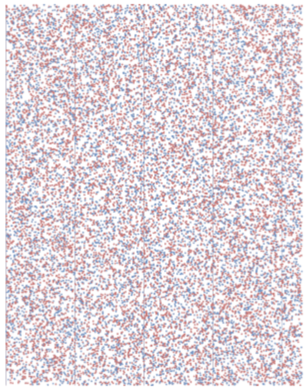
CS 190C
Science Education in Computational Thinking



RANDOMNESS:

- Floating-Point Numbers & Issues
- Using Randomness
- (Pseudo) Random Numbers
- Monte Carlo Methods

Hoffmann, 2008

Which is not a Random Event?

A. Color of first car crossing Stadium Ave after 12 noon

B. 101^{st} digit in expansion of π is even

C. Fair coin toss

D. June 1, 2008, is a cloudy day

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Use of Randomness

- Simulations:
  - Agent-based simulations: people, traffic
  - Event simulations: server/client, temperature effects, system component failure
  - Environmental parameters: porosity, composition of materials
  - Simulated annealing
- Integration and solving stochastic problems

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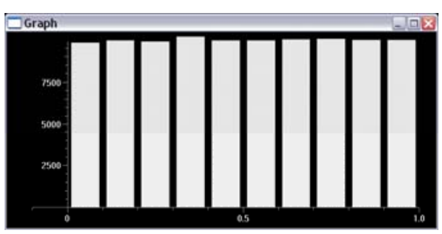
Pseudo-Random Numbers

- Look randomly distributed
- Pass various tests of acceptability
  - e.g. uniform distribution and bins



100,000 trials
First bin 9,964 vs. 10,000, less than 0.4%

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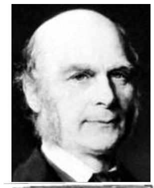
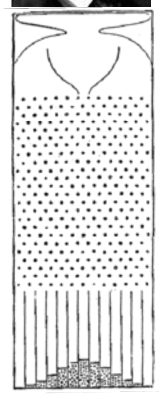
Beyond Uniform Distributions



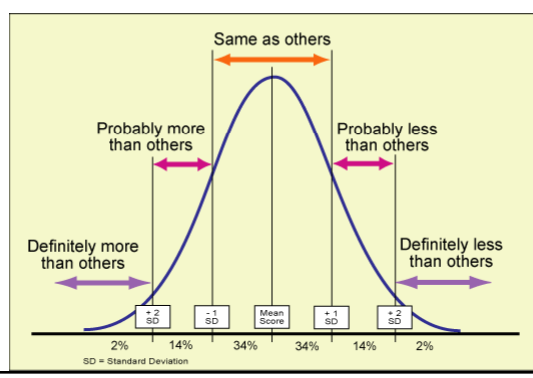


- Random number in a fixed range, each value equally likely
  - Example: toss of a coin
- Probability of having a run of 10 consecutive tosses being *heads* is 1:1024
- Binomial distributions:
  - Toss m coins at each trial
  - Drop balls into Francis Galton's board (1889, Quincunx)
  - Probability $\dfrac{\binom{n}{k}}{2^n}$
- As n grows in binomial distribution, we get the uniform distribution

Normal Distribution

- Bell curve:
  - standard deviation σ
  - area 1 under curve

$$\frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(x-\mu)^2}{2\sigma^2})$$



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Python's *Random* Class

`random()` – uniformly distributed numbers in [0,1]:

```
from random import *
 X = Random()
 X.seed(1)
 v = X.random()
```

```
X = Random()
v = X.random()
```

`randrange(b,e,s)` – **`int`** in **`range(b,e,s)`**
`randint(l,u)` – **`=randrange(l,u+1)`**
`normalvariate(μ,σ)` – Gauss distribution

pgm_1

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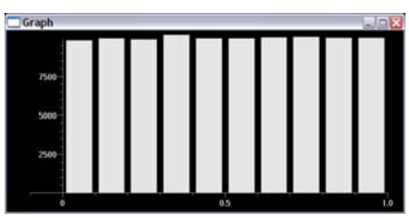
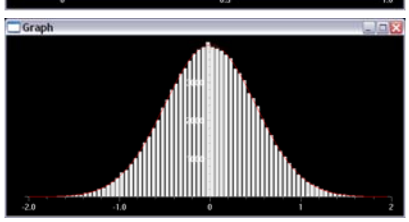
Visual Randomness Test

- Histogram is the basic tool, but also mappings





pgm_2

100,000 trials each

pgm_3

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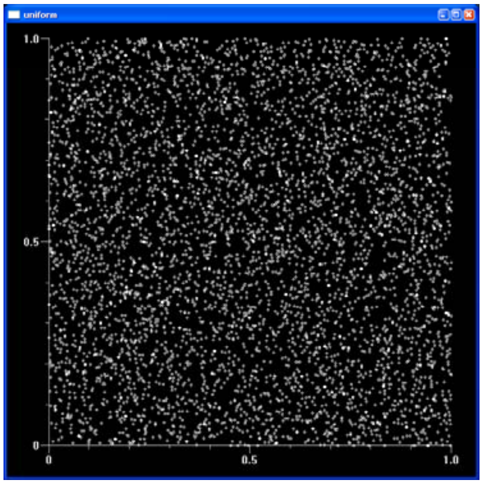
2D Mappings



5,000 points, uniform

pgm$_4$

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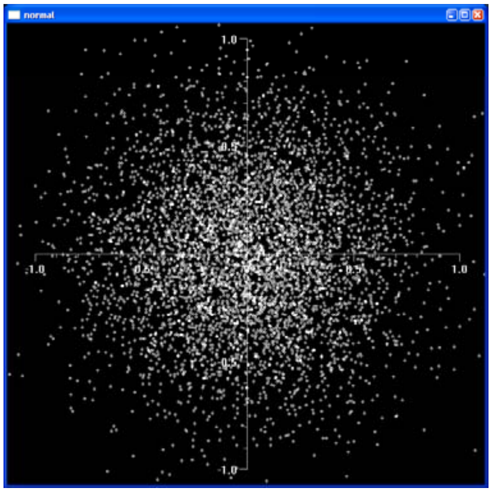
2D Mappings



5,000 points, normal

pgm$_5$

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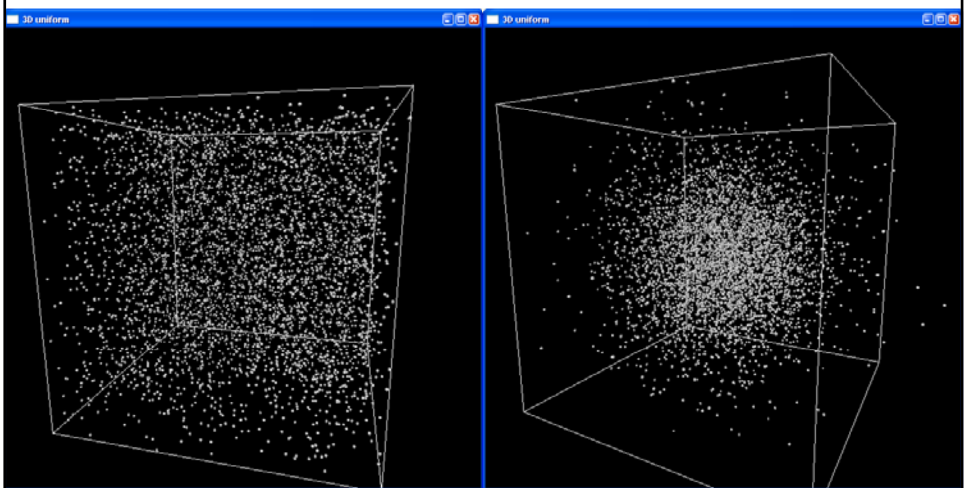
3D Mappings



pgm$_6$ 5,000 points pgm$_7$

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Poor Generators

- Linear congruence: $X_{k+1} = (aX_k+c) \% m$
  - period is at most m
  - careful with choice of a, c, m: a and m should be relative primes
- But note that even then things tend to lie in hyperplanes, exhibiting an unwanted correlation…

pgm$_8$

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Common MC Applications

1. **Classical Monte Carlo:** samples drawn from a probability distribution, e.g., the Boltzmann distribution, to obtain thermodynamic properties, minimum-energy structures and/or rate coefficients.
2. **Quantum Monte Carlo:** random walks to compute quantum-mechanical energies and wavefunctions, e.g., to solve electronic structure problems
3. **Path-integral quantum Monte Carlo:** quantum statistical mechanical integrals computed to obtain thermodynamic properties, using Feynman's path integral as a formal starting point);
4. **Volumetric Monte Carlo:** random and quasirandom number generators used to generate molecular volumes and sample molecular phase-space surfaces
5. **Simulation Monte Carlo:** stochastic algorithms to generate initial conditions for quasi-classical trajectory simulations, to simulate processes using scaling arguments to establish time scales or by introducing stochastic effects into molecular dynamics

The results of "Molecular Monte Carlo" calculations can be used to predict thermally-averaged structures, molecular charge distributions, reaction rate constants, free energies, dielectric constants, compressibilities, heat capacities, phase transition temperatures - just about anything.

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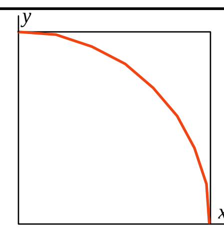
Integration



- Find π:
  - Area of unit circle is π, so integrate $\sqrt{1-x^2}$ for $\pi/4$
- Methods of integration:
  - divide axis into regular intervals and add average area
  - sample random points on axis and add average values
  - divide domain into regular grid and add square areas that are inside
  - sample by generating random points and computing fraction inside circle area

pgm$_9$

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Experiments

- Regular grid, regular average evaluation is better than Monte Carlo, but it requires full evaluation.
  - – refine by subdividing
- Monte Carlo can do the integration until a particular criterion is reached.
  - – refine by additional trials
- Can adapt sampling density to the problem

pgm

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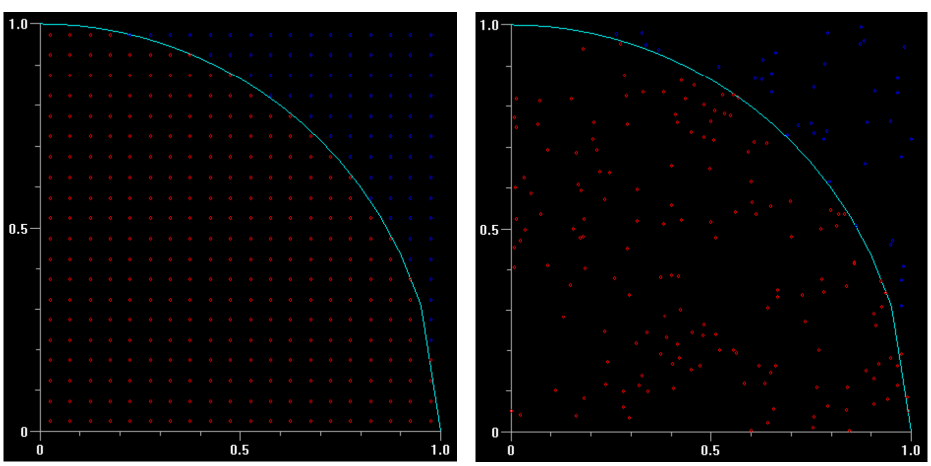
Example



pgm_A

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Percolation

- Given a grid in which some squares/boxes are blocked and some are free, can fluid percolate through the grid?
- If the probability *p* that a given square/box is blocked, does the grid allow percolation?
- Example applications:
  - Soil contamination models
  - Cerro Negro steam caused by water percolation
  - Absorption/run-off of rain water in suburbs

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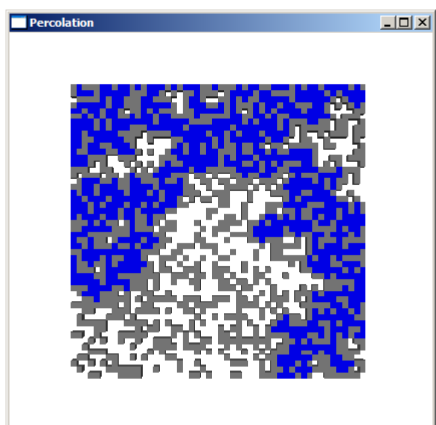
Percolation



Probability for percolation given probability of generating the grid
Critical probability is 0.5

pgm$_{B,C}$

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Demon Algorithm for Ideal Gas

- Randomized momentum transfer
- Demon to hold the residual system energy