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Advanced Monte Carlo Methods: Direct Simulation

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Direct Simulation

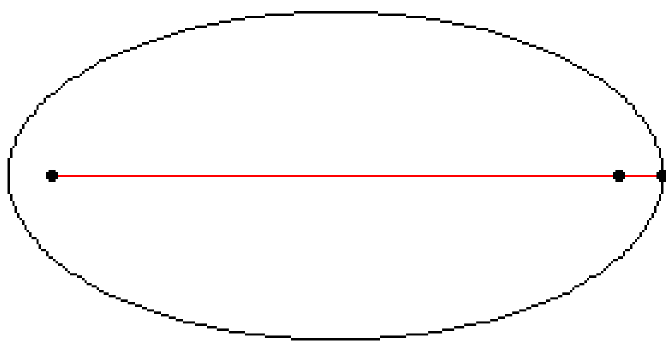
- Probabilistic Problem or Model
  - Directly simulate the physical random processes of the original problem
  - Replace complicated “blocks” with randomized outcomes (neutronics)
  - Direct the simulation’s random outcomes with random numbers
- Examples
  - Controlling floodwater and construction of new dams on the Niles
    - The quantity of water in the river varies randomly from season to season
    - Use records of weather, rainfall, and water levels extending over many years
    - Examine what may happen to the water if certain dams are built and certain possible policies of water control are exercised
    - Evaluate artificial lake impact on people, agriculture, transportation, antiquities

Direct Simulation (Cont.)

- Examples (Cont.)
  - Telephone networks
  - Computer networks
  - Growth of an insect population on the basis of certain assumed vital statistics of survival and reproduction
  - Service rates (queuing theory)
  - Operations research problems
  - Actuarial simulations
    - Insurance risk from tabulated date (mortality)
    - Risk assessment of investment portfolios
  - Computer games
  - Roadway design simulation
  - War gaming

Direct Simulation of the Lifetime of Comets

- A Long-period Comet
  - Described as a sequence of elliptic orbits
    - Sun at one focus of the orbit ellipse
    - Energy of a comet is inversely proportional to the length of the semi-major axis of the ellipse



Direct Simulation of the Lifetime of Comets (Cont.)

- Behavior of the Comet
  - Most of the time
    - Moves at a great distance from the sun
  - A relatively short time (instantaneous)
    - Passes through the immediate vicinity of the sun and the planets
    - At this instant, the gravitational field of the planet perturbs the cometary energy by a random component
    - Successive energy perturbations (in suitable units of energy) may be taken as independent normally distributed random variables $\eta_1, \eta_2, \eta_3, \ldots, \eta_n$
    - $\eta_1, \eta_2, \eta_3, \ldots, \eta_n$ can be normalized to, for example, a standard normal distribution, $N(0,1)$
    - Computing the perturbations exactly is daunting

Direct Simulation of the Lifetime of Comets (Cont.)

- Comets under perturbation
  - A comet, starting with an energy, $G = -z_0$, has subsequent energies
    - $-z_0$, $-z_1=-z_0+\eta_1$, $-z_2=-z_1+\eta_2$, …
  - The process continues until the first occasion on which z changes sign (negative = bound state; positive = free state)
    - Once z changes sign, the comet departs on a hyperbolic orbit and is lost from the solar system
- Kepler's Third Law
  - the time taken to describe an orbit with energy $-z$ is $z^{-3/2}$
  - the total lifetime of the comet is

$$G = \sum_{i=0}^{T-1} z_i^{-3/2}$$

    - z_T is the first negative quantity in the sequence of z_0, z_1, …

Direct Simulation of the Lifetime of Comets (Cont.)

- Problem is to determine distribution of G given z_o
  - Very difficult problem in theoretical mechanics
  - Easy to simulate using probabilistic model
- Seek CDF: $P(G \leq g)$
  - N times: $p(g) =$ proportion of G's $\leq g$
  - Standard error of estimate: $[p(g)(1-p(g))/N]^{1/2}$

Direct Simulation of the Lifetime of Comets (Cont.)

- Monte Carlo trick: use analytic/deterministic information when it is available
  - Probability of escape in one orbit (available from N(0,1) tables:

$$F = P(\eta_1 \geq z_0) = \frac{1}{\sqrt{2\pi}} \int_{z_0}^{\infty} e^{-t^2/2}\, dt$$

  - Know also:

$$1 - P(G \leq g) = \begin{cases} 1 & \text{if } g < z_0^{-3/2} \\ F & \text{if } g = z_0^{-3/2} \end{cases}$$

Direct Simulation of the Lifetime of Comets (Cont.)

- Now we need to estimate:

$$P(G > g) = 1 - P(G \leq g) \text{ for } g > z_0^{-3/2}$$

- **When $g > z_0^{-3/2}$, we know $T > 1$**
- N^* samples (subsample) out of N have $T > 1$
- Let $1-p^*(g)$ be the proportion of values in the subsample with $G>g$

Direct Simulation of the Lifetime of Comets (Cont.)

- Using conditional probability we have:

Estimator of $P(G > g)$ is $[1 - p^*(g)]F$ with std. error $[p^*(g)\{1 - p^*(g)\}/N^*]^{1/2}F$, and is smaller than original std. error by the factor (approx.)

$$\left[1 - \frac{(1-F)\{1-p(g)\}}{Fp(g)}\right]^{1/2}$$

A Robotics Problem

- Take symmetric, concentric objects, O_1 and O_2 in random orientations: what is the distribution of the smallest angle needed to rotate one into coincidence with the other?
- There is an analytic solution, but for simulation need to generate random orientations via random 3x3 orthogonal matrices

A Robotics Problem (Cont.)

- Let $\boldsymbol{Q_o} = [\boldsymbol{x}; \boldsymbol{y}; \boldsymbol{z}]$ where the vectors $\boldsymbol{x}$, $\boldsymbol{y}$, $\boldsymbol{z}$ are uniformly distributed on S_2
- $\boldsymbol{x} = (x_1, x_2, x_3) | \boldsymbol{x} |^{-1}$ is uniform on S_2 when x_1, x_2, x_3 are i.i.d. $N(0,1)$ random variables
- Similarly define $\boldsymbol{y}^* = (y_1, y_2, y_3) | \boldsymbol{y}^* |^{-1}$
- Take $\boldsymbol{y} = (\boldsymbol{y}^* - P\boldsymbol{x})/(1 - P^2)^{1/2}$ where $P = \boldsymbol{x} \cdot \boldsymbol{y}^*$ (Gram-Schmidt procedure)

A Robotics Problem (Cont.)

- Finally, let ***z*** = ***x*** x ***y*** which is orthogonal to the others
- Alternatively, let x_0, x_1, x_2, x_3 be normalized i.i.d. $N(0,1)$, then

$$\begin{pmatrix} 1-2x_2^2-2x_3^2 & 2x_1x_2+2x_0x_3 & 2x_3x_1-2x_0x_2 \\ 2x_1x_2-2x_0x_3 & 1-2x_1^2-2x_3^2 & 2x_2x_3+2x_0x_1 \\ 2x_3x_1+2x_0x_2 & 2x_2x_3-2x_0x_1 & 1-2x_1^2-2x_2^2 \end{pmatrix}$$

is a random orthogonal matrix

Dimensional Analysis

- Consider the "Traveling Salesman" problem: given *n* towns to visit, no order, minimize the Hamiltonian path through the Euclidean weighted complete graph
- Let
  - *l* be the length of the shortest path
  - *A* total area of region containing cities
  - *n/A* is the density of cities

Dimensional Analysis (Cont.)

- Assume $l = A^a(n/A)^b = n^b A^{(a-b)}$
- Units
  - l – length
  - n – dimensionless (number)
  - A – (length)^2
- Implies $a-b = ½$

Dimensional Analysis (Cont.)

- Multiply the area by f while keeping the density constant, l is also multiplied by f
  - fA replaces A
  - fn replaces n
  - fl replaces l
- $l = n^b A^{1/2}$ implies $fl = f^b n^b f^{1/2} A^{1/2}$ so $b = ½$
- $l = k\,(nA)^{1/2}$ strictly via dimensional analysis