Doing Physics with Random Numbers

Andrew J. Schultz

Department of Chemical and
Biological Engineering
University at Buffalo
The State University of New York

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State University of New York

Concepts

- Random numbers can be used to measure things that aren't so random
- Uncertainty in averages can be estimated from the measurements themselves
- A Markov process can be used to sample from a probability distribution
- Physical properties can be computed using a Markov process

Monte Carlo Simulation: Buffon's Needle

- Consider a grid of equally spaced lines, separated by a distance *d*
- Take a needle of length *l*, and repeatedly toss it at random on the grid
- Record the number of "hits", times that the needle touches a line, and "misses", times that it doesn't
  - OK, do it! (Buffon's toothpick)

Monte Carlo Simulation: Buffon's Needle

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- Take a needle of length *l*, and repeatedly toss it at random on the grid
- Record the number of "hits", times that the needle touches a line, and "misses", times that it doesn't
- Buffon showed that the probability of a "hit" is

$$P = \frac{2l}{\pi d}$$

- This experiment provides a means to evaluate π

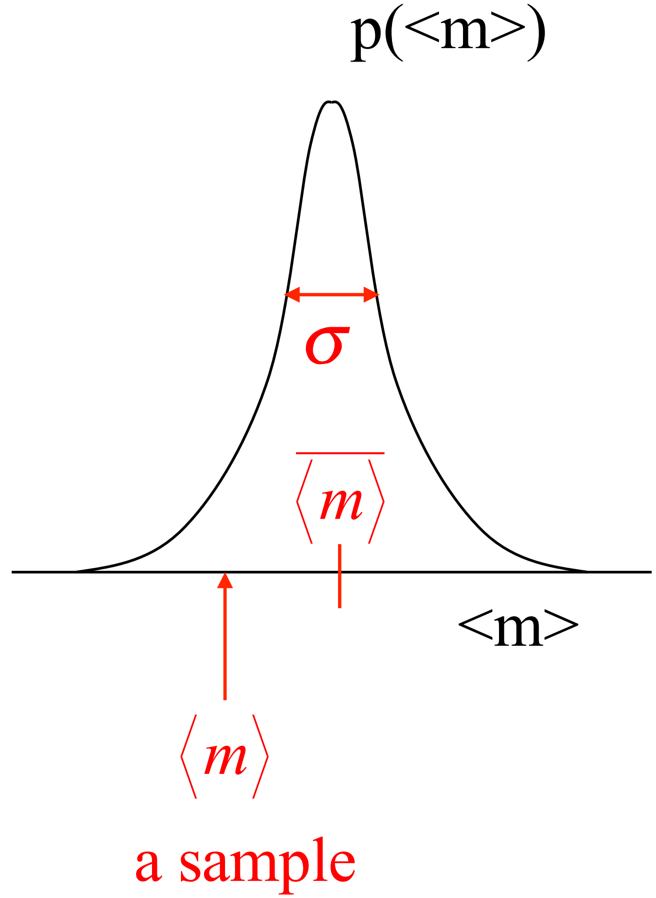
$$\pi = \frac{2l}{Pd}$$

Quantifying Uncertainty

- Averages <m> obtained by a stochastic process are known to follow a Gaussian distribution
- Any given <m> will represent a sample from this distribution
- The width of the distribution is related to the standard deviation of the same set of numbers used to compute <m>

$$\sigma^2_{\langle m \rangle} = \frac{1}{n}\sigma^2_m$$

- Use this to quantify uncertainty in <m>



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The Weather

- Model the weather as having three states:
  - Sunny, Cloudy, Rainy
- The weather tomorrow is related to the weather today
  - For example, Cloudy today:
    - 10% chance it will be Cloudy again tomorrow
    - 50% chance it will be Sunny tomorrow
    - 40% chance it will be Rainy tomorrow
- *Transition probabilities* define the likelihood of the state of the weather tomorrow given the state of the weather today
- We might ask, knowing all (9) transition probabilities, what are the fraction of days that are Sunny, Cloudy, and Rainy?

Markov Processes

- Random walk
  - movement through a series of well-defined states in a way that involves some element of randomness ("stochastic")
- Markov process
  - random walk that has no "memory"
    - selection of next state depends only on current state, and not on prior states
  - process is fully defined by a set of transition probabilities p_{ij}
  - p_{ij} = probability of selecting state j next, given that presently in state i.

Transition-Probability Matrix

- Example
  - system with three states

1 = Cloudy

2 = Sunny

3 = Rainy

$$\Pi \equiv \begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{pmatrix} = \begin{pmatrix} 0.1 & 0.5 & 0.4 \\ 0.9 & 0.1 & 0.0 \\ 0.3 & 0.3 & 0.4 \end{pmatrix}$$

If Cloudy, will stay Cloudy tomorrow, with probability 0.1

If Cloudy, will be Rainy tomorrow with probability 0.4

Never Rainy tomorrow if Sunny today

- Requirements of transition-probability matrix
  - all probabilities non-negative, and no greater than unity
  - sum of each row is unity
  - probability of staying in present state may be non-zero

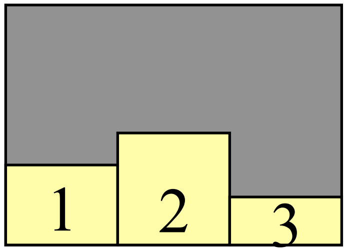
Distribution of State Occupancies

- Consider process of repeatedly moving from one state to the next, choosing each subsequent state according to Π
  - $1 \to 2 \to 2 \to 1 \to 3 \to 2 \to 2 \to 3 \to 3 \to 1 \to 2 \to 3 \to$ etc.
- Histogram the occupancy number for each state
  - $n_1 = 3$
  - $n_2 = 5$
  - $n_3 = 4$

$p_1 = 0.33$ (Cloudy)

$p_2 = 0.42$ (Sunny)

$p_3 = 0.25$ (Rainy)



- After very many steps, a limiting distribution emerges
- Click here for an applet that demonstrates a Markov process and its approach to a limiting distribution

Some Uses of Markov Processes

- Physics (molecular simulation)
- Chemistry (modeling kinetics)
- Designing tests
- Speech recognition
- Information science
- Queuing theory
- Google PageRank
- Economics and Finance
- Social sciences
- Mathematical biology
- Genetics
- Games
- Algorithmic music composition
- Text generators

http://en.wikipedia.org/wiki/Markov_chain

Designer Transition Probabilities

- Say we want to sample states with a desired probability distribution (p_i are given), using a Markov process
- How do we design transition probabilities p_{ij}?
- Many choices are possible for a given distribution
- *Metropolis algorithm* provides a good choice

$$p_{ij} = \min\left(\frac{p_j}{p_i}, 1\right)$$

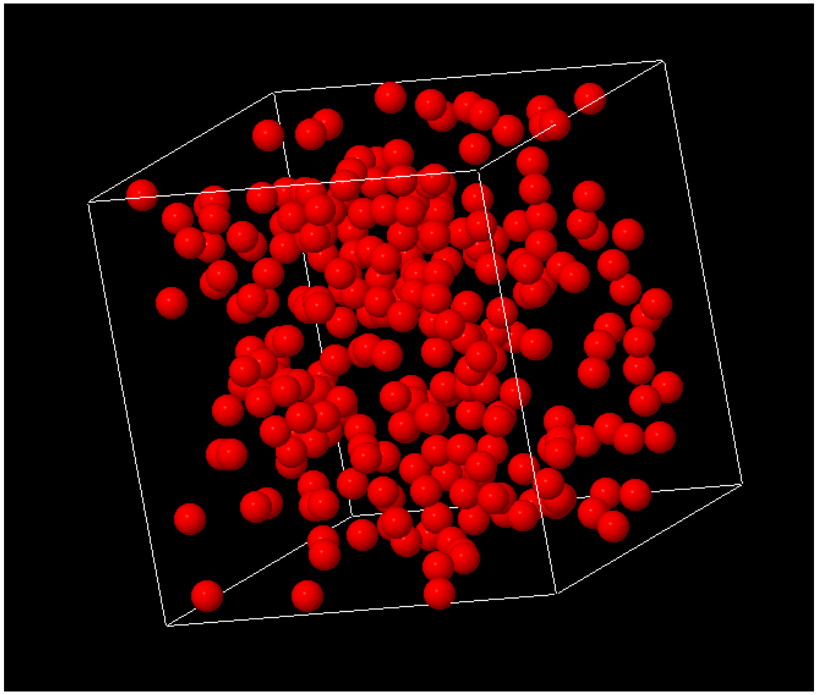
$$p_{ii} = 1 - \sum_{j \neq i} p_{ij}$$

In-class Markov Process

- Three groups
  - Group 1: $p_1 = 0.3$
  - Group 2: $p_2 = 0.1$
  - Group 3: $p_3 = 0.6$
- For state at group *n*, perform trial:
  - Select one of the other states (*m*) with equal probability
  - Compare state probabilities
    - If $p_m > p_n$, let new state be *m*; done with trial
    - Otherwise, select a random number *r* in (0, 1)
    - If $p_m / p_n > r$, let new state be *m*; done with trial
    - Otherwise, let new state be *n* (again); done with trial
- Repeat

Calculating Physical Properties

- Molecular simulation
- Generate box of atoms/ molecules
- Postulate a model for how they interact
- Generate configurations appropriate to postulated model
- Record averages over generated configurations



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Generating Configurations

- Monte Carlo
  - Sample configurations using a Markov process
  - Atoms move around randomly, but in a controlled way
  - Movements aren't physically meaningful, but the sampled distribution of configurations are
- Molecular dynamics
  - Sample configurations according to Newton's laws
    - F = ma
  - Move/accelerate all atoms at once
  - Direction and amount depends on current velocities and forces
  - Movements looks realistic, like a movie
- Let's see some demos…

An Application of Molecular Simulation

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