algorithm:
  - Generate a random number $r \in (0,1)$
  - Compare r to the current value of the fraction of particles n/N, on the left side of the box.
  - If $r \le n/N$, move a particle from left to right, otherwise, move a particle from right to left.
  - Increase the "time" by unity.

Program **box** implements in a straightforward way the algorithm and plots the evolution of particle number *n*.

```
PROGRAM box
! Simulation of the particles in a box problem
CALL initial(N,tmax)
CALL move(N,tmax)          ! Move particles through hole
END

SUB initial(N,tmax)
      RANDOMIZE
      INPUT prompt " number of particles = ": N
      LET tmax = 20*N
      SET WINDOW -0.01*tmax, 1.01*tmax,-0.01*N,1.01*N
      CLEAR
      BOX LINES 0,tmax,0,N
      SET COLOR "blue"
      PLOT 0,0.5*N;tmax,0.5*N        ! Equilibrium values
ENS SUB
```

```
SUB move(N,tmax)
        LET nleft = N          ! Initially all particles on left side
        SET COLOR "red"
        FOR t = 1 to tmax
                ! Generate random number and move particles
                LET r = int(N*rnd) + 1
                IF r <= nleft then
                    LET nleft = nleft - 1
                ELSE
                    LET nleft = nleft + 1
                END IF
                PLOT t, nleft
        NEXT t
END SUB
```

Monte Carlo

- Such probabilistic method for simulating the approach to equilibrium is an example of **MONTE CARLO** methods.
- Monte Carlo methods are especially useful for large N, why?
- Due to its random nature, we need to do Monte Carlo simulation **many times** and average over the results to obtain meaningful averages.

Questions to be Answered

- How long does it take for the system to reach the equilibrium?
- How does this time depend on particles number?
- What is the magnitude of the ***fluctuations***?
- If there are $n(t)$ particles on the left side, then the change in $n(t)$ in time interval Δt is:

$$\frac{\Delta n}{\Delta t} = -\frac{n(t)}{N} + \frac{N - n(t)}{N} \quad \Rightarrow \frac{dn}{dt} = 1 - \frac{2n(t)}{N}$$

→ $n(t) = N/2\,[1 + \exp(-2t/N)]$

where the initial condition is $n(t = 0) = N$.

Introduction to Random Walk

Drunken sailor problem:

- A drunkard begins at a lamp post and takes N steps of equal length in random directions, how far will the drunkard be from the lamp post?
- Such motion is an example of **random walk**.
- Physically, this is similar to the trajectory of a particle that can move in any direction with equal probability.

One-dimensional Random Walk

- Suppose the walker begins at $x = 0$ and that each step is of equal length l.
- At each time interval, the walker has a probability p of a step to the right and a probability $q = 1 - p$ of a step to the left.
- The direction of each step is **independent** of the preceding one.
- Then the displacement and its square of a walker after N steps are

$$x(N) = \sum_{i=1}^{N} s_i \text{ and } x^2(N) = \left(\sum_{i=1}^{N} s_i \right)^2 \text{ where } s_i = \pm l$$

One-dimensional Random Walk

$$\langle x(N)\rangle = \sum_{i=1}^{N}(pl - ql) = (p-q)lN \text{ and}$$

$$\langle x^2(N)\rangle = \sum_{i=1}^{N}\langle s_i^2\rangle + \sum_{i\neq j=1}^{N}\langle s_i s_j\rangle = Nl^2 + N(N-1)(p-q)^2 l^2$$

$$\langle \Delta x^2(N)\rangle \equiv \left\langle \left(x(N) - \langle x(N)\rangle\right)^2 \right\rangle$$

$$= \langle x^2(N)\rangle - \langle x(N)\rangle^2$$

$$= Nl^2 + N(N-1)(p-q)^2 l^2 - N^2(p-q)^2 l^2$$

$$= \left[1 - (p-q)^2\right] Nl^2$$

$$= 4pqNl^2$$

What are we interested?

- **Asymptotic scaling law:**

  for sufficiently large N, one has

  $$\langle \Delta x^2(N) \rangle \sim N^{2\nu} \quad \text{for } (N >> 1)$$

  For 1D, $\nu = 1/2$.

  For 2D and 3D, ν =?

- **Correlation among walkers:**

  $< x(i)\, x(j) >$, *etc.*

- **Simulation technique**

Performing Monte Carlo simulation of the random walk is simple, the difficult part is associated with the bookkeeping.

Use of array is one of the useful tricks.

```
PROGRAM random_walk
! Simulation of a random walk in one dimension
DIM xcum(64), x2cum(64)
CALL initial (p,N,xcum(),x2cum(),ntrial)
FOR itrial = 1 to ntrial
        CALL walk(p,N,xcum(),x2cum())
NEXT itrial
CALL output(N,xcum(),x2cum(),ntrial)
END
```

```
SUB initial(p,N,xcum(),x2cum(),ntrial)
      RANDOMIZE (initialize random number sequence)
      IPUT prompt " maximum number of steps N " : N
          LET p = 0.5
      LET ntrial = 1000              !Number of trials
      FOR istep = 1 to N
            LET xcum(istep) = 0  ! Not necessary in True Basic
            LET x2cum(istep) = 0
      NEXT istep
END SUB

SUB walk(p,N,xcum(),x2cum())
       LET x = 0                     ! Initial position of walker for each trial
       FOR istep = 1 to N
             IF rnd <= p then
                LET x = x +1
             ELSE
                LET x = x - 1
             END IF
             ! collect data after every step
             CALL data(x,xcum(),x2cum(),istep)
        NEXT istep
END SUB
```

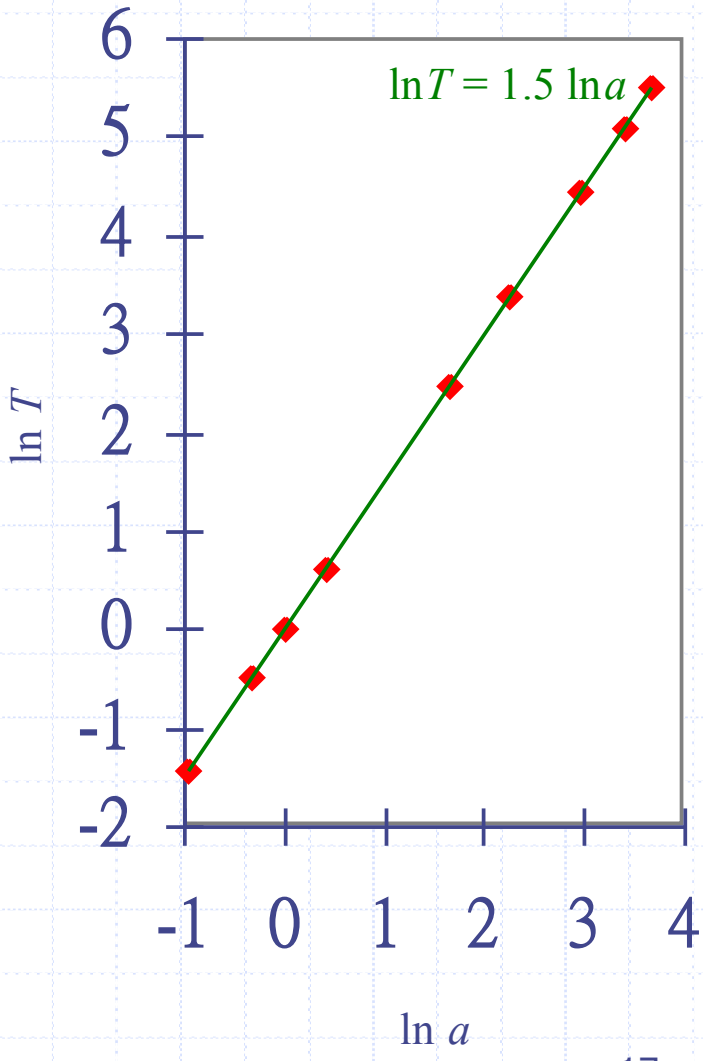
```
SUB data(x,xcum(),x2cum(),istep)
      LET xcum(istep) = xcum(istep) + x
      LET x2cum(istep) = x2cum(istep) + x*x
END SUB

SUB output(N,xcum(),x2cum(),ntrial)
       PRINT "# steps","<x>","<x^2>","<x^2>-<x>^2"
       PRINT
       FOR istep 1 to N
              LET xbar = xcum(istep)/ntrial
              LET x2bar = x2cum(istep)/ntrial
              LET variance = x2bar -  xbar*xbar
              PRINT istep, xbar, x2bar, variance
        NEXT istep
END SUB
```

Data Analysis

- After simulation, with a collection of data (x(i), etc.), how do we get useful information?
- This is a necessary step in all experiments, e.g., coffee cooling constant, Kepler's law.
- Graphic is an intuitive approach. However, it could be biased. Is there any analytical approach?

Plot of ln*T* vs ln*a*

Planet	*T* (earth years)	*a* (AU)
Mercury	0.241	0.387
Venus	0.615	0.723
Earth	1.00	1.00
Mars	1.88	1.523
Jupiter	11.86	5.202
Saturn	29.5	9.539
Uranus	84	19.18
Neptune	165	30.06
Pluto	248	39.44



Why 1.5, not 1.53 or 1.588???

Method of Least Squares

- A common method for finding the best straight line fit to a series or measured points (linear regression).
- Suppose that we have n pairs of measurements (x_1,y_1), (x_2,y_2), $\cdots$, (x_n,y_n) and that the errors are entirely in the values of y.
- We want to obtain the best fit to the linear function

$$y = mx + b, \qquad y = \sum_{k=0}^{p} a_k x^k .$$

Covered, see Data_Modeling.pdf

Random Walks & the Diffusion Equation

- One reason random walks are very useful in simulating many physical processes and modelling many differential equations of physical interest is that their behaviour is closely related to the solution of the ***diffusion equation***.
- Consider the one-dimensional diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2},$$

where D is the self-diffusion coefficient and $P(x,t)dx$ is the probability of a particle being in the interval between x and $x+dx$ at time t.

Random Walks & the Diffusion Equation

At infinity position, P is *zero*, $P(x = \pm\infty, t) = 0$,
and all the spatial derivative of P are *zero*,

$$\left.\frac{\partial P(x,t)}{\partial x}\right|_{x=\pm\infty} = 0.$$

The average of any function of x can be written as

$$\langle f(x,t)\rangle = \int_{-\infty}^{\infty} dx f(x) P(x,t).$$

Multiply both sides of the diffusion equation by x and performing integration:

$$\int_{-\infty}^{\infty} dx\, x \frac{\partial P(x,t)}{\partial t} = D\int_{-\infty}^{\infty} dx x \frac{\partial^2 P(x,t)}{\partial x^2}.$$

Random Walks & the Diffusion Equation

The left-hand side is

$$\int_{-\infty}^{\infty} dx x \frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial t}\int_{-\infty}^{\infty} dx x P(x,t) = \frac{\partial}{\partial t}\langle x \rangle.$$

We do integration by parts to the right hand side

$$D\int_{-\infty}^{\infty} dx x \frac{\partial^2 P(x,t)}{\partial x^2} = Dx\frac{\partial P(x,t)}{\partial x}\bigg|_{x=-\infty}^{x=\infty} - D\int_{-\infty}^{\infty} dx \frac{\partial P(x,t)}{\partial x}.$$

Both terms are zero and we find that

$$\frac{\partial}{\partial t}\langle x \rangle = 0 \quad \Rightarrow \quad \langle x \rangle = 0 \quad \text{for all } t.$$

Random Walks & the Diffusion Equation

- Similarly, we would get (two integrations by parts)

$$\frac{\partial}{\partial t}\left\langle x^2 \right\rangle = 2D \quad \Rightarrow \quad \left\langle x^2(t) \right\rangle = 2Dt$$

- The random walk and diffusion equation have the same time dependence if we identify t with $N\Delta t$ and $2D$ with $l^2/\Delta t$.
- In three dimensions the second derivative $\partial^2/\partial x^2$ is replaced by the Laplacian operator ∇^2. $2D$ is replace by $2dD$.

Other Topics

- The Poisson Distribution & Nuclear Decay
- Problems in Probability
  (*see references and random number*)
- Method of Least Squares
  (*see LSQ*)
- A Variational Monte Carlo Method