Monte Carlo *and* Simulation

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Section 1

Introduction

Monte Carlo: principle

$$\mathbb{E}[\varphi(X)] \approx \frac{1}{N}\sum_{n=1}^{N}\varphi(X_n)$$

with $\varphi : \mathcal{X} \to \mathbb{R}$.

Rationale: MSE, Law of large number, central limit theorems.

Also: **confidence intervals**!

Need for *simulation* methods. Note that simulation has other uses beyond Monte Carlo.

Bibliography

- Stats, MCMC: *Monte Carlo statistical methods*, C.P Robert, Springer
- IID simulation: *non-uniform random variate generation*, L. Devroye, Springer
- in French: *La simulation de Monte Carlo*, B. Tuffin, Lavoisier
- QMC: *Monte Carlo and quasi-Monte Carlo sampling*, C. Lemieux, Springer
- finance: *Monte Carlo methods in financial engineering*, P. Glasserman, Springer

Section 2

Pseudo-random number generators

Famous quotes, outline

Anyone who uses software to produce random numbers is in a "state of sin''. John von Neumann

One should not use a random method to generate random numbers. Donald Knuth

A PRNG is a *convenient fiction*. Ideally, it should:

- be *fast*,
- be *reproducible*,
- look *random* (at least according to statistical tests, e.g. "die-hard").

PRNGs: a few facts

- The general structure of a PRNG: $x_t = f(x_{t-1})$, where $x_t \in \{0, \ldots, 2^k - 1\}$; by construction, x_t is **periodic**.
- LCG (linear congruential generators):

$$x_{t+1} = (ax_t + c) \pmod{m}$$

  and take $u_t = x_t/m$ so that the u_t's are in $[0, 1]$.
- Take $c = 0$ for simplicity (then seed 0 is forbidden; and 0 is never generated, provided m is prime, and $a < m$).
- Assuming m is prime, the period is $m - 1$ iff $a^k - 1$ is a multiple of m for $k = m - 1$, but not $k \leq m - 2$.

Lattice structure

- Vectors of dim d lie on at most $(d!m)^{1/d}$ hyperplanes in the d-dimensional unit cube; e.g. for $m = 2^{31} - 1$, 108 for $d = 3$ and 39 for $d = 10$.
- RANDU, the most ill-conceived random number generators ever designed... has $a = 65539 = 2^{16} + 3$, $c = 2^{31}$, and is such that $x_t = 6x_{t-1} - 9x_{t-2}$.
- See Table 2.1 p 44 of Glasserman for better choices of (a,c).
- note that if a is not small, then computing $a * x$ is not easy even using floating point operations. We could take $a = 2^k$, but then generators typically have bad properties (see RANDU).

More modern PRNGs

- basic LCGs (even with *good* values of a and c) are now considered obsolete.
- Combine several generators to (a) increase period; and (b) reduce lattice structure: e.g. take the sum of K generators modulo one (Wichmann-Hill).
- Mersenne twister: very popular 32-bit PRNG (Python, R, Matlab, etc), has period $2^{19937} - 1$.
- Also push for 64-bit PRNG.

Main conclusion

- **DO NOT** use C standard implementation `rand()`.
- **DO NOT** implement your own PRNG.
- **DO** resort to some **modern** implementation of a **modern** generator, such as Mersenne twister; see e.g. GSL in C.

Section 3

Non-uniform simulation

Outline

A few general recipes:

- inversion
- rejection
- chain rule

plus several specialised ones (e.g. Box-Muller).

inversion

inversion algorithm

If X has CDF F, take

$$X = F^{-1}(U), \quad U \sim \mathcal{U}[0,1].$$

Applications: exponential, Laplace, Gaussian?

Box-Muller

Box-Muller

$$\begin{cases} X & = \sqrt{-2\log(U)} * \cos(2\pi V) \\ Y & = \sqrt{-2\log(U)} * \sin(2\pi V) \end{cases}$$

Then $X,\ Y \sim N(0,1)$, independently.

A sneaky introduction to rejection

To understand the coming slides, note that the following algorithm

Rejection

```
Repeat $X \sim \mathcal{U}(\mathcal{A})$
Until $X \in \mathcal{B}$.
```

draws from $\mathcal{U}(\mathcal{B})$ (provided $\mathcal{B} \subset \mathcal{A}$).

Modified Box-Muller

Box-Muller with rejection

```
Repeat
    $U,\ V \sim \mathcal{U}[-1,1]$
Until $S := U^2 + V^2 \leq 1$.
Return
```

$$\begin{cases} X & = U\sqrt{-2\log(S)/S} \\ Y & = V\sqrt{-2\log(S)/S} \end{cases}$$

Then $X,\ Y \sim N(0,1)$, independently.

Note: avoid computing sin and cos.

Rejection

Let f, g PDFs such that $f \leq Mg$ (with $M \geq 1$).

Accept-reject

```
Repeat
                    $X \sim g, \quad U \sim \mathcal{U}[0,1]$,
Until $U \leq f(X)/Mg(X)$.
```

Properties: $X \sim f$, number of draws until acceptance is Geometric$(1/M)$.

Justification: uniform sampling under the graph, see next slide.

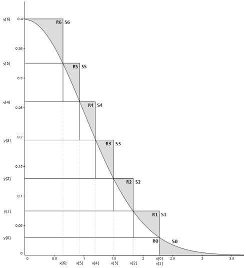
Uniform sampling under the graph

For a function f, let $\mathcal{G} = \{(x, y) \in \mathbb{R}^2 :\, 0 \le y \le Mf(x)\}$, then

$$(X, Y) \sim \mathcal{U}(\mathcal{G}) \Leftrightarrow \begin{cases} X & \sim f \\ Y|X = x & \sim \mathcal{U}[0, Mf(x)] \end{cases}$$

Note: this construction is in fact not restricted to real-valued random variables.

Ziggurat algorithm for $N(0,1)$ (Marsaglia, 60?)



K Slices $S_k = [-x_k, x_k] \times [y_k, y_{k+1}]$ constructed to have the same area.

1. Choose slice k (uniformly).
2. Sample (X, Y) within slice k.
3. If $X \leq x_{k+1}$, return X, else, if $Y \leq \varphi(X)$, return X, else go to 1.

Note: If slice 0 is selected, extra steps required (truncated Gaussian distribution).

Multivariate simulation: chain-rule decomposition

The inverse transform method is restricted to real-valued random variables, the inverse transform *is not*.

General recipe to generate jointly (X, Y, Z), with PDF $f(x, y, z)$:

1. `Generate` $X \sim f_X(x)$ (marginal). Call x the output.
2. `Generate` $Y|X = x \sim f_{Y|X}(y|x)$ (conditional given $X = x$). Call y the output.
3. `Generate` $Z|X = x, Y = y \sim f_{Z|Y,X}(z|x, y)$ (full conditional). Call z the output.

Gaussian vectors

The standard method to generate $X \sim N_d(\mu, \Sigma)$ is:

- `Generate` $Z_1, \ldots, Z_d \sim N(0,1)$.
- `Compute` $C = \mathrm{Choleksy}(\Sigma)$. (i.e. $\Sigma = CC^T$, and C is lower triangular)
- `Return` $X = \mu + CZ$.

The Cholesky decomposition costs $\mathcal{O}(d^3)$.

Section 4

Non-uniform simulation in spaces other than $\mathbb{R}^d$

Outline

Some recipes to sample specific cases of

- distributions over constrained sets
- discrete distributions

How to sample N sorted uniforms

Naive method: `sample` $U_n \sim \mathcal{U}[0,1]$ for $n = 1, \ldots, N$, `return` sort$(U_{1:N})$.
Cost is $\mathcal{O}(N \log N)$ (not bad).

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Smart $\mathcal{O}(N)$ method:

- `Sample` $E_1, \ldots, E_{N+1} \sim \mathrm{Exp}(1)$.
- `Compute` $V_{1:(N+1)} = \mathrm{cumsum}(E_{1:(N+1)})$.
- `Return` $(V_1/V_{N+1}, \ldots, V_N/V_{N+1})$.

How to sample uniformly on the sphere

- `Sample` $X \sim N_d(0, I_d)$.
- `Return` $X/\|X\|$.

How to sample from a discrete distribution over $\mathbb{N}$

The inverse methods extends to the discrete case. Simply define:

$$F^{-1}(u) = \inf\{x : F(x) \geq u\}$$

In practice:

- `Sample` $U \sim \mathcal{U}[0,1]$
- `If` $U \leq p_0$, `return` 0
- `If` $p_0 < U \leq p_0 + p_1$, `return` 1
- etc

What if N and K are large

Suppose we want to sample N times from a distribution over $\{0, \ldots, K-1\}$. If we run the algorithm of the previous slide N times, we do $\mathcal{O}(NK)$ operations (on average). Can we do better?

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Suppose we want to sample N times from a distribution over $\{0, \ldots, K-1\}$. If we run the algorithm of the previous slide N times, we do $\mathcal{O}(NK)$ operations (on average). Can we do better?

Solution: use as input N sorted uniforms. Then cost is $\mathcal{O}(N+K)$.

Application: (weighted) bootstrap.

Inverse CDF algorithm

```
def inversecdf(su,W):
    """ Input:  su[0:N] sorted uniforms
                W[0:K]  normalised weights (sum to one)
        Output: A[0:N]  indexes (in {0,...,K-1})
    """
    j=0; s=W[0]; N = su.shape[0]
    A = empty(N,'int')
    for n in xrange(N):
        while su[n]>s:
            j += 1
            s += W[j]
        A[n] = j
    return A
```

How to sample a permutation

"Naive" $\mathcal{O}(N \log N)$ method: $\sigma = \mathrm{argsort}(U_{1:N})$.

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Smart $\mathcal{O}(N)$ method:

- Let $\sigma = (1, 2, \ldots, N)$.
- $I \sim \mathcal{U}(1, \ldots, N)$, swap $\sigma(1)$ and $\sigma(I)$.
- $I \sim \mathcal{U}(2, \ldots, N)$, swap $\sigma(2)$ and $\sigma(I)$.
- etc.

Section 5

Variance reduction

Objectives, outline

Given a certain quantity

$$I = \mathbb{E}[\varphi(X)] = \int_{\mathcal{X}} f(x)\varphi(x)\,dx$$

find a Monte Carlo estimator with smaller variance than the standard estimator

$$\frac{1}{N}\sum_{n=1}^{N}\varphi(X_n).$$

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Recipes:

- antithetic variables
- control variates

Antithetic variables

In cases where $\varphi(-X)$ has the same distribution as $\varphi(X)$, use:

$$\hat{I}_{\mathrm{anti}} = \frac{1}{2N} \sum_{n=1}^{N} \{\varphi(X_n) + \varphi(-X_n)\}$$

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Lemma:

$$\mathrm{Var}(\hat{I}_{\mathrm{anti}}) \leq \mathrm{Var}(\hat{I})$$

Note: we have less variance, but twice as many evaluations of $\varphi\ldots$

Control variates (univariate case)

Let Z a real-valued r.v. such that $\mathbb{E}(Z) = 0$. For any β,

$$\hat{I}_{\mathrm{cv}} = \frac{1}{N}\sum_{n=1}^{N}\{\varphi(X_n) - \beta Z_n\}$$

is an unbaised estimator of $I = \mathbb{E}[\varphi(X)]$.

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The smallest variance is obtained by taking

$$\beta_{\mathrm{opt}} = \frac{\mathrm{Cov}(\varphi(X), Z)}{\mathrm{Var}(Z)}.$$

Control variates (multivariate case)

$Z^1, \ldots, Z^K$ are mean-zero real-valued r.v. Take

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Control variates (multivariate case)

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In practice, replace β_k by $\hat{\beta}_k$, the OLS estimate for regression:

$$\varphi(X_n) = \alpha + \sum_{k=1}^{K}\beta_k Z_n^k + \varepsilon_n.$$

Variance reduction and Rao-Blackwellisation

Often variance reduction techniques may be cast as particular **Rao-Blackwellisation** schemes, i.e. the idea that

$$\mathrm{Var}\left[\mathbb{E}[\varphi(X)|Z]\right] \leq \mathrm{Var}[\varphi(X)].$$

Section 6

Importance sampling

A simple identity

$$\begin{aligned}\mathbb{E}[\varphi(X)] &= \int_{\mathcal{X}} \varphi(x) f(x)\,dx \\ &= \int_{\mathcal{X}} \varphi(x) \frac{f(x)}{g(x)} g(x)\,dx = \mathbb{E}_g\left[\frac{f(X)}{g(X)}\varphi(X)\right]\end{aligned}$$

assuming $\mathrm{Supp}(f) \subset \mathrm{Supp}(g)$.

Any expectation w.r.t. PDF f may be rewritten thusly as an expectation w.r.t. PDF g (which may be easier to simulate from):

$$\hat{I}_{IS} = \frac{1}{N}\sum_{n=1}^{N} \frac{f(X_n)}{g(X_n)}\varphi(X_n).$$

How to choose proposal g?

1. Check that variance exists, $\Leftrightarrow \mathbb{E}_g\left[\varphi(X)^2\frac{f(X)^2}{g(X)2}\right] < \infty$. (Sufficient condition: $f/g \leq M$, and $\mathbb{E}_f[\varphi^2] < \infty$.)

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2. Optimal g (in terms of minimizing variance) is

$$g_{\mathrm{opt}}(x) \propto f(x)|\varphi(x)|.$$

It is often not possible to simulate from g_{opt}, so more generally, it is recommended to take $g \approx f$.

Auto-normalised IS

Sometimes either f or g are known only up to a constant: $f = f_u/Z_f$, $g = g_u/Z_g$, and Z_f, Z_g are intractable. In that case, we use the auto-normalised IS estimator:

$$\hat{I}_{\mathrm{AIS}} = \frac{\sum_{n=1}^{N} w_n \varphi(X_n)}{\sum_{n=1}^{N} w_n}, \quad w_n = \frac{f_u(X_n)}{g_u(X_n)}.$$

This estimator is biased, and asymptotically Gaussian:

$$\sqrt{N}\left(\hat{I}_{\mathrm{AIS}} - I\right) \Rightarrow N(0, v_{f/g})$$

with $v_{f/g} = \mathbb{E}_g[\left(\frac{f}{g}\right)^2 (\varphi - I)^2]$ (assuming this quantity is $< \infty$).

How to choose g (bis repetita)

Same points as for standard IS:

1. Check that at least $v_{f/g} < \infty$; sufficient condition is (a) $f/g < \ M$ and (b) $\mathrm{Var}_f(\varphi) < \infty$.
2. Optimal g is
$$g_{\mathrm{opt}}(x) \propto f(x)|\varphi(x) - I|$$
which depends on I... In practice, take $g \approx f$.

Estimating the Z's, effective sample size

Note that AIS also provides an estimate of Z_f/Z_g:

$$\mathbb{E}\left[\frac{1}{N}\sum_{n=1}^{N} w_n\right] = \frac{Z_f}{Z_g}$$

and of $v_{f/g}$:

$$\frac{N\sum_{n=1}^{N} w_n^2 \left\{\varphi(X_n) - \hat{I}\right\}^2}{\left(\sum_{n=1}^{N} w_n\right)^2}.$$

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Similarly, the **effective sample size**

$$\frac{\left(\sum_{n=1}^{N} w_n\right)^2}{\sum_{n=1}^{N} \left(w_n\right)^2} \in [1, N]$$

is a good indicator of AIS efficiency.

Curse of dimensionality

For $\mathcal{X} = \mathbb{R}^d$, $f(x) = \prod_{i=1}^d f_1(x_i)$, $g(x) = \prod_{i=1}^d g_1(x_i)$, one has:

$$\mathbb{E}_g[f^2/g^2] = C^d, \quad C \geq 1.$$

We expect the variance of IS to grow exponentially with the dimension.

Resampling

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Simply draw randomly $\tilde{X}_n$ from

$$\sum_{n=1}^{N} W_n \delta_{X_n}, \quad W_n = \frac{w_n}{\sum_{m=1}^{N} w_m}$$

(as in the bootstrap).

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(as in the bootstrap).

See previous chapter on multinomial sampling.

Section 7

Quasi-Monte Carlo

Principle

Often one may rewrite quantity of interest as:

$$I = \mathbb{E}[\varphi(U)], \quad U \sim \mathcal{U}[0,1]^d$$

and then use

$$\hat{I} = \frac{1}{N} \sum_{n=1}^{N} \varphi(U_n).$$

Principle

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Can we construct (deterministic or random) points $U_1, \ldots, U_N$ in $[0,1]^d$ so that the approximation error is smaller than with standard Monte Carlo (i.e. U_n are IID uniforms)?

Stratification ($d = 1$)

- Generate N/K uniforms in each interval $[(k-1)/K, k/K]$, $k = 1, \ldots, K$. (Note the connection with antithetic variables.)

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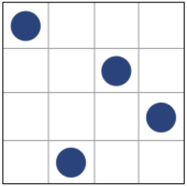
- Or even take $K = N$, i.e. generate $U_n \sim \mathcal{U}[(n-1)/N, n/N]$.
- or even take $u_n = (2n-1)/2N$, the (deterministic) centre of interval $[(n-1)/N, n/N]$).

Stratification for $d > 1$: Latin hypercube sampling



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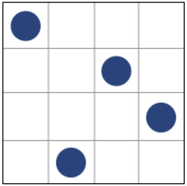

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Tip: use random permutations.

Koksma–Hlawka inequality

$$|\hat{I} - I| \leq V(\varphi) D^\star(u_{1:N})$$

where $V(\varphi)$ is the variation of φ (in the sense of Hardy and Krause), and

$$D^\star(u_{1:N}) = \sup_{[0,b]\subset[0,1]^d} \left| N^{-1} \sum_{n=1}^{N} \mathbb{I}_{[0,b]}(u_n) - \prod_{i=1}^{d} b_i \right|$$

is the **star discrepancy**.

Proof for $d = 1$

$$N^{-1}\sum_{n=1}^{N}\varphi(u_n) - \int_0^1 \varphi(u)\,du = \int_0^1 \delta(u)\varphi'(u)\,du$$

where $\delta(u) = u - N^{-1}\sum_{n=1}^{N}\mathbf{1}(u_n \leq u)$.

Why is the previous inequality so important?

Because we know how to construct:

- point-sets such that $D^\star(u_{1:N}) = \mathcal{O}\left(\frac{(\log N)^{d-1}}{N}\right)$
- sequences such that $D^\star(u_{1:N}) = \mathcal{O}\left(\frac{(\log N)^{d}}{N}\right)$

hence we can do **better** than Monte Carlo, i.e. $\mathcal{O}_P(\frac{1}{\sqrt{N}})$.

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hence we can do **better** than Monte Carlo, i.e. $\mathcal{O}_P(\frac{1}{\sqrt{N}})$.

Side note: there are good reasons to believe that these rates are optimal.

$d = 1$

Take $u_n = (2n-1)/2N$, $n = 1, \ldots, N$. Then

$$D^{\star}(u_{1:N}) = \frac{1}{2N}.$$

Van der Corput (sequence for $d = 1$)

In base b, for $n = \sum_{j=0}^{k} a_j(n) b^j$, take

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e.g. for $b = 2$: $1/2$, $1/4$, $3/4$, $1/8$, $\dots$

For $b = 3$: $1/3$, $2/3$, $1/9$, $\dots$

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e.g. for $b = 2$: $1/2$, $1/4$, $3/4$, $1/8$, $\ldots$

For $b = 3$: $1/3$, $2/3$, $1/9$, $\ldots$

Then $D^\star(u_{1:N}) = \mathcal{O}(\log N/N)$.

$d > 1$: Halton & Hammersley

Halton sequence: component j is a van der Corput sequence in base b_j, where the b_j are the first d prime numbers. Discrepancy is $\mathcal{O}((\log N)^d/N)$.

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Hammersley point set (of size N): take N first elements of Halton sequence of dimension d, replace last component by n/N.
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Note however that for large d, both Halton and Hammersley require many points to cover the space...

Other low-discrepancy sequences and point sets

- Niederreiter
- Faure
- Sobol'
- . . .

RQMC (randomised QMC)

QMC is purely deterministic. It lacks a simple way to evaluate the numerical error. Imagine we are able to randomise $U_{1:N}$ so that

1. $U_n \sim \mathcal{U}[0,1]^d$ (marginally).
2. $U_{1:N}$ is still a low-discrepancy point-set (or sequence).

Then

$$\mathbb{E}\left[\frac{1}{N}\sum_{n=1}^{N}\varphi(U_n)\right] = \mathbb{E}[\varphi(U)]$$

and we can evaluate the numerical error through the empirical variance (over repeated runs).

RQMC: random shift

The simplest RQMC strategy is to generate a low-discrepancy point set $v_{1:N}$, $W \sim \mathcal{U}[0,1]^d$, then take:

$$U_n = v_n + W \pmod 1 \qquad \text{(componentwise)}$$

RQMC: a surprising result

Owen (1998) showed that for smooth functions φ

$$\mathrm{Var}[\hat{I}] = \mathcal{O}\left(\frac{(\log N)^{(d-1)/2}}{N^3}\right)$$

when scrambling (a particular RQMC technique) is used.

conclusion: QMC vs MC

- QMC has a better convergence rate.
- But for large d, QMC might need a very large N to beat MC.
- With MC, the (square) error is simple to estimate, whereas for QMC, we have only a deterministic bound, which is hard to evaluate, and is often pessimistic. See RQMC however.
- Variance reduction: may be used in conjunction with (R)QMC. (Recommendation is to do variance reduction, *then* replace MC with QMC).
- Practical recommendation: scrambled Sobol' seems like a good default choice (or Latin Hypercube sampling for very high dimensions).

Section 8

Markov chain Monte Carlo

Outline

In some settings, simulating *independently* $X \sim \pi(dx)$ is difficult, but it is possible to simulate a Markov chain (X_n) that leaves $\pi(dx)$ **invariant**. Then, we still have

$$\frac{1}{N}\sum_{n=1}^{N}\varphi(X_n) \approx \mathbb{E}_\pi[\varphi(X)]$$

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This is the case in particular when density π is known only up to a constant.

Definitions

- A **Markov kernel** $K(x, dy)$ is an application $\mathcal{X} \to \mathcal{P}(\mathcal{X})$.

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- A Markov kernel K leaves distribution π **invariant** iff

$$\int_{\mathcal{X}} \pi(dx)K(x, dy) = \pi(dy).$$

- A Markov kernel is **reversible** w.r.t. π iff

$$\pi(dx)K(x, dy) = \pi(dy)K(y, dx).$$

This implies that π is invariant.

Metropolis-Hastings

Let $Q(x, dy)$ a Markov kernel, such that $Q(x, dy) = q(x, y)dy$.

Hastings-Metropolis step

Input: X_{n-1}

1. Generate $Y \sim Q(X_{n-1}, dy)$
2. With probability $1 \wedge r(X_{n-1}, Y)$, where
$$r(x, y) = \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}$$
accept Y, i.e. $X_n = Y$; otherwise $X_n = X_{n-1}$.

Property: This kernel is reversible (w.r.t. π).

An important practical point

Note that Hastings-Metropolis may be implemented even if π is known only up to a constant: $\pi(x) = \pi_u(x)/Z$, Z is intractable. Then

$$r(x, y) = \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)} = \frac{\pi_u(y)q(y, x)}{\pi_u(x)q(x, y)}$$

Examples of MH algorithms

1. $q(x,y) = q(y,x)$, for instance $q(x,y) = N(y; x, \Sigma)$ (Gaussian **random walk**); then

$$r = \frac{\pi(y)}{\pi(x)}$$

2. $q(x,y) = q(y)$: **independent Metropolis**; then

$$r = \frac{\pi(y)q(x)}{\pi(x)q(y)}$$

3. Langevin proposal:

$$Y \sim N(x + \frac{1}{2}\Sigma\nabla \log \pi(x), \Sigma)$$

(two-block) Gibbs sampling

Assume $X = (X_1, X_2)$, $\pi(x) = \pi(x_1, x_2)$, with conditional distributions $\pi_{1|2}(x_1|x_2)$, $\pi_{2|1}(x_2|x_1)$.

Gibbs sampling step

Input: $X_{n-1} = (X_{n-1,1}, X_{n-1,2})$

1. `Generate` $X_{n,1} \sim \pi_{1|2}(\bullet|X_{n-1,2})$.
2. `Generate` $X_{n,2} \sim \pi_{2|1}(\bullet|X_{n,1})$.

Again, this leaves invariant π. Gibbs can be generalised to $k > 2$ blocks.

Combining chains

1. If K_1, K_2 leave π invariant, then so does $K_1 K_2$.
2. **Within** Gibbs, we can replace the exact simulation of $X_1|X_2$ (say) by a Metropolis step that leaves invariant $\pi_{1|2}$.

MCMC in practice

1. Assess how long it takes for the chain to reach stationarity;
2. When chain seems stationary, check for intra-correlations, i.e. look at ACF (Auto-Correlation Function).

Then we compute averages

$$\frac{1}{N - N_0} \sum_{n=N_0+1}^{N} \varphi(X_n)$$

where N_0 is burn-in time, and $N - N_0$ is sufficiently large relative to the **auto-correlation time** (i.e. time k so that X_n and X_{n+k} are nearly uncorelated).

scaling random walk Metropolis

One big hurdle with random walk Metropolis is the choice of Σ, in the proposal $N(x, \Sigma)$. If too small, chain moves slowly, if too large, proposals always get rejected.

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Theory (e.g. Roberts and Rosenthal, 2004) indicates that one should take

$$\Sigma = c\Sigma_\pi$$

where Σ_π is the covariance matrix of target π, and c calibrated so that acceptance rate is ≈ 0.25.

a tiny bit of MCMC theory

1. From an arbitrary starting point $X_0 = x_0$, and any $\varepsilon > 0$, we have

   $$\|K^n(x_0, dx_n) - \pi(dx_n)\|_{\mathrm{TV}} \leq \varepsilon$$

   for n large enough.

2. CLT:

   $$\sqrt{N}\left(\frac{1}{N}\sum_{n=1}^{N}\varphi(X_n) - I\right) \Rightarrow N(0, V(\varphi))$$

   with

   $$V(\varphi) = \mathrm{Var}_\pi(\varphi) + 2\sum_{k=1}^{\infty}\gamma_k(\varphi)$$

   and $\gamma_k(\varphi) = \mathrm{Cov}[\varphi(X_n), \varphi(X_{n+k})]$.

Adaptive MCMC?

Can we use past samples to automatically calibrate Metropolis-Hastings? e.g. at time t, do a random walk Metropolis step, of size $\Sigma = c\hat{\Sigma}_t$, where $\hat{\Sigma}_t$ is the empirical covariance matrix computed from $X_0, \ldots, X_{t-1}$.

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Big theoretical problem: we are not simulating a Markov chain any more (X_t depends on the whole past). Convergence is more difficult to establish.

Section 9

Interlude: Bayesian classification

Outline

Consider model with responses $y_i \in \{-1, 1\}$, covariates $x_i \in \mathbb{R}^p$, likelihood

$$L(x, y; \beta) = \prod_{i=1}^{n_d} F(y_i \beta^T x_i)$$

with $F = \Phi$ (probit), or $F = L$ (logit), and prior

$$\pi(\beta) = 1$$

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with $F = \Phi$ (probit), or $F = L$ (logit), and prior

$$\pi(\beta) = 1$$

The posterior is

$$\pi(\beta | x, y) \propto \prod_{i=1}^{n_d} F(y_i \beta^T x_i)$$

We will use this example to discuss many of the approaches seen so far.

Laplace approximation

Taylor expansion of log posterior density around its mode, $\widehat{\beta} = \arg\max \pi(\beta|x,y)$ (MLE):

$$\log \pi(\beta|x,y) \approx \log \pi(\widehat{\beta}|x,y) - \frac{1}{2}(\beta - \widehat{\beta})^T H(\beta - \widehat{\beta})$$

implies a Gaussian approximation of the posterior: $\approx N(\widehat{\beta}, H^{-1})$.

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In practice, this Gaussian approximation may be:

1. obtained numerically (Newton);
2. used as a proposal in various approaches (e.g. importance sampling).

Section 10

Monte Carlo optimisation

Objectives

Numerical maximisation:

$$\max_{\theta \in \Theta} \psi(\theta)$$

when

1. ψ can be evaluated point-wise, but is difficult to maximise by standard methods: **Exploration**
2. ψ is an (intractable) expectation:

$$\psi(\theta) = \mathbb{E}_\theta[h(X,\theta)]$$

Stochastic approximation

Statistical applications: MLE

Exploration

When ψ can be evaluated point-wise, one may sample N times from some distribution $\pi(d\theta)$, and return $\max_{n=1,\ldots,N}\psi(\theta_n)$; for instance if Θ is compact, take $\pi(d\theta)$ to be the Uniform dist. over Θ.

Exploration

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In particular, consider

$$\pi_\lambda(\theta) \propto \exp\{\lambda\psi(\theta)\}.$$

When λ (inverse temperature) increases, support of π_λ gets more concentrated around modal regions, but in return it may be more difficult to sample from π_λ.

Simulated annealing

Simulate a (inhomogeneous) Markov chain as follows: at iteration t, do a Metropolis step w.r.t. π_{λ_t}, and make λ_t increase at a logarithmic rate.

The Cross-Entropy method

For some parametric family $\{f_\xi,\, \xi \in \Xi\}$, choose initial ξ_0, then iteratively:

1. Sample $\theta_1, \ldots, \theta_n \sim f_{\xi_t}$.
2. Estimate (using e.g. MLE) ξ_{t+1} from the 10% best of the θ_i (in terms of $\psi(\theta_i)$).

Other heuristic optimisation procedures

- genetic algorithms
- tabu search
- ant colony algorithm

and also more specialised ones.

Stochastic approximation

One has: $\psi(\theta) = \mathbb{E}_\theta[h(X, \theta)]$ (double dependence on θ). Possible approaches:

1. If Expectation is w.r.t. a fixed dist' f, $\psi(\theta) = \mathbb{E}[h(X, \theta)]$, generate $X_1, \ldots, X_n \sim f$, maximise $\theta \to N^{-1} \sum_{n=1}^{N} h(X_n, \theta)$.
2. Gradient-based approach, e.g.

$$\theta_{t+1} = \theta_t + \alpha_t \hat{\nabla} \psi(\theta_t)$$

   where $\hat{\nabla}\psi(\theta_t)$ is some MC estimate of the gradient of ψ.

Robins-Monroe

Take α_t such that $\alpha_t \to 0$, and $\sum_t \alpha_t = \infty$; e.g. $\alpha_t = Ct^{-b}$, $1/2 < b \leq 1$.

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To estimate the gradient, if $\psi(\theta) = \mathbb{E}_\theta[h(X)]$, one has

$$\nabla\psi(\theta) = \mathbb{E}_\theta[h(X)s_\theta(X)], \quad s_\theta(x) = \frac{\partial}{\partial\theta}\log f_\theta(x)$$

and thus a possible choice is:

$$\hat{\nabla}\psi(\theta) = \frac{1}{N}\sum_{n=1}^{N} h(X_n)s_\theta(X_n)$$

Section 11

Selected applications of Monte Carlo

Outline

1. Derivative pricing
2. Statistical applications: MCEM, Bayesian inference, ABC
3. Enumeration
4. Go playing. . .

Derivative pricing: statement

There, X is continuous-time process on $[0, T]$, and φ could be:

- $\varphi(X) = (K - X_T)^+$
- $\varphi(X) = (K - \frac{1}{k}\sum_i X_{t_i})^+$
- $\varphi(X) = (K - \int X_t dt)^+$
- $\varphi(X) = \mathbb{I}\{\tau_b > T\}(X_T - K)^+$, with $\tau_b = \inf\{t : X_t \leq b\}$
- etc.

Simulating Brownian paths

For a Brownian motion $\{W_t\}$, several ways to simulate *exactly* vector $(W_{t_1}, \ldots, W_{t_k})$:

- random walk: $W_{t_i} | W_{t_{i-1}} \sim N(W_{t_{i-1}}, t_i - t_{i-1})$
- Brownian bridge: $W_{t_i} | W_{t_{i-1}}, W_{t_{i+1}} \sim$

$$N\left(\frac{(t_{i+1} - t_i)W_{t_{i-1}} + (t_i - t_{i-1})W_{t_{i+1}}}{t_{i+1} - t_{i-1}}, \frac{(t_{i+1} - t_i)(t_i - t_{i-1})}{t_{i+1} - t_{i-1}}\right)$$

  and order times according to a van der Corput sequence: first t_k, then $t_{k/2}$, $t_{k/4}$, and so on.
- principal components

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  $$N\left(\frac{(t_{i+1} - t_i) W_{t_{i-1}} + (t_i - t_{i-1}) W_{t_{i+1}}}{t_{i+1} - t_{i-1}}, \frac{(t_{i+1} - t_i)(t_i - t_{i-1})}{t_{i+1} - t_{i-1}} \right)$$

  and order times according to a van der Corput sequence: first t_k, then $t_{k/2}$, $t_{k/4}$, and so on.
- principal components

Try to think about the implications for QMC. . .

QMC and Brownian paths

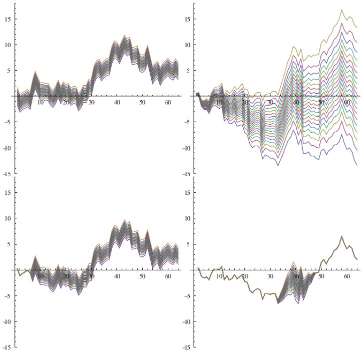

Fig. 8.6 Paths of Brownian motion obtained by the forward construction (*left*) and the Brownian bridge construction (*right*). All but one parameters are fixed

Top: all but first component fixed; bottom, all but seventh component fixed

Source: Chap. 8 of Leobacher and Pillichshammer (2014).

Euler discretization

In general, diffusion processes need to be discretized:

$$dX_t = \mu(X_t)dt + \sigma(X_t)dW_t$$

becomes

$$X_{t+1} - X_t = \delta\mu(X_t) + \sigma(X_t)\epsilon_t, \quad \epsilon_t \sim N(0, \delta)$$

where δ is the discretization step.

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Choice of δ: trade-off between discretization bias and CPU time.

Multi-level Monte Carlo

Consider a sequence of decreasing steps: $\delta_0 > \ldots > \delta_L$; say $\delta_l = 2^{-l}$.

$$\mathbb{E}_{\delta_L}(\varphi) = \mathbb{E}_{\delta_0}(\varphi) + \sum_{l=1}^{L} \left\{ \mathbb{E}_{\delta_l}(\varphi) - \mathbb{E}_{\delta_{l-1}}(\varphi) \right\}$$

To get a low-variance estimate for each level, use **coupling**: e.g. use Brownian bridge construction to obtain the finer level from the coarser level.

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To get a low-variance estimate for each level, use **coupling**: e.g. use Brownian bridge construction to obtain the finer level from the coarser level.

To minimise variance, choose N_l (number of samples for level l) to be:

$$N_l \propto \sqrt{V_l / C_l}$$

where V_l (resp. C_l) is variance (resp. CPU cost per sample) of estimate for level l.

Other worthy points

- control variates: simulation involves many Gaussian variables, with known mean and variance
- antithetic variables (Gaussians variables are symmetric)
- QMC very popular nowadays in option pricing

Statistical applications

- Bayesian estimation: already covered, see MCMC
- Frequentist estimation: MC for the E part of EM
- Likelihood-free inference

MCEM = Monte Carlo EM

For a statistical model involving a latent X and an observed y, maximise iteratively:

$$\theta_{t+1} = \arg\max_{\theta} \mathbb{E}[\log L(X, y; \theta)]$$

where the expectation is w.r.t. the distribution of X given $Y = y$ and $\theta = \theta_t$.

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See also SAEM.

ABC (likelihood-free inference)

Data $y^\star$, model $p(y|\theta)$ such that (a) one can simulate from $p(y|\theta)$; (b) one cannot compute the likelihood $p(y|\theta)$. (Many scientific models fall in this category.)

ABC (likelihood-free inference)

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ABC (Approximate Bayesian inference) samples from:

$$p_\varepsilon(\theta, y|y^\star) \propto p(\theta)p(y|\theta)\mathbb{I}(\|s(y) - s(y^\star)\| \leq \varepsilon).$$