Monte Carlo Integration and Random Numbers

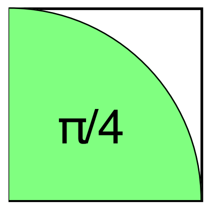
Higher dimensional integration

- Simpson rule with M evaluations in
  - one dimension the error is order M^{-4}
  - d dimensions the error is order $M^{-4/d}$
- In general an order-n scheme in one dimensions is order-n/d in d dimensions
- The phase space of physical N-body problems are usually very high-dimensional
  - classical mechanics: $d=6N$ (positions and velocities)
  - classical spin problem: $d=2N$ (two angles)
  - quantum spin-S problem: $d=(2S+1)^N$

Throwing stones into a pond

- How can we estimate the size of a pond with stones?
- How can we calculate π by throwing stones?

- Let us take a square surrounding the area we want to measure:



- Choose *M* random points and count how many lie in the interesting area
- Again we have a Mathematica notebook for this problem

Monte Carlo integration

- Consider an integral $\langle f \rangle = \int_\Omega f(x)dx \Big/ \int_\Omega dx$
- Instead of evaluating it at equally spaced points evaluate it at *M* points x_i chosen randomly in W:

$$\langle f \rangle \approx \frac{1}{M}\sum_{i=1}^{M} f(\vec{x}_i)$$

- This is a Monte Carlo estimate for the integral

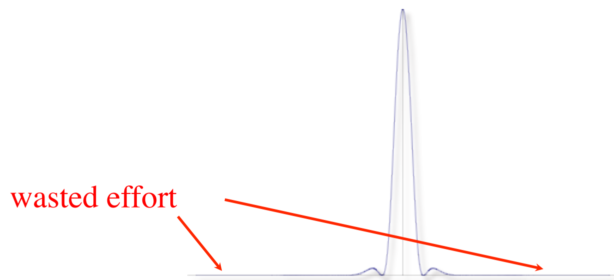
- The error is statistical:

$$\Delta = \sqrt{\frac{\mathrm{Var}\, f}{M-1}} \propto M^{-1/2}$$

$$\mathrm{Var}\, f = \langle f^2 \rangle - \langle f \rangle^2$$

- In *d*>8 dimensions Monte Carlo is better than Simpson!

Sharply peaked functions



- In many cases a function is large only in a tiny region
- Lots of time wasted in regions where the function is small
- The sampling error is large since the variance is large

Importance sampling

- Simple sampling as discussed before is slow if the variance is big (function large in some regions, small in others)
- Then importance sampling is better. We choose points not uniformly but with probability p(x):

$$\langle f \rangle = \left\langle \frac{f}{p} \right\rangle_p := \int_\Omega \frac{f(x)}{p(x)} p(x) dx \Big/ \int_\Omega dx$$

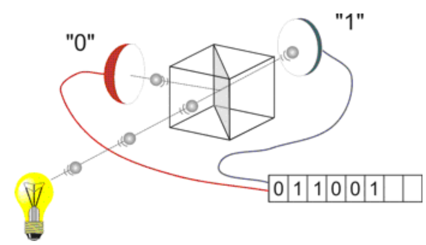
- The error is now determined by the variance of *f/p*
- We want to choose *p* similar to *f* and such that p-distributed random numbers are easily available
- Example can also be found on the Mathematica file

$$f(x) = \exp(-x^2) \qquad p(x) = \exp(-x)$$

Generating random numbers

- Real random numbers are hard to obtain
  - classical or thermal chaos (atmospheric noise)
  - quantum mechanics
- Commercial products: quantum random number generators
  - based on photons and semi-transparent mirror
  - 4 Mbit/s from a USB device, too slow for most MC simulations

http://www.idquantique.com/



Pseudo Random numbers

- Are generated by an algorithm
- Not random at all, but completely deterministic
- Look nearly random however when algorithm is not known and may be good enough for our purposes
- Never trust pseudo random numbers however!

Linear congruential generators

- are of the simple form $x_{n+1}=f(x_n)$, with f usually a linear function
- A good choice is the GGL generator

$$x_{n+1} = (ax_n + c) \bmod m$$

with $a = 16807$, $c = 0$, $m = 2^{31}-1$, $x_0=667790$

- quality depends sensitively on a,c,m and the seed value x_0
- Periodicity is a problem with such 32-bit generators
  - The sequence repeats identically after $2^{31}-1$ iterations
  - With modern computers that is just a few seconds!
  - Nowadays such 32-bit generators should not be used!

Lagged Fibonacci generators

- $$x_n = x_{n-p} \otimes x_{n-q} \bmod m$$
- Good choices for 64-bit floating point numbers (m=1)
  - (55,24,+)
  - (607,273,+)
  - (2281,1252,+)
  - (9689,5502,+)
  - (44497,23463,+)
- Seed blocks usually generated by linear congruential
- Has very long periods since large block of seeds
- no data dependencies for min(p,q) iterations
  - can be vectorized on vector CPUs
  - can be pipelined on scalar CPUs

More advanced generators

- As well-established generators fail new tests, better and better generators get developed
  - Mersenne twister (Matsumoto & Nishimura, 1997)
    http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html
  - Well generator (Panneton and L'Ecuyer , 2004)
    http://www.iro.umontreal.ca/~panneton/WELLRNG.html

Are these numbers really random?

- No!
- Are they random enough?
  - Maybe?
- How can we test?
  - Statistical tests for distribution
  - Statistical tests for short time correlations
  - Statistical tests for long time correlations
  - …
- Are these tests enough?
  - No! Your calculation could depend in a subtle way on hidden correlations!
- What is the ultimate test?
  - Run your simulation with various random number generators and compare the results

Easiest: graphical

- Before discussing statistical tests there is a simple first tool:
  - Create random pairs *(x,y)* and plot them
  - Create random triples *(x,y,z)* and plot them
- Can you see correlations?
- A Mathematica Notebook for these plots is on the web page of this course

Some simple RNG tests

- Graphical correlations test:
  - Create random n-tuplets ($x_1, x_2, \ldots, x_n$) and plot them (see *Mathematica* notebook).
- Correlations test: $$\frac{1}{N}\sum_{i=1}^{N} x_i x_{i+n} = \langle x\rangle^2 + \mathcal{O}(N^{-1/2}) \qquad \forall n$$
- Moments test: $$\left|\frac{1}{N}\sum_{i=1}^{N} x_i^k - \frac{1}{k-1}\right| \sim \mathcal{O}(N^{-1/2})$$
- Best known (free) testsuite: Diehard from George Marsaglia. See: http://stat.fsu.edu/pub/diehard/.

Marsaglia's diehard tests

- Birthday spacings: Choose random points on a large interval. The spacings between the points should be asymptotically Poisson distributed. The name is based on the birthday paradox.
- Overlapping permutations: Analyze sequences of five consecutive random numbers. The 120 possible orderings should occur with statistically equal probability.
- Ranks of matrices: Select some number of bits from some number of random numbers to form a matrix over {0,1}, then determine the rank of the matrix. Count the ranks.
- Monkey tests: Treat sequences of some number of bits as "words". Count the overlapping words in a stream. The number of "words" that don't appear should follow a known distribution. The name is based on the infinite monkey theorem.
- Count the 1s: Count the 1 bits in each of either successive or chosen bytes. Convert the counts to "letters", and count the occurrences of five-letter "words".
- Parking lot test: Randomly place unit circles in a 100 x 100 square. If the circle overlaps an existing one, try again. After 12,000 tries, the number of successfully "parked" circles should follow a certain normal distribution.

Marsaglia's diehard tests (cont.)

- Minimum distance test: Randomly place 8,000 points in a 10,000 x 10,000 square, then find the minimum distance between the pairs. The square of this distance should be exponentially distributed with a certain mean.
- Random spheres test: Randomly choose 4,000 points in a cube of edge 1,000. Center a sphere on each point, whose radius is the minimum distance to another point. The smallest sphere's volume should be exponentially distributed with a certain mean.
- The squeeze test: Multiply 231 by random floats on [0,1) until you reach 1. Repeat this 100,000 times. The number of floats needed to reach 1 should follow a certain distribution.
- Overlapping sums test: Generate a long sequence of random floats on [0,1). Add sequences of 100 consecutive floats. The sums should be normally distributed with characteristic mean and sigma.
- Runs test: Generate a long sequence of random floats on [0,1). Count ascending and descending runs. The counts should follow a certain distribution.
- The craps test: Play 200,000 games of craps, counting the wins and the number of throws per game. Each count should follow a certain distribution.

Non-uniform random numbers

- we found ways to generate pseudo random numbers *u* in the interval [0,1[
- How do we get other uniform distributions?
  - uniform in [*a*,*b*[: *a+(b-a) u*
- Other distributions:
  - inversion of integrated distribution
  - acceptance-rejection method

The probability density function of a distribution

- The probability density function $p(x)$ Gives the probability of finding a number in an infinitesimal interval dx around x
- The probability of finding a number x in an interval $[a,b[$ is

$$P[a \leq x < b] = \int_a^b p(x)dx$$

- The integrated probability function $P(x)$ is the integral of $p(x)$

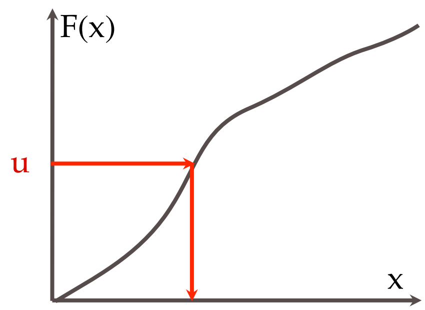
$$P(x) = \int_{-\infty}^{x} p(t)dt$$

Non-uniform distributions

- How can we get a random number x distributed with f(x) in the interval [a,b[from a uniform random number u?
- Look at probabilities:

$$P[x<y]=\int_a^y f(x)dx =: F(y) \equiv P[u<F(y)]$$

$$\Rightarrow x = F^{-1}(u)$$



- This method is feasible if the integral can be inverted easily
  - exponential distribution f(x)=λ exp(-λx)
  - can be obtained from uniform by x=-1/λ ln(1-u)

Normally distributed numbers

- The normal distribution

$$f(x)=\frac{1}{\sqrt{2\pi}}\exp\left(-x^2/2\right)$$

  can be easily integrated in 2 dimensions

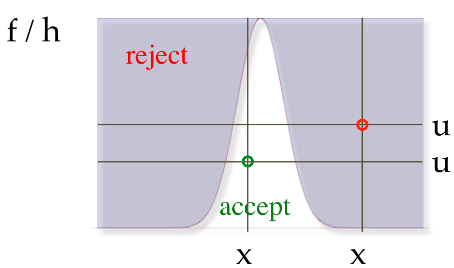
- We can obtain two normally distributed numbers from two uniform ones (Box-Muller method)

$$n_1 = \sqrt{-2\ln(1-u_1)}\sin u_2$$
$$n_2 = \sqrt{-2\ln(1-u_1)}\cos u_2$$

Uniform random numbers on N-sphere

- random points ***s*** on the surface of an N-sphere
- using acceptance-rejectance
  - get uniform random vector ***x*** with each component in [-1,1[
  - if norm is greater then one choose new one
  - normalize length to one
- using Box-Muller
  - start with uniform random vector ***x***
  - use Box-Muller to get normally distributed vector ***n***
  - normalize the length to one: the angles are uniformly distributed
- first method better only for very small N

Rejection method (von Neumann)



- Look for a simple distribution h that bounds f: f(x) < λh(x)
  - Choose an h-distributed number x
  - Choose a uniform random number 0 <= u < 1
  - Accept x if u < f(x)/ λh(x), otherwise reject x and get a new pair (x,u)
- Needs a good guess h to be efficient

The Boost random library

- Has become part of the C++03 standard and in a modifed form in C++11
- For now get it from Boost: http://www.boost.org/
- It contains
  - Random number generators
  - Distribution functions

Generators in the Boost random library

- All generators have members such as:

```
class RNG {
  public:
    typedef … result_type; // can be int, double,…
    RNG();

    void seed(); // the default seed
    template <class Iterator>
    Iterator seed(Iterator first, Iterator last);
    // seed from a range of unsigned int

    result_type min() const;
    result_type max() const;

    result_type operator(); // get the next random number
};
```

- They can be uniform floating point or integer generators with range between `min()` and `max()`

Useful and good generators

- `#include <boost/random.hpp>`

```
// Mersenne-twisters (modern, improved lagged Fibonacci generators)
boost::mt11213b rng1;
boost::mt19937 rng2;

// standard lagged Fibonacci generators
boost::lagged_fibonacci607 rng3;
boost::lagged_fibonacci1279 rng4;
boost::lagged_fibonacci2281 rng5;

// linear congruential generators
boost::minstd_rand0 rng6;
boost::minstd_rand rng7;
```

- Read the documentation for more generators and details

Distributions in the Boost random library

- Uniform distributions
  - Integer: `boost::uniform_int<int> dist1(a,b)`
  - Floating point: `boost::uniform_real<double> dist2(a,b)`
- Exponential distribution

$$p(x) = \frac{1}{\lambda}\exp(-\lambda x)$$

  - `boost::exponential_distribution<double> dist3(lambda)`
- Normal distribution

$$f(x) = \frac{1}{\sqrt{2\pi}}\exp\left(-(x-\mu)^2 / 2\sigma^2\right)$$

  - `boost::normal_distribution<double> dist4(mu,sigma)`
- Read the documentation for more distributions and details

Combining generators with distributions

- Is done using `boost::variate_generator`

```
// define the distribution
boost::normal_distribution<double> dist(0.,1.);

// define the random number generator engine
boost::mt19937 engine;

// create a normally distributed generator
boost::variate_generator<boost::mt19937&,
  boost::normal_distribution<double> >
  rng(engine,dist);

// use it
 for (int i=0;i<100;++i)
  std::cout << rng() << “\n”;
```

- Read the documentation for more details