Introduction to Monte Carlo (MC) methods

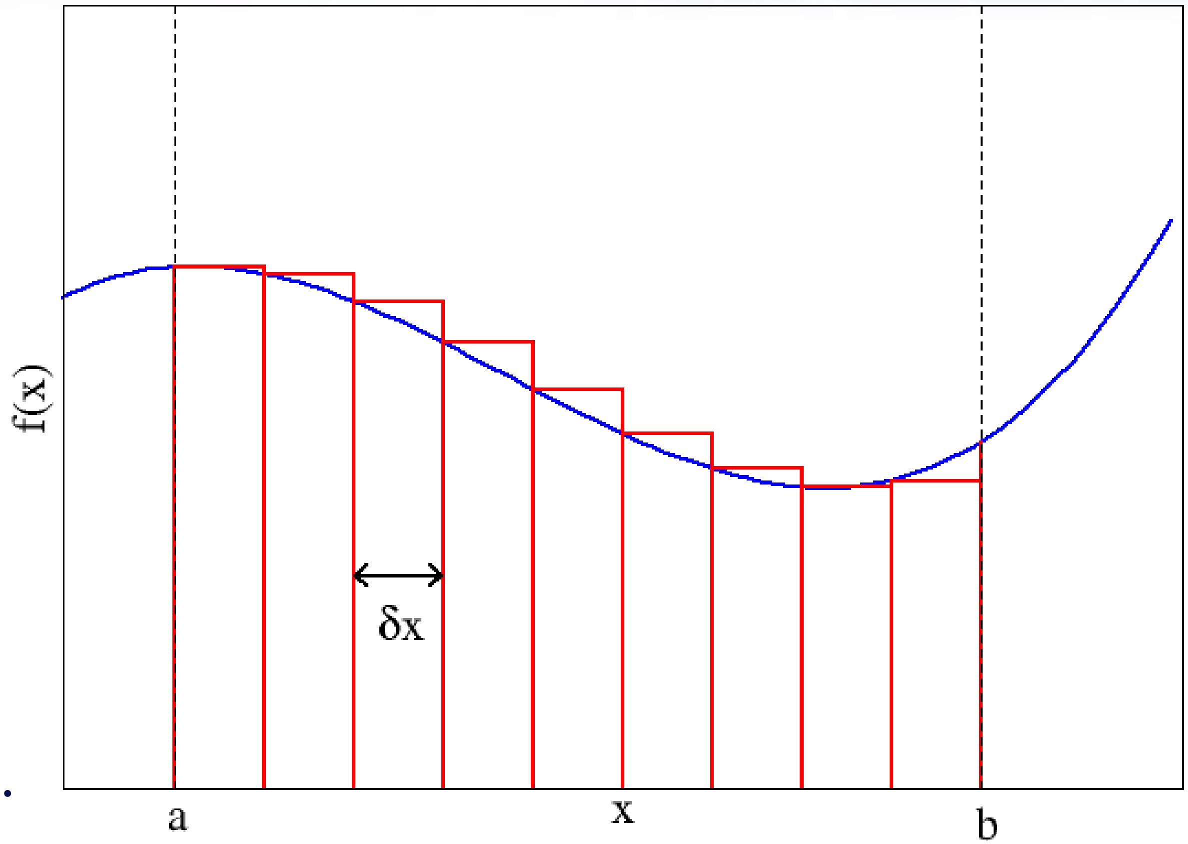
Why Scientists like to gamble

Overview

- Integration by random numbers
  - Why?
  - How?
- Uncertainty, Sharply peaked distributions
  - Importance sampling
- Markov Processes and the Metropolis algorithm
- Examples
  - statistical physics
  - finance
  - weather forecasting

Integration – Area under a curve

Tile area with strips of height *f(x)* and width *δx*



Analytical:

$$\delta x \to dx \to 0$$

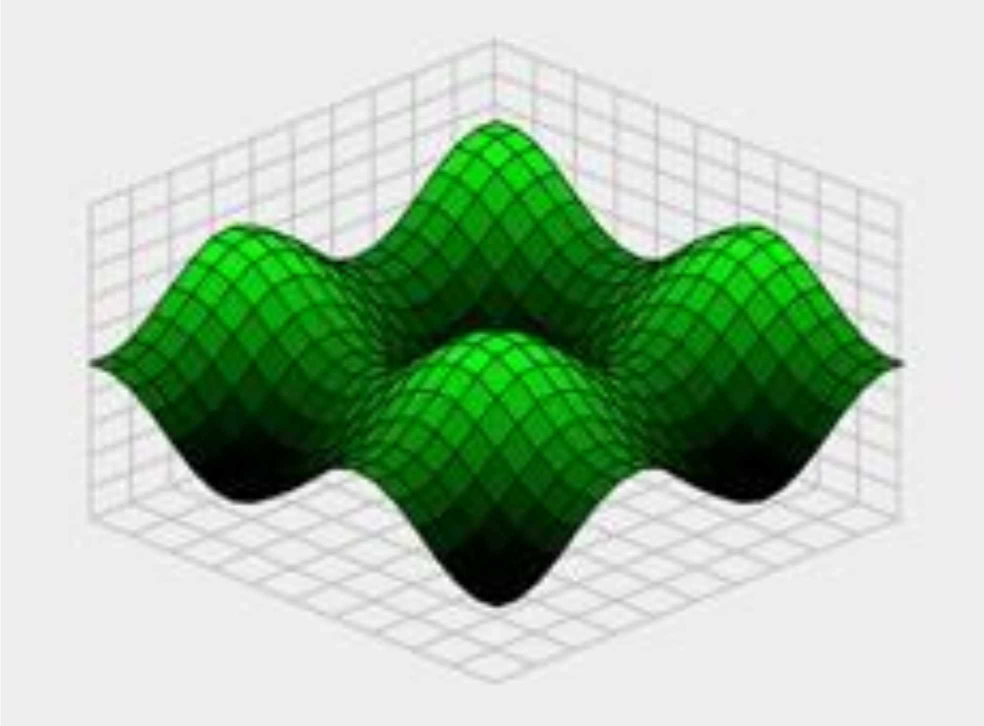
Numerical: integral replaced with a sum.

Uncertainty depends on size of *δx* (N points) and order of scheme, (Trapezoidal, Simpson, etc)

Multi-dimensional integration

1d integration requires N points

2d integration requires N^2



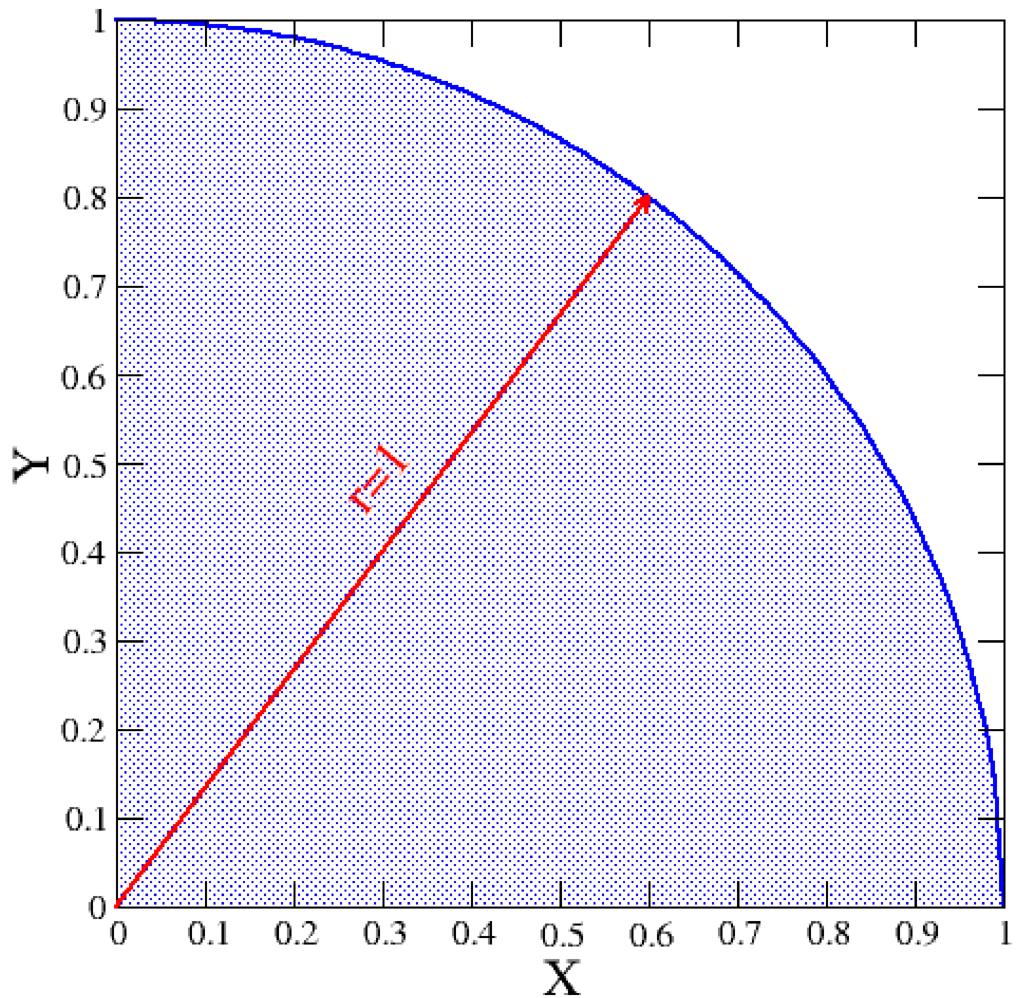
Problem of dimension m requires N^m

Curse of dimensionality

Calculating π by MC

Area of circle = πr^2
Area of unit square, $s = 1$
Area of shaded arc,
$c = \pi/4$
$c/s = \pi/4$

Estimate ratio of shaded to non-shaded area to determine π

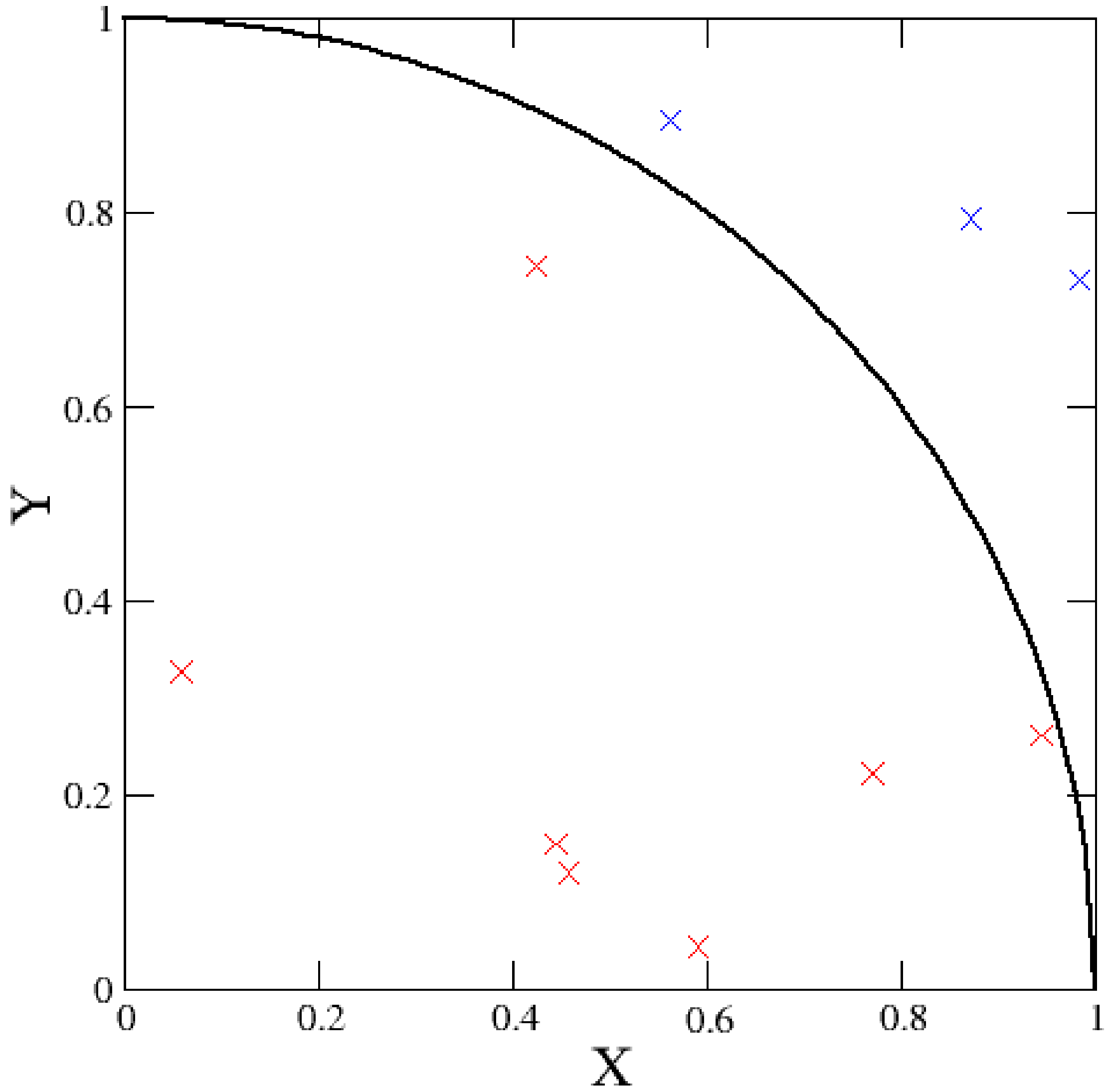


The algorithm

- `y = rand()/RAND_MAX // float {0.0:1.0}`
- `x = rand()/RAND_MAX`
- `P=x*x + y*y  // x*x + y*y = 1 eqn of circle`
- `If(P<=1)`
  - `isInCircle`
- `Else`
  - `IsOutCircle`
- `Pi=4*isInCircle / (isOutCircle+isInCircle)`

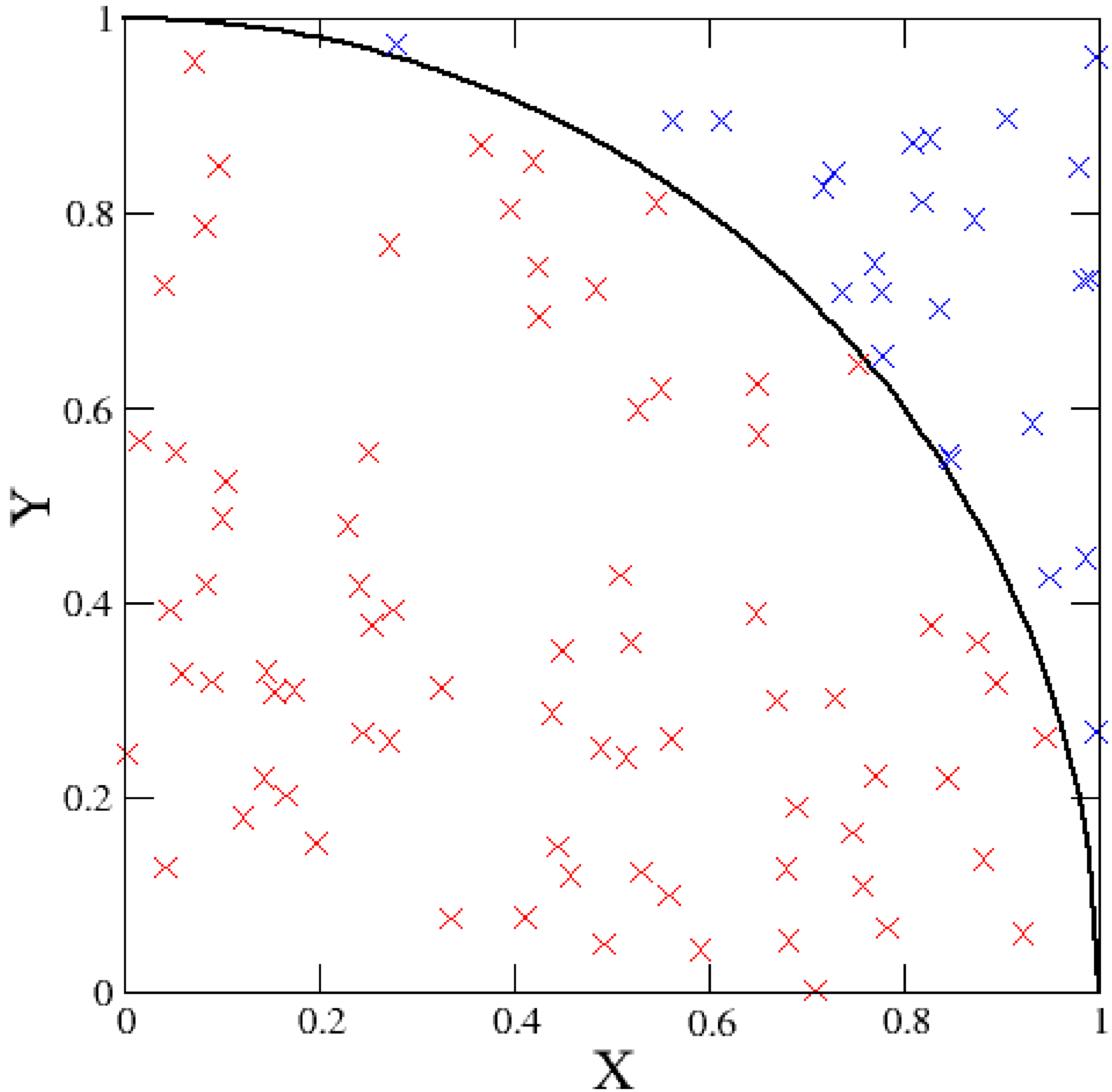
π from 10 darts

$\pi = 2.8$



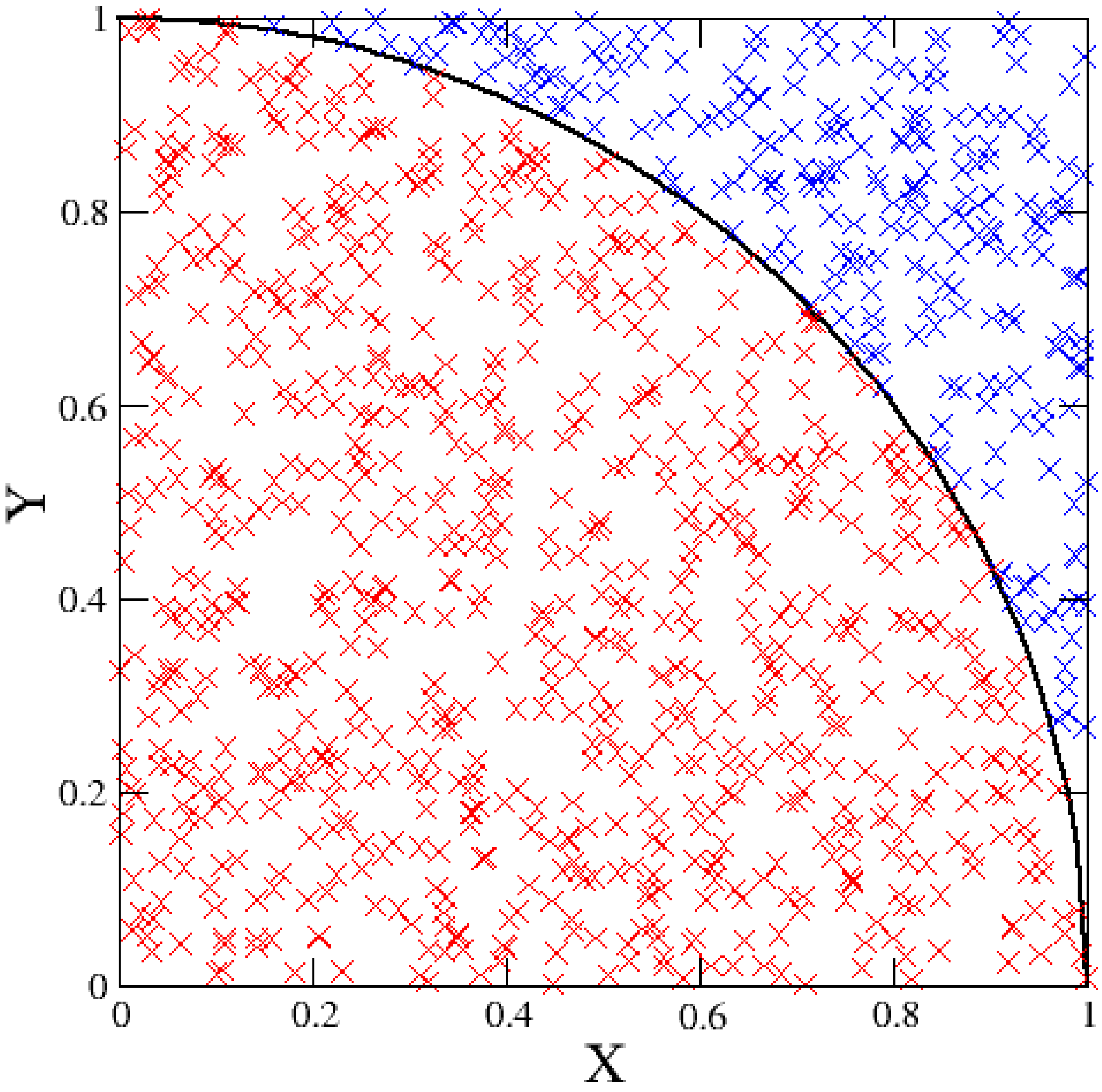
π from 100 darts

$\pi = 3.0$



π from 1000 darts

$\pi = 3.12$

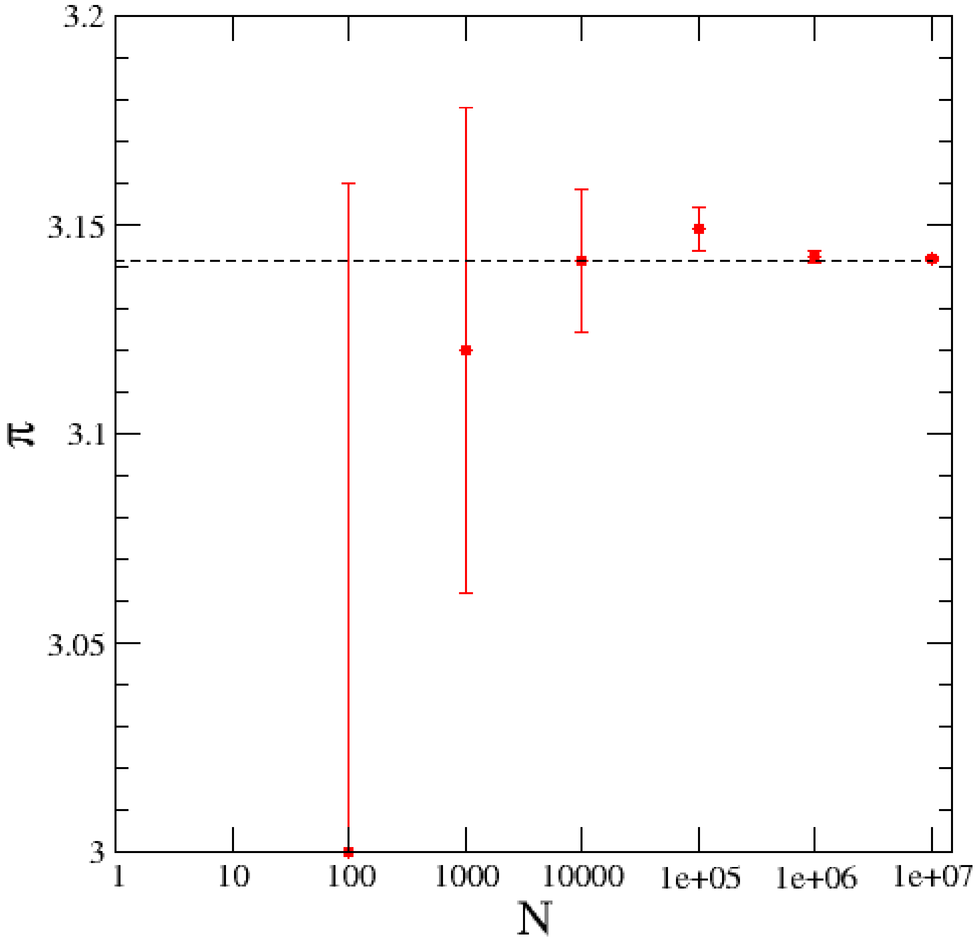


Estimating the uncertainty

- Stochastic method
  - –Statistical uncertainty
- Estimate this
  - –Run each measurement 100 times with different random number sequences
  - –Determine the variance of the distribution

$$\sigma^2 = \left(\bar{x} - x\right)^2 / k$$

- Standard deviation is σ
- How does the uncertainty scale with N, number of samples



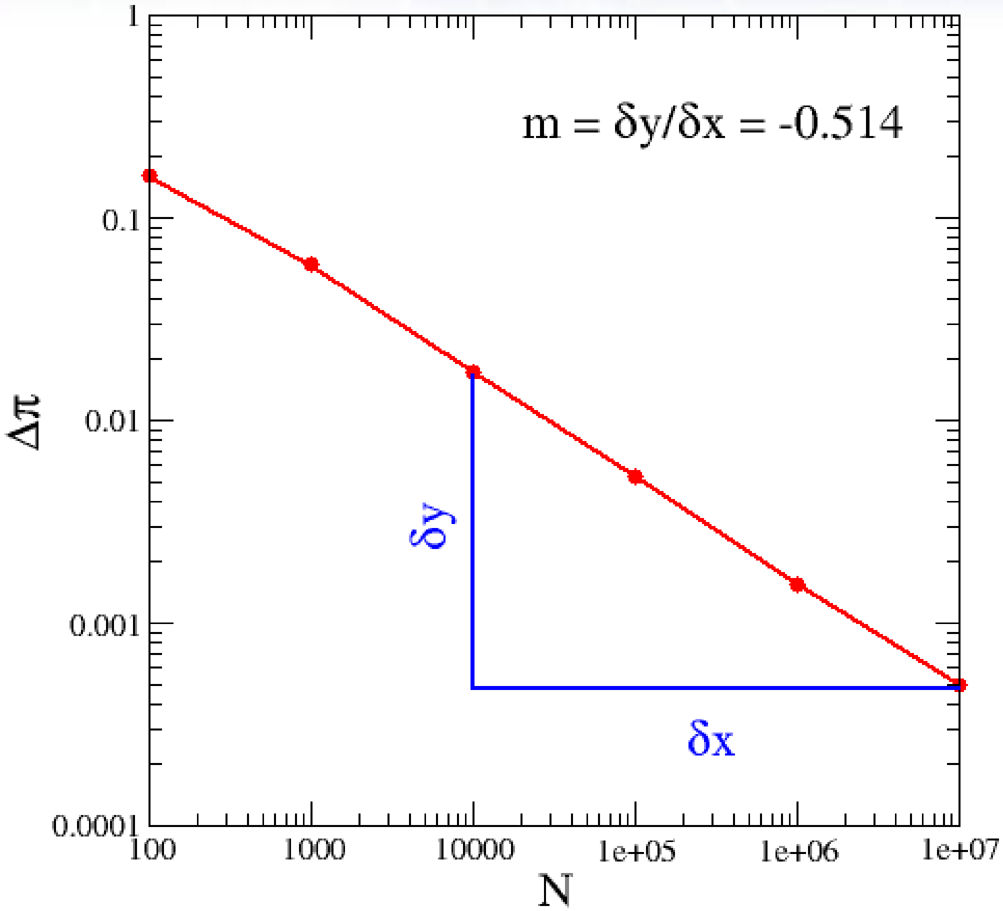
Uncertainty versus N

- Log-log plot

$$y = ax^{b}$$

$$\log y = \log a + b \log x$$

- Exponent b, is gradient
- b ≈ -0.5
- Law of large numbers and central limit theorem



$$\boxed{\Delta \sim 1/\sqrt{N}}$$

True for *all* MC methods

More realistic problem

- Imagine traffic model
  - can compute average velocity for a given density
  - this in itself requires random numbers ...
- What if we wanted to know average velocity of cars over a week
  - each day has a different density of cars (weekday, weekend, ...)
  - assume this has been measured (by a man with a clipboard)

Density	Frequency
0.3	4
0.5	1
0.7	2

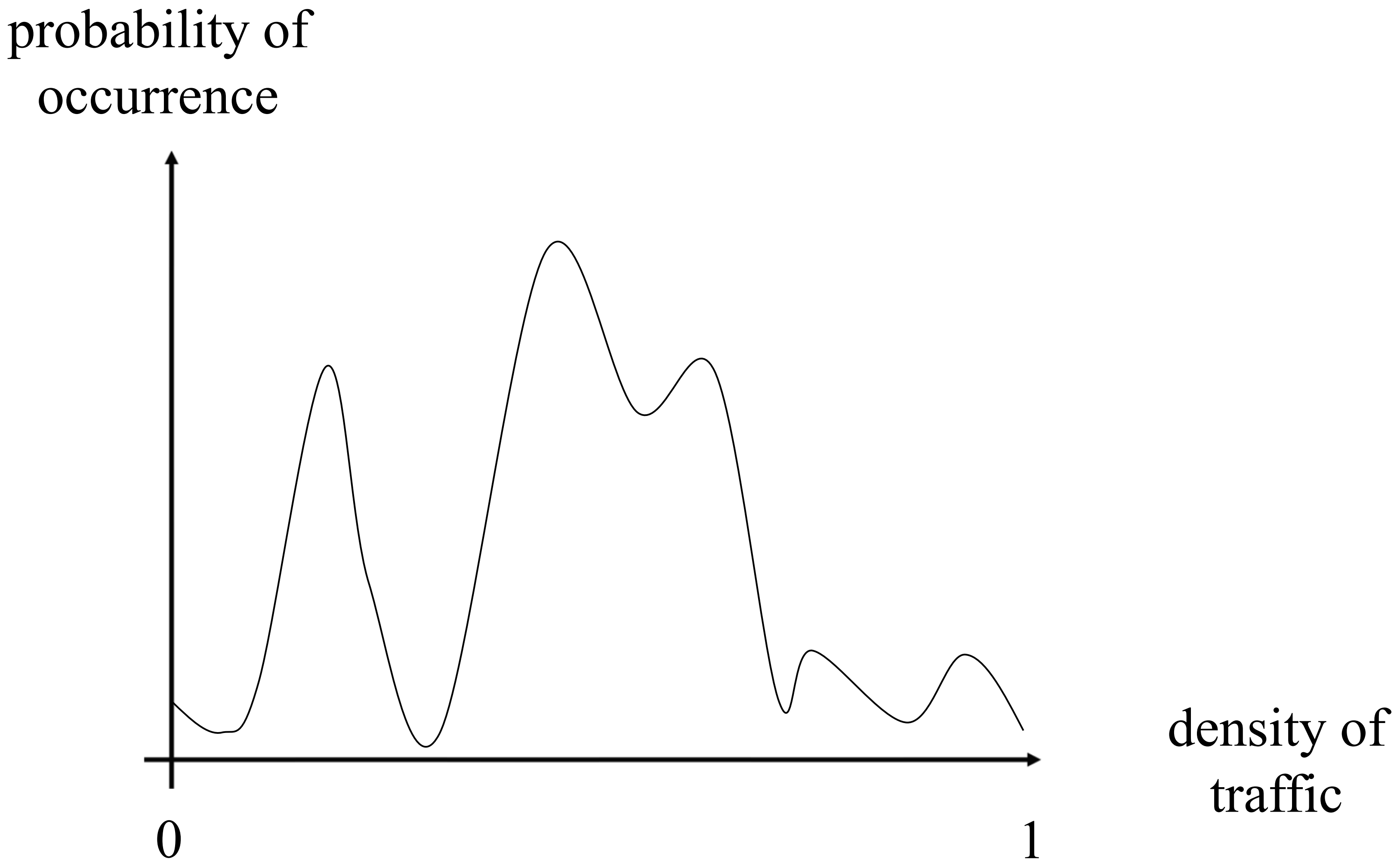
Expectation values

- Procedure:
  - run a simulation for each density to give average car velocity
  - compute average over week by weighting by probability of that density
  - i.e. velocity = 1/7* (4 * velocity(density = 0.3) +
    1 * velocity(density = 0.5) +
    2 * velocity(density = 0.7))

- In general, for many states x_i (e.g. density) and some function $f(x_i)$ (e.g. velocity) need to compute *expectation value* <f>

$$\sum_{1}^{N} p(x_i) * f(x_i)$$

Continuous distribution



Aside: A highly dimensional system

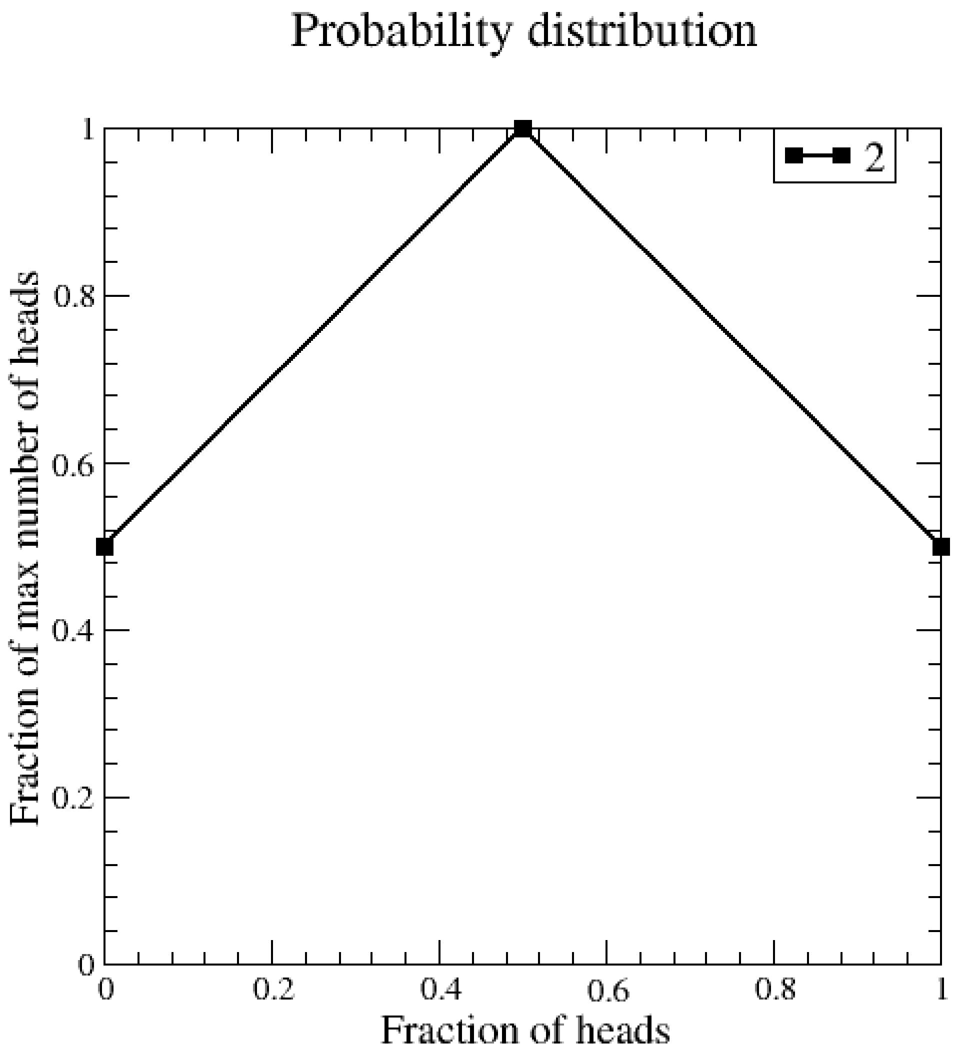
A high dimensional system

- 1 coin has 1 degree of freedom
  - Two possible states Heads and Tails
- 2 coins have 2 degrees of freedoms
  - Four possible micro-states, two of which are the same
  - Three possible states 1*HH, 2*HT, 1*TT
- n coins have n degrees of freedom
  - 2^n microstates: n+1 states
  - Number of micro-states in each state is given by the binomial expansion coefficient

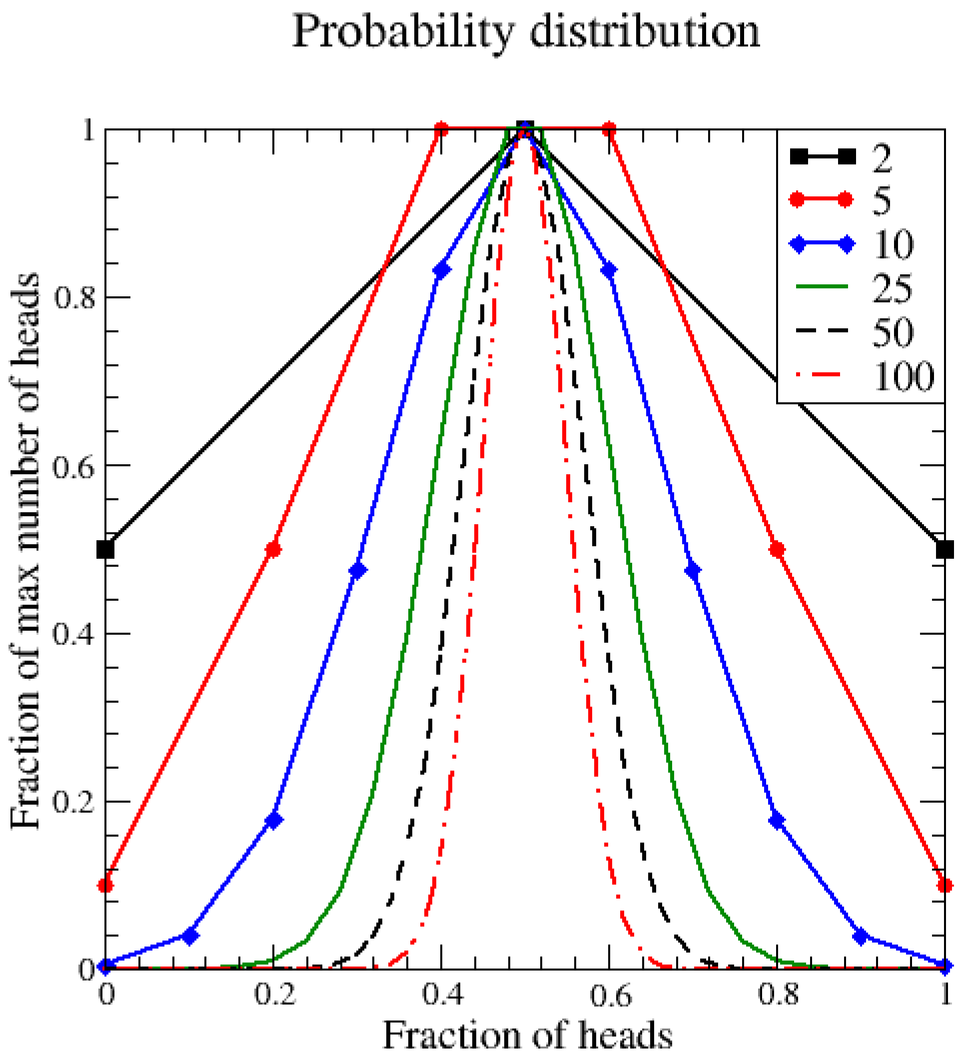
$$\Omega = 2^n = \sum_{r=0}^{n} {}^rC_n H^r T^{n-r}$$

$${}^rC_n = \frac{n!}{r!(n-r)!}$$

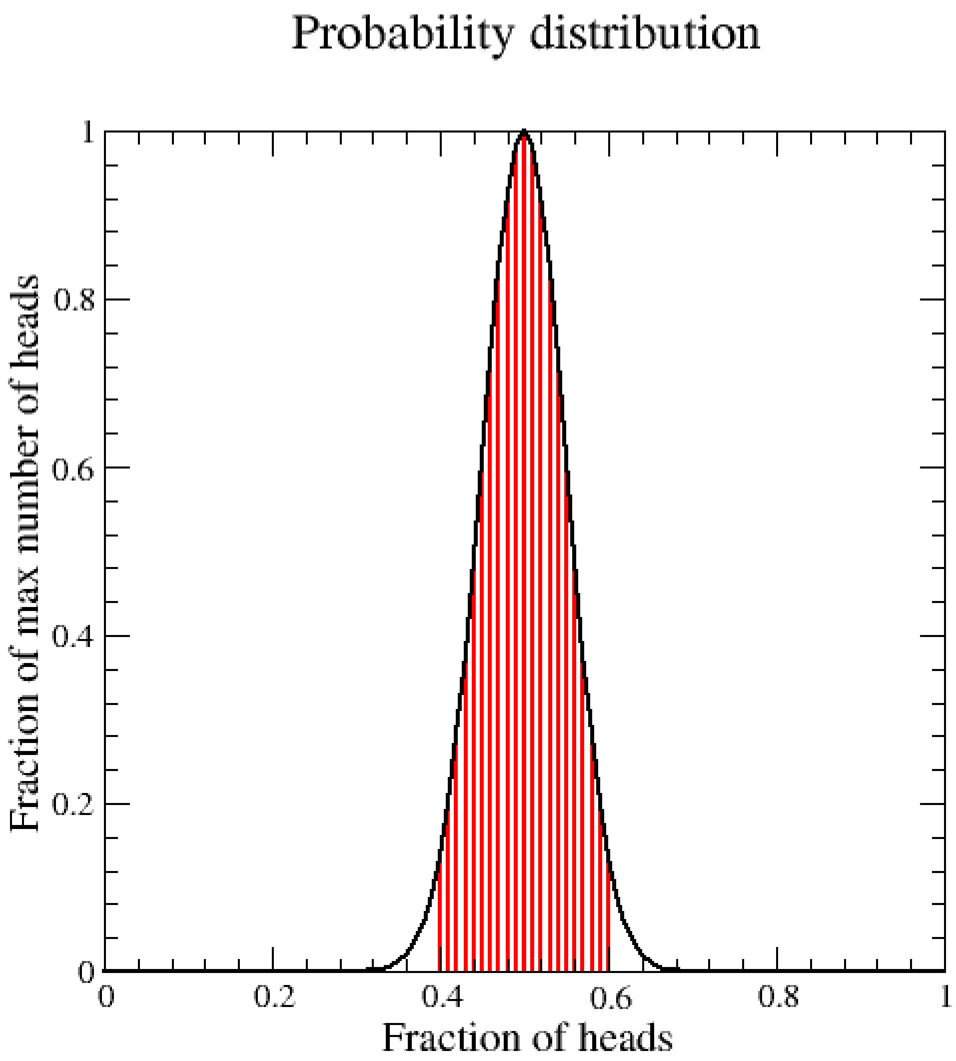
Highly peaked distribution



Highly peaked distribution



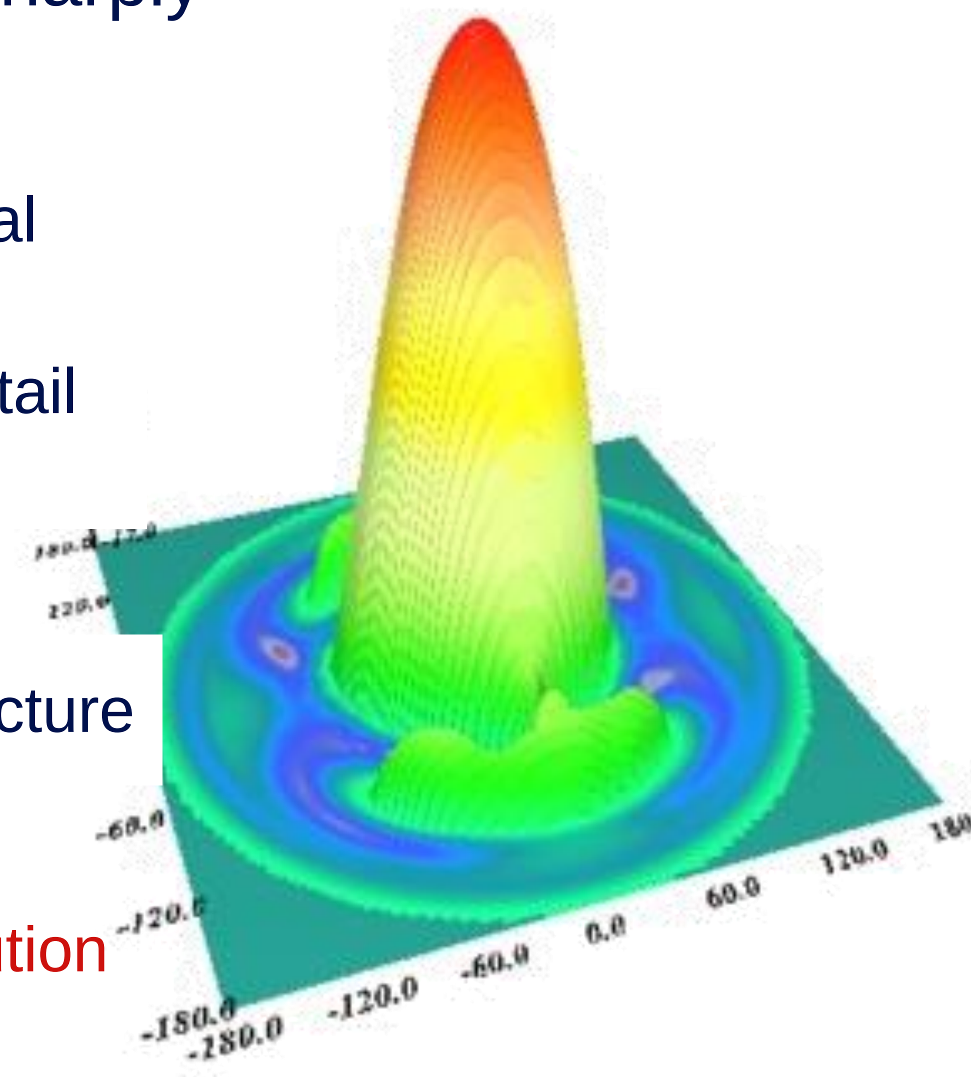
100 Coins



- 96.48% of all possible outcomes lie between 40 – 60 heads

Importance Sampling (i)

- The distribution is often sharply peaked
  - especially high-dimensional functions
  - often with fine structure detail
- Random sampling
  - $p(x_i) \sim 0$ for many x_i
  - N large to resolve fine structure
- Importance sampling
  - generate weighted distribution
  - proportional to probability



Importance Sampling (ii)

- With random (or uniform) sampling

$$<f> = \sum_1^N p(x_i) * f(x_i)$$

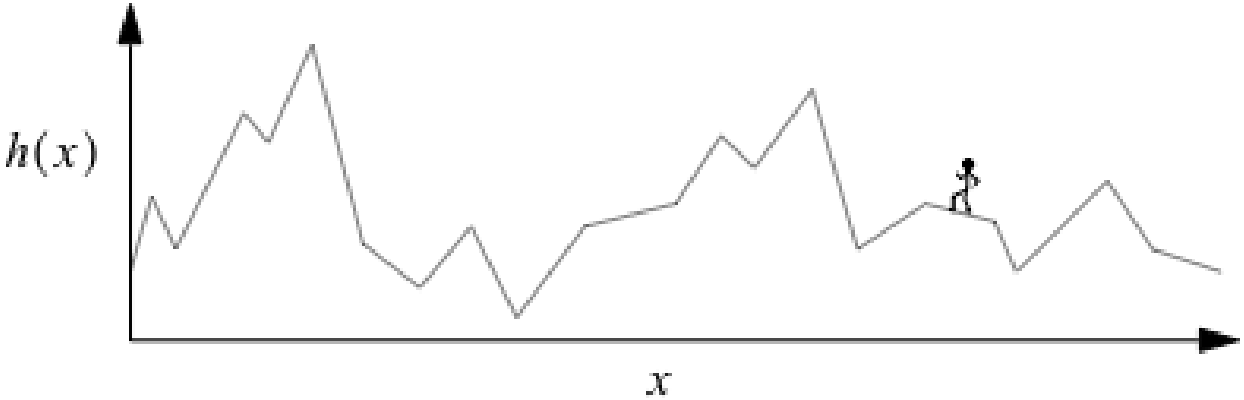
  - but for highly peaked distributions, $p(x_i) \sim 0$ for most cases
  - most of our measurements of $f(x_i)$ are effectively wasted
  - large statistical uncertainty in result
- If we generate x_i with *probability proportional* to $p(x_i)$

$$<f> = \frac{1}{N} \sum_1^N f(x_i)$$

  - all measurements contribute equally
- But how do we do this?

Hill-walking example

- Want to spend your time in areas proportional to height $h(x)$



  - walk randomly to explore all positions x_i
  - if you always head up-hill or down-hill
    - get stuck at nearest peak or valley
  - if you head up-hill or down-hill with equal probability
    - you don't prefer peaks over valleys
- Strategy
  - take both up-hill and down-hill steps but with a *preference* for up-hill

Markov Process

- Generate samples of $\{x_i\}$ with probability $p(x)$
- x_i no longer chosen independently
- Generate new value from old – evolution

$$x_{i+1} = x_i + \delta x$$

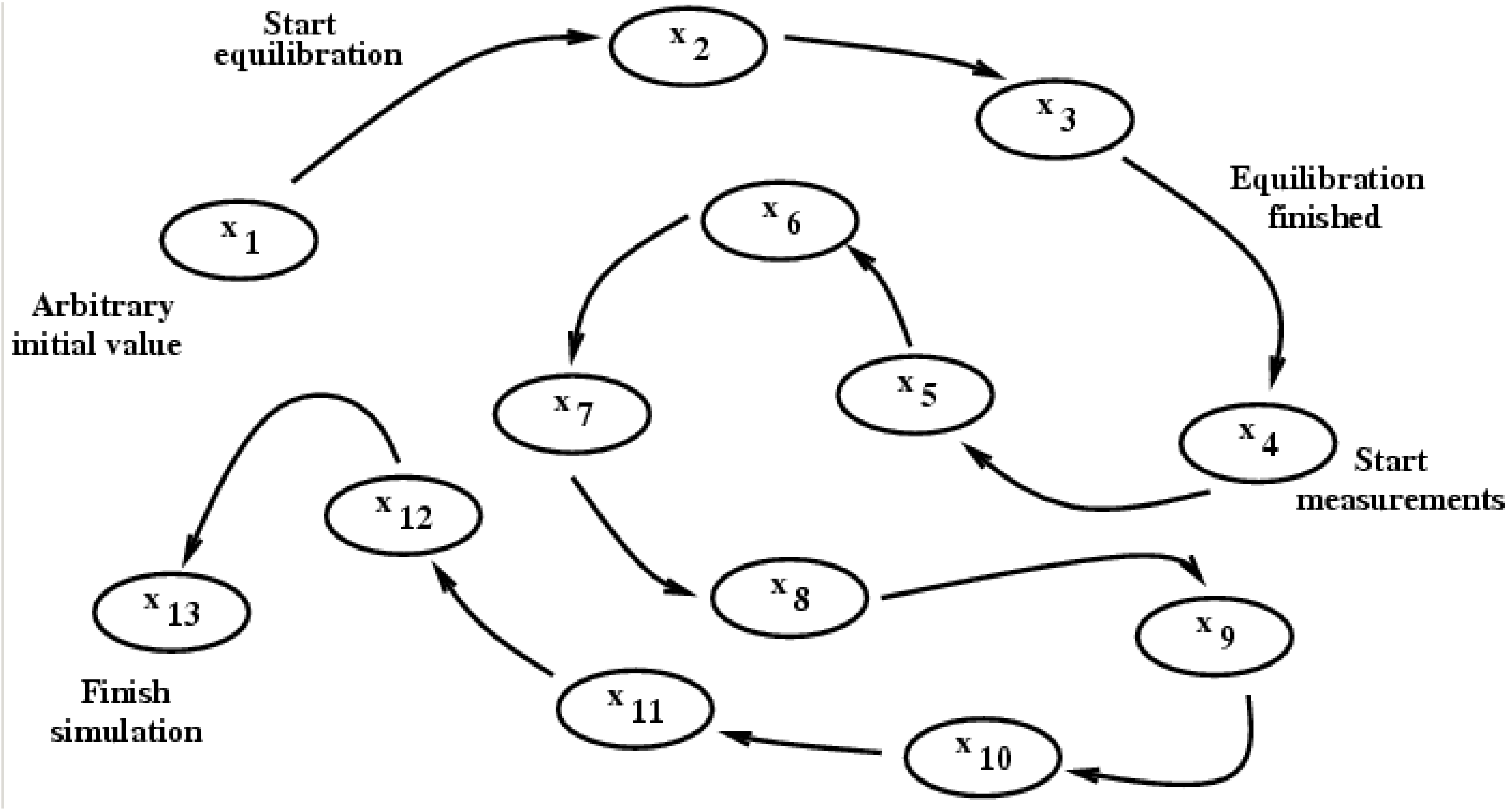
- Accept/reject change based on $p(x_i)$ and $p(x_{i+1})$
  - if $p(x_{i+1}) > p(x_i)$ then accept the change
  - if $p(x_{i+1}) < p(x_i)$ then accept **with probability** $\frac{p(x_{i+1})}{p(x_i)}$
- Asymptotic probability of x_i appearing is proportional to $p(x)$
- Need random numbers
  - to generate random moves δx and to do accept/reject step

AA Markov 1856-1922

Markov Chains

- The generated sample forms a Markov chain
- The update process must be ergodic
  - Able to reach *all x*
  - If the updates are non-ergodic then some states will be absent
  - Probability distribution will not be sampled correctly
  - computed expectation values will be incorrect!
- Takes some time to equilibrate
  - need to forget where you started from
- Accept / reject step is called the Metropolis algorithm

Markov Chains and Convergence



$$\langle f \rangle = \frac{1}{10} \sum_{i=4}^{13} f(x_i)$$

Statistical Physics

- Many applications use MC
- Statistical physics is an example
- Systems have extremely high dimensionality
  - e.g. positions and orientations of millions of atoms
- Use MC to generate “snapshots” or configurations of the system
- Average over these to obtain answer
  - Each individual state has no real meaning on its own
  - Quantities determined as averages across all the states

MC in Finance

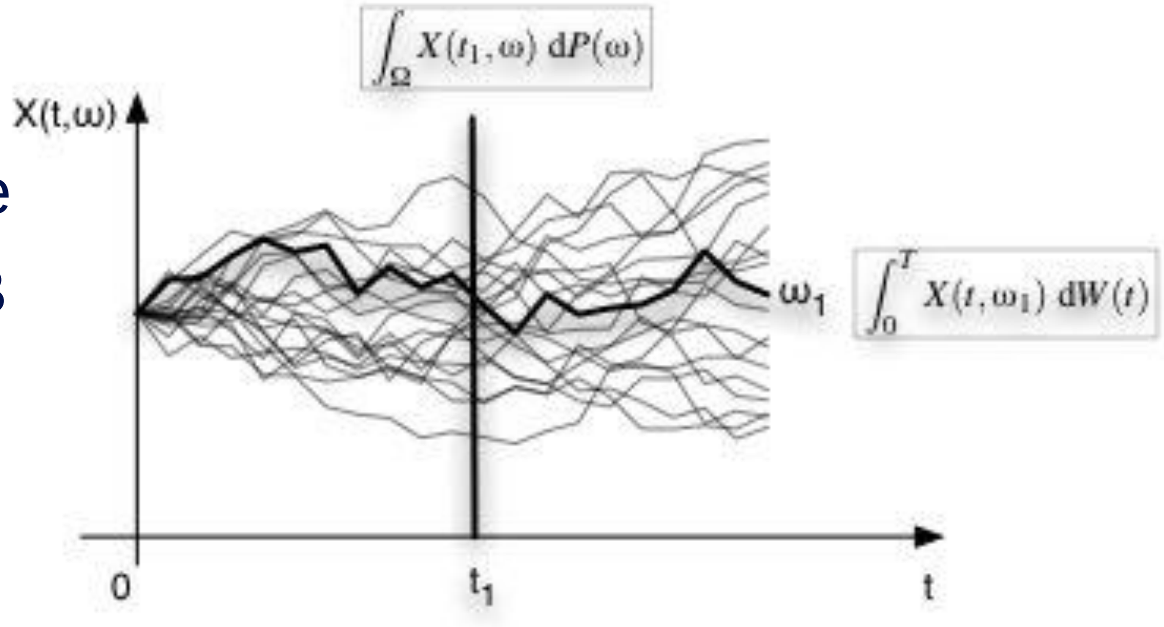
- Used to price *options*
- An option is a contract, holder has the *right*
  - buy an asset – *call*
  - sell an asset – *put*
  - at some time in the future (T)
  - For a predetermined price (*strike* price) X
- Terminal pay off for the holder is then

$$\max(\pm(S_T - X), 0)$$

  - where S_T is the price of the underlying asset at time T
  - $\pm$ call/put
- How much should the option cost?

MC in Finance II

- Price model called Black-Scholes equation
  - Partial differential equation
  - based on geometric brownian motion (GMB) of underlying asset
- Assumes a "perfect" market
  - markets are not perfect, especially during crashes!
  - Many extensions
  - area of active research
- Use MC to generate many different GMB paths
  - statistically analyse ensemble



Numerical Weather Prediction

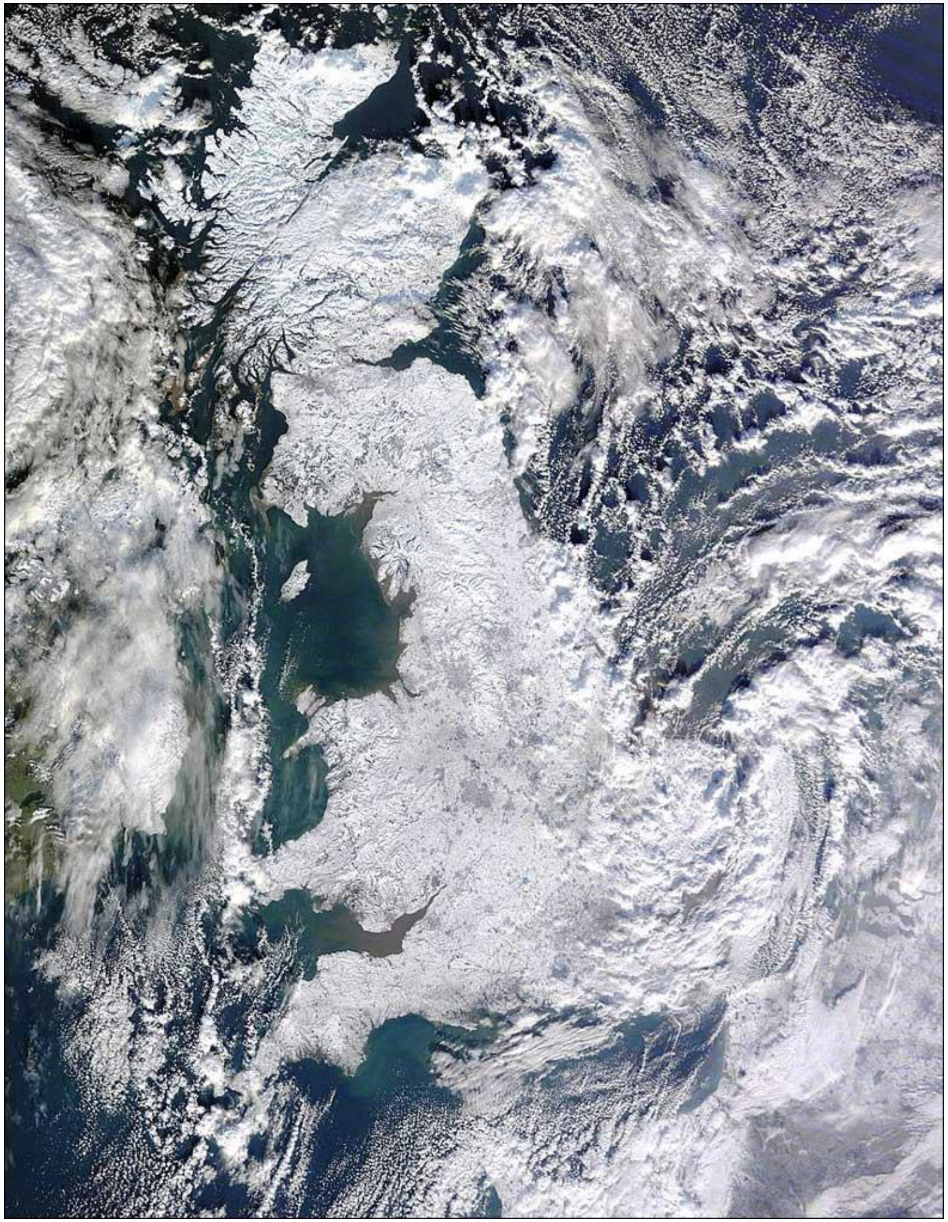


Image taken by NASA's Terra Satellite
7^{th} January 2010

Britain in the grip of a very cold spell of weather

NWP in the UK

- Weather forecasts used by the media in the UK (e.g. BBC news) are generated by the UK Met office
  - Code is called the Unified Model
  - Same code runs climate model and weather forecast
  - Can cover the whole globe

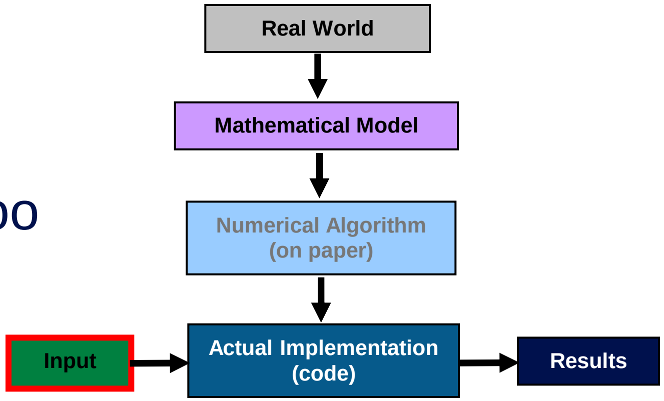
- Newest supercomputer
  - Cray XC40
  - almost half a million processor-cores
  - weighs 140 tonnes

(http://www.bbc.co.uk/news/science-environment-29789208)

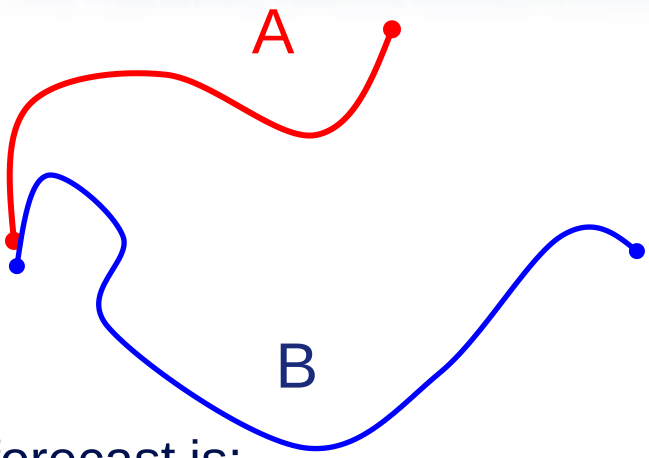
Initial conditions and the Butterfly effect

- The equations are extremely sensitive to initial conditions
  - Small changes in the initial conditions result in large changes in outcome
- Discovered by Edward Lorenz *circa* 1960
  - 12 variable computer model
  - Minute variations in input parameters
  - Resulted in grossly different weather patterns

- The Butterfly effect
  - The flap of a butterfly's wings can effect the path of a tornado
  - My prediction is wrong because of effects too small to see



Chaos, randomness and probability



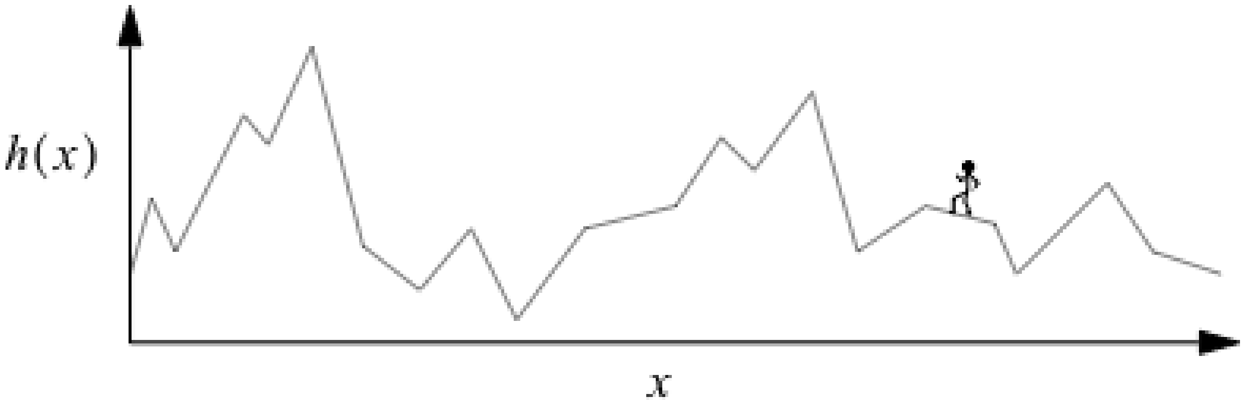
- A Chaotic system evolves to very different states from close initial states
  - – no discernible pattern
- We can use this to estimate how reliable our forecast is:
- Perturb the initial conditions
  - –Based on uncertainty of measurement
  - –Run a new forecast
- Repeat many times (random numbers to do perturbation)
  - –Generate an “ensemble” of forecasts
  - –Can then estimate the probability of the forecast being correct
- If we ran 100 simulations and 70 said it would rain
  - –probability of rain is 70%
  - –called **ensemble** weather forecasting

Optimisation Problems

- Optima of function rather than averages
- Often need to minimise or maximise functions of many variables
  - minimum distance for travelling salesman problem
  - minimum error for a set of linear equations
- Procedure
  - take an initial guess
  - successively update to progress towards solution
- What changes should be proposed?
  - could reduce/increase the function with each update (steepest descent/ascent) ...
  - ... but this will only find the local minimum/maximum

Stochastic Optimisation

- Add a random component to updates
- Sometimes make "bad" moves
  - possible to escape from local minima
  - but want more up-hill steps than down-hill ones
- Hill-walking example
  - find the highest peak in the Alps by maximising $h(x)$



Simulated Annealing

- Monte Carlo technique applied to optimisation
- Analogy with Metropolis and Statistical Mechanics
- Initial "high-temperature" phase
  - accept both up-hill and down-hill steps to explore the space
- Intermediate phase
  - start to prefer up-hill steps to look for highest mountain
- Final "zero-temperature" phase
  - only accept up-hill steps to locate the peak of the mountain
- A lot of freedom in how you vary the temperature ...

Summary

- Random numbers used in many simulations

- Mainly to efficiently sample a large space of possibilities

- One state generated from another: Markov Chain
  - Metropolis algorithm gives a guided random walk

- Real simulations can require trillions of random numbers!
  - parallelisation introduces additional complexities ...