Monte Carlo Methods for Uncertainty Quantification

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Lecture outline

Lecture 1: Introduction and Monte Carlo basics

- some model applications
- random number generation
- Monte Carlo estimation
- Central Limit Theorem and confidence interval

Lecture 2: Variance reduction

- basic manipulations
- control variate
- importance sampling
- stratified sampling
- Latin Hypercube
- randomised quasi-Monte Carlo

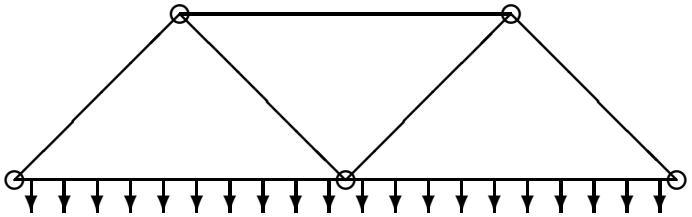
Lecture outline

Lecture 3: multilevel Monte Carlo and applications

- weak and strong convergence
- mean square error decomposition
- multilevel Monte Carlo
- PDEs with uncertainty

Application 1

Consider a bridge with 7 elements and pinned joints:



Design will compute a force balance, work out compression / extension of each element, and therefore determine the natural length to be cast.

However, the manufactured elements will vary from design in both length and extensibility – 14 uncertain inputs.

If two supporting joints have fixed position, then analysis has 6 unknowns (coordinates of free joints) and 6 equations (force balance at free joints).

Application 1

Given manufacturing data on the variability of the natural length and extensibility, what might we want to know?

- RMS deviation of joint position from design
- RMS deviation of forces from design
- probability of maximum compression / extension force being outside some specified range

Note: if we turn this into a full finite element analysis, then the computational cost becomes much larger.

Application 2

Consider a square trampoline, with vertical position given by

$$T\left(\frac{\partial^2 Z}{\partial x^2}+\frac{\partial^2 Z}{\partial y^2}\right)=L(x,y), \qquad 0<x<1,\ 0<y<1$$

where T is the tension and $L(x,y)$ is the applied load.

Here the uncertainty could be in the boundary conditions:

- simplest case would be uncertainty in the 4 corner values of $Z(x,y)$ with straight line interpolation along each edge
- a more complicated case might add a Fourier decomposition of the perturbation from the straight line interpolation

$$Z(x,0)=(1-x)\,Z_{0,0}+x\,Z_{1,0}+\sum_{n=1}^{\infty} a_n \sin(n\pi x)$$

Could also have uncertainty in the tension and the loading.

Application 2

Again there are various outputs we might be interested in:

- average values for $\min Z(x,y)$ and $\max Z(x,y)$
- RMS varation in these due to uncertainty

Note: biggest displacements likely to occur in the middle, not significantly affected by high order Fourier perturbations on the boundary.

Application 3

In modelling groundwater flow in nuclear waste repositories, or oil flow in oil reservoirs, we use Darcy's Law:

$$\nabla\cdot\Big(\kappa\nabla p\Big)=0$$

where p is the pressure and κ is the permeability of the rock.

The uncertainty here is in $\kappa(x)$ – typically might know the values at a few bore holes, but there is a large amount of uncertainty elsewhere.

We do know that if two points x_1, x_2 are close, then $\kappa(x_1)\approx\kappa(x_2)$, but if they are far apart then they can be quite different. Hence, often model $\log\kappa$ as having a Normal distribution, with a spatial covariance of the form

$$\mathrm{cov}(\log\kappa(x_1),\log\kappa(x_2))=\sigma^2\exp(-\|x_1-x_2\|/\lambda)$$

where λ is the correlation length.

Application 3

What does this application require?

- generation of samples of the stochastic field $\log \kappa(x)$ with correct distribution
- computation of $p(x)$ by solving Darcy PDE
- evaluation of outputs of interest (e.g. water or oil flux across some boundary)
- Monte Carlo simulation to obtain average value, RMS variation, probability of exceeding some threshold, etc.

Random Number Generation

Monte Carlo simulation starts with random number generation, usually split into 2 stages:

- generation of independent uniform $(0, 1)$ random variables
- conversion into random variables with a particular distribution (e.g. Normal)

Very important: never write your own generator, always use a well validated generator from a reputable source

- Matlab
- NAG
- Intel MKL
- AMD ACML

Uniform Random Variables

Pseudo-random number generators use a deterministic (i.e. repeatable) algorithm to generate a sequence of (apparently) random numbers on $(0, 1)$ interval.

What defines a good generator?

- a long period – how long it takes before the sequence repeats itself
  2^{32} is not enough – need at least 2^{40}
- various statistical tests to measure "randomness"
  well validated software will have gone through these checks
- trivially-parallel Monte Carlo simulation on a compute cluster requires the ability to "skip-ahead" to an arbitrary starting point in the sequence

  first computer gets first 10^6 numbers
  second computer gets second 10^6 numbers, etc

Uniform Random Variables

For information see

- Intel MKL information
  `www.intel.com/cd/software/products/asmo-na/eng/266864.htm`
- NAG library information
  `www.nag.co.uk/numeric/CL/nagdoc_cl08/pdf/G05/g05_conts.pdf`
- Matlab information
  `www.mathworks.com/moler/random.pdf`
- Wikipedia information
  `en.wikipedia.org/wiki/Random_number_generation`
  `en.wikipedia.org/wiki/List_of_random_number_generators`
  `en.wikipedia.org/wiki/Mersenne_Twister`

Normal Random Variables

$N(0,1)$ Normal random variables (mean 0, variance 1) have the probability distribution

$$p(x) \;=\; \phi(x) \;\equiv\; \frac{1}{\sqrt{2\pi}}\,\exp(-\tfrac{1}{2}x^2)$$

The Box-Muller method takes two independent uniform $(0,1)$ random numbers y_1, y_2, and defines

$$\begin{aligned} x_1 &= \sqrt{-2\log(y_1)}\;\cos(2\pi y_2) \\ x_2 &= \sqrt{-2\log(y_1)}\;\sin(2\pi y_2) \end{aligned}$$

It can be proved that x_1 and x_2 are $N(0,1)$ random variables, and independent:

$$p_{\text{joint}}(x_1, x_2) = p(x_1)\;p(x_2)$$

Inverse CDF

A more flexible alternative uses the cumulative distribution function $CDF(x)$ for a random variable X, defined as

$$CDF(x) \;=\; \mathbb{P}(X < x)$$

If Y is a uniform $(0,1)$ random variable, then can define X by

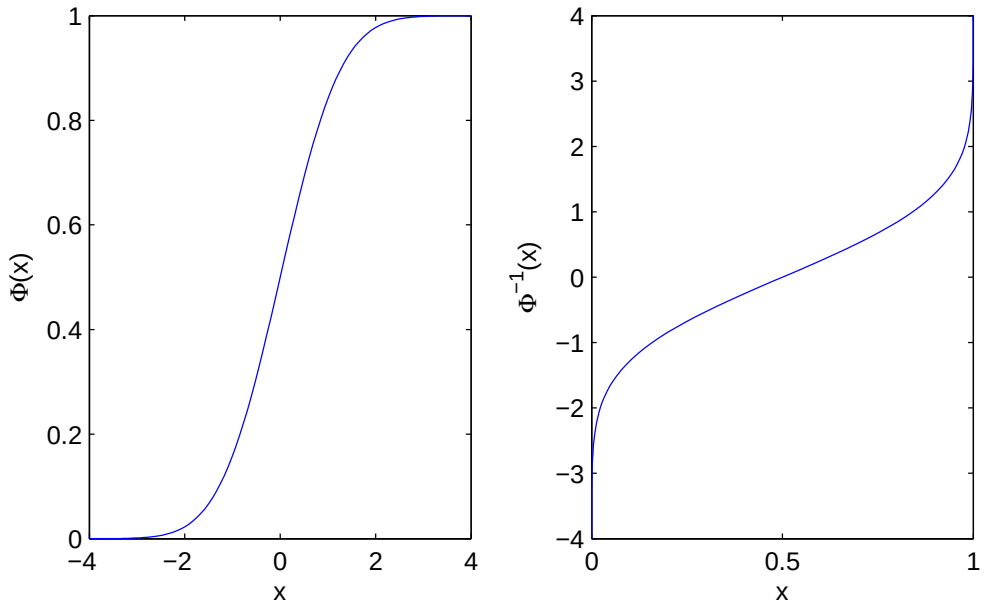
$$X = CDF^{-1}(Y).$$

For $N(0,1)$ Normal random variables,

$$CDF(x) \;=\; \Phi(x) \;\equiv\; \int_{-\infty}^{x} \phi(s)\,\mathrm{d}s \;=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x} \exp\left(-\tfrac{1}{2}s^2\right)\,\mathrm{d}s$$

$\Phi^{-1}(y)$ is approximated in software in a very similar way to the implementation of $\cos, \sin, \log$.

Normal Random Variables



Normal Random Variables

Some useful weblinks:

- `en.wikipedia.org/wiki/Normal_distribution`
  Wikipedia definition of Φ matches mine
- `mathworld.wolfram.com/NormalDistribution.html`
  `mathworld.wolfram.com/DistributionFunction.html`
  Good Mathworld items, but their definition of Φ is slightly different; they call the cumulative distribution function $D(x)$.
- `lib.stat.cmu.edu/apstat/241/`
  single and double precision code in FORTRAN
- `http://people.maths.ox.ac.uk/gilesm/erfinv/`
  My GPU CUDA code for inverse error function `erfinv`

Normal Random Variables

The Normal CDF $\Phi(x)$ is related to the error function $\mathrm{erf}(x)$ through

$$\Phi(x) = \tfrac{1}{2} + \tfrac{1}{2}\,\mathrm{erf}(x/\sqrt{2}) \quad \Longrightarrow \quad \Phi^{-1}(y) = \sqrt{2}\,\mathrm{erf}^{-1}(2y-1)$$

This is the function I use in Matlab:

```
% x = ncfinv(y)
%
% inverse Normal CDF

function x = ncfinv(y)

x = sqrt(2)*erfinv(2*y-1);
```


Correlated Normal Random Variables

We often need a vector y of Normally distributed variables with a prescribed covariance matrix, so that $\mathbb{E}[y\,y^T] = \Sigma$.

Suppose x is a vector of independent $N(0,1)$ variables, and define $y = L\,x$. Each element of y is Normally distributed, $\mathbb{E}[y] = L\,\mathbb{E}[x] = 0$, and

$$\mathbb{E}[y\,y^T] = \mathbb{E}[L\,x\,x^T L^T] = L\;\mathbb{E}[x\,x^T]\;L^T = L\,L^T$$

since $\mathbb{E}[x\,x^T] = I$ because

- elements of x are independent $\Longrightarrow \mathbb{E}[x_i\,x_j] = 0$ for $i \neq j$
- elements of x have unit variance $\Longrightarrow \mathbb{E}[x_i^2] = 1$

Hence choose L so that $LL^T = \Sigma$. One choice is a Cholesky factorisation in which L is lower-triangular. Another is PCA in which $L = U\,\Lambda^{1/2}$ with U the matrix of eigenvectors of Σ, and Λ the diagonal eigenvalue matrix.

Expectation and Integration

If X is a random variable uniformly distributed on $[0,1]$ then the expectation of a function $f(X)$ is equal to its integral:

$$\overline{f} = \mathbb{E}[f(X)] = I[f] = \int_0^1 f(x)\,\mathrm{d}x.$$

The generalisation to a d-dimensional "cube" $I^d = [0,1]^d$, is

$$\overline{f} = \mathbb{E}[f(X)] = I[f] = \int_{I^d} f(x)\,\mathrm{d}x.$$

Thus the problem of finding expectations is directly connected to the problem of numerical quadrature (integration), often in very large dimensions.

Expectation and Integration

Suppose we have a sequence $X^{(n)}$ of independent samples from the uniform distribution.

An approximation to the expectation/integral is given by

$$I_N[f] = N^{-1} \sum_{n=1}^{N} f(x^{(n)}).$$

Two key features:

- Unbiased: $\mathbb{E}\left[I_N[f]\right] = I[f]$
- Convergent: $\lim_{N\to\infty} I_N[f] = I[f]$

Central Limit Theorem

In general, define

- error $\varepsilon_N(f) = I[f] - I_N[f]$
- bias $= \mathbb{E}[\varepsilon_N(f)]$
- RMSE, "root-mean-square-error" $= \sqrt{\mathbb{E}[(\varepsilon_N(f))^2]}$

The Central Limit Theorem proves (roughly speaking) that for large N

$$\varepsilon_N(f) \sim \sigma\, N^{-1/2}\, Z$$

with Z a $N(0,1)$ random variable and σ^2 the variance of f:

$$\sigma^2 = \mathbb{E}[(f-\overline{f})^2] = \int_{I^d} \left(f(x) - \overline{f}\right)^2 \, \mathrm{d}x.$$

Central Limit Theorem

More precisely, provided σ is finite, then as $N \longrightarrow \infty$,

$$\mathrm{CDF}(N^{1/2}\sigma^{-1}\varepsilon_N) \longrightarrow \mathrm{CDF}(Z)$$

so that

$$\mathbb{P}\left[N^{1/2}\sigma^{-1}\varepsilon_N < s\right] \longrightarrow \mathbb{P}[Z < s] = \Phi(s)$$

and

$$\mathbb{P}\left[\left|N^{1/2}\sigma^{-1}\varepsilon_N\right| > s\right] \longrightarrow \mathbb{P}[|Z| > s] = 2\,\Phi(-s)$$

$$\mathbb{P}\left[\left|N^{1/2}\sigma^{-1}\varepsilon_N\right| < s\right] \longrightarrow \mathbb{P}[|Z| < s] = 1 - 2\,\Phi(-s)$$

Central Limit Theorem

Given N samples, the empirical variance is

$$\widetilde{\sigma}^2 = N^{-1}\sum_{n=1}^{N}\left(f(x^{(n)}) - I_N\right)^2 = I_N^{(2)} - (I_N)^2$$

where

$$I_N = N^{-1}\sum_{n=1}^{N} f(x^{(n)}), \qquad I_N^{(2)} = N^{-1}\sum_{n=1}^{N}\left(f(x^{(n)})\right)^2$$

$\widetilde{\sigma}^2$ is a slightly biased estimator for σ^2; an unbiased estimator is

$$\widehat{\sigma}^2 = (N-1)^{-1}\sum_{n=1}^{N}\left(f(x^{(n)}) - I_N\right)^2 = \frac{N}{N-1}\left(I_N^{(2)} - (I_N)^2\right)$$

Central Limit Theorem

How many samples do we need for an accuracy of $\overline{\varepsilon}$ with probability c?

Since

$$\mathbb{P}\left[N^{1/2}\sigma^{-1}|\varepsilon| < s\right] \approx 1 - 2\,\Phi(-s),$$

define s so that $1 - 2\,\Phi(-s) = c$

c	0.683	0.9545	0.9973	0.99994
s	1.0	2.0	3.0	4.0

Then $|\varepsilon| < N^{-1/2}\,\sigma\, s$ with probability c, so to get $|\varepsilon| < \overline{\varepsilon}$ we can put

$$N^{-1/2}\,\widehat{\sigma}\, s(c) = \overline{\varepsilon} \quad \Longrightarrow \quad N = \left(\frac{\widehat{\sigma}\, s(c)}{\overline{\varepsilon}}\right)^2.$$

Note: twice as much accuracy requires 4 times as many samples.

Expectation and Integration

How does Monte Carlo integration compare to grid based methods for d-dimensional integration?

MC error is proportional to $N^{-1/2}$ independent of the dimension.

If the integrand is sufficiently smooth, trapezoidal integration with $M = N^{1/d}$ points in each direction has

$$\text{Error} \;\propto\; M^{-2} \;=\; N^{-2/d}$$

This scales better than MC for $d < 4$, but worse for $d > 4$.
i.e. MC is better at handling high dimensional problems.

Other outputs

Using Monte Carlo we can compute more than just simple averages.

First of all, can compute quantities like the standard deviation:

$$\sigma_f^2 = \mathbb{E}\left[(f - \mathbb{E}[f])^2\right]$$

and other higher moments.

Other outputs

We can also approximate the cumulative distribution function

$$C(s) \;=\; \mathbb{P}[f(X) < s] \;=\; \mathbb{E}[\mathbf{1}_{f(X)<s}]$$

or the probability density function, $P(s) = \dfrac{\mathrm{d}C}{\mathrm{d}s}$, in various ways:

- Maximum Entropy reconstruction – uses $\mathbb{E}[f^m]$ for $m = 1, 2, \ldots, M$ to construct PDF approximation $P(s) \approx \exp(p(s))$, where $p(s)$ is a polynomial and $P(s)$ has the same moments
- Alternatively, can evaluate $C(s_j)$ for a set of values s_j, and then interpolate to approximate the full $C(s)$

Summary so far

- Monte Carlo quadrature is straightforward and robust
- confidence bounds can be obtained as part of the calculation
- can calculate the number of samples N needed for chosen accuracy
- much more efficient than grid-based methods for high dimensions
- accuracy $= O(N^{-1/2})$, CPU time $= O(N)$

  $\Longrightarrow$ accuracy $= O(\text{CPU time}^{-1/2})$

  $\Longrightarrow$ CPU time $= O(\text{accuracy}^{-2})$

- the key now is to reduce number of samples required by reducing the variance