Advanced Statistical Computing

Fall 2016

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Outline

Today

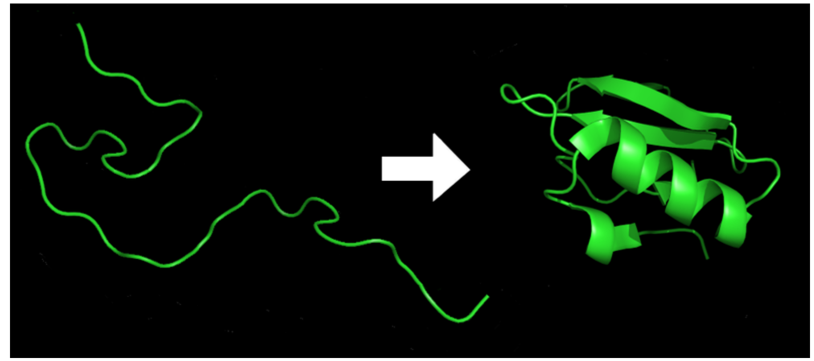
- Introduction to Monte Carlo strategy and methods,
- Random number generation,
- Importance sampling.

Next lectures

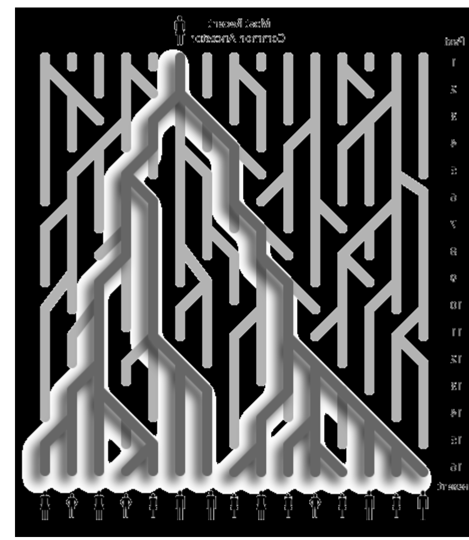
- MCMC
  - Gibbs Sampler,
  - Metropolis-Hastings algorithms.
- MCMC (cont.)
  - Check for convergence,
  - Techniques to accelerate Markov chain mixing.
- Applications
  - Implementations of Monte Carlo methods,
  - Examples of MCMC applications.

Examples

- How protein fold
  molecular dynamics



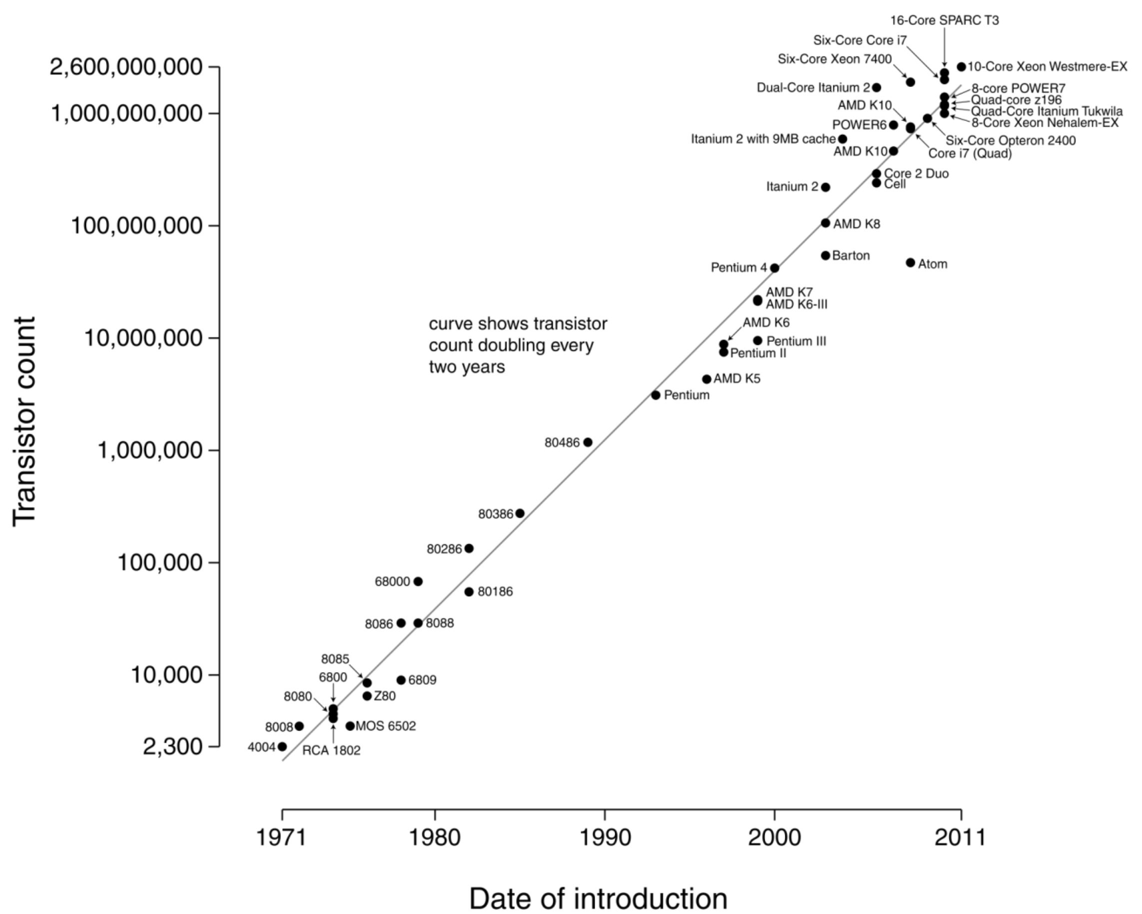
- Phylogeny, inheritance
  pattern in large pedigree



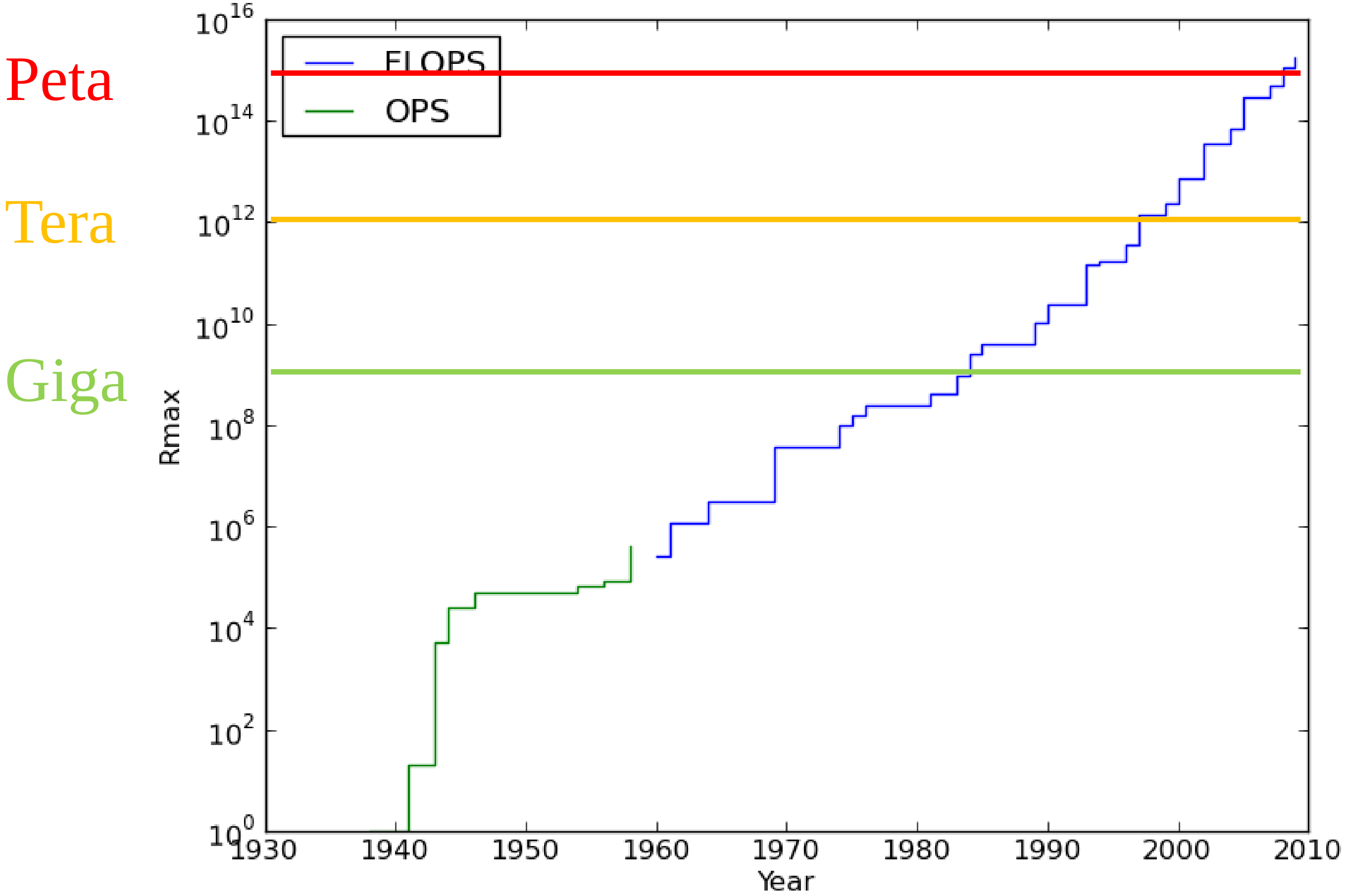
- Next generation sequencing
  mapping, assembly, …

Moore’s law

Microprocessor Transistor Counts 1971-2011 & Moore’s Law



Computation speed



Computation speed

• Intel Core i750	7 GFlops.
• The Intel Core2Quad	6.9 GFlops.
• AMD Phenom II X4	7.5 Gflops.
• Core2Dup E8200	2.9 GFlops.
Celeron M 540	0.9 GFlops.
• Pentium4	0.74 GFlops.
• nVidia GeForce 8800GS	264 Gflops
• nVidia GeForce 9800GT	336 GFlops.

(Results from MaxxPi^2)

What is Monte Carlo?

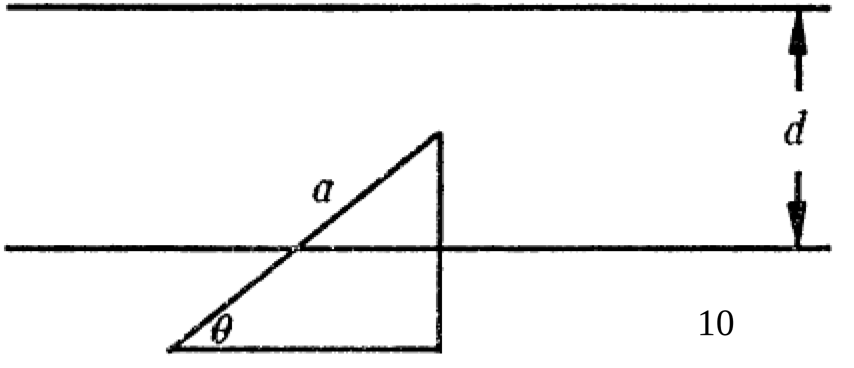
- Rely on repeated sampling to study the results of a experiment or study the properties of certain procedure.
  - Often used in complex and uncertain scenarios
  - Difficult to formulate, high correlation.
  - Cheap
  - Take advantage of faster computers
- History
  - John von Neumann, Stanislaw Ulam, Nicholas Metropolis

Buffon's needle

Georges-Louis Leclerc, Comte de Buffon

(1707-1788)

Given a needle of length *a* and an infinite grid of parallel lines with common distance *d* between them, what is the probability *P*(*E*) that a needle, tossed at the grid randomly, will cross one of the parallel lines?



Buffon's needle

- Assume $a < d$

$$P(E) = \int_0^\pi \frac{a \sin\theta d\theta}{\pi d} = (a/\pi d) \int_0^\pi \sin\theta d\theta = 2a/\pi d.$$

http://web.student.tuwien.ac.at/~e9527412/buffon.html

Random variate generation

- Generate uniform r.v.

  Uniform (0,1)
- Important techniques
  - Direct method
  - Inverse method
  - Relationship to other distributions
  - Accept-reject method

Direct method

Directly use the definition of the distribution.

– Bernoulli distribution *Bernoulli*(p)

  Generate $r \sim Uniform\ (0,1)$

– Binomial distribution *Binom*(*n*,*p*)

  Generate $r_1,\ldots,r_n$ $iid \sim Uniform\ (0,1)$

Inverse method

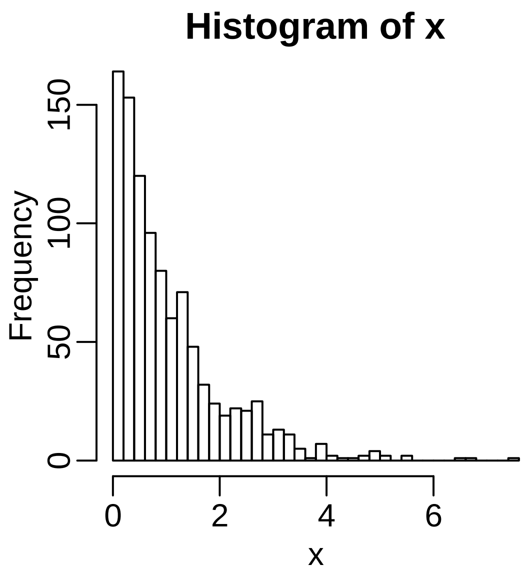
- Theorem: If $U \sim \mathit{Uniform}\ (0,1)$, then using $X = F^{-1}(U)$ generates a random number X from a continuous distribution with specified cdf F.
  - Exponential: generate $r \sim \mathit{Uniform}\ (0,1)$,

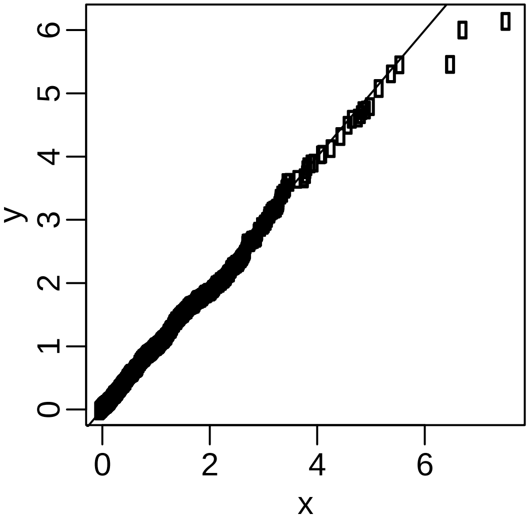
    $F(x) = 1 - e^{-x}$

    then $-\log(1 - r)$ or $-\log(r) \sim \mathit{Exponential}(1)$

Example

```
r=runif(1000) ## generate 1000 U(0,1) random numbers
x=-log(1-r) ## convert to exp(1) random numbers
## compare with exp(1)
y=rexp(1000)
qqplot(x,y); abline(0,1)
```





Numerical approximation

- Is Monte Carlo a “exact” method?
- Use numerical method to approximate complex functions, then use in inverse method to simulate random variates.
- Example: Abramowitz and Stegun 1964 provided numerical approximation to the normal cdf.
  – Error order 10^{-8}

Transformation method (I)

- If a distribution *f* is linked to another distribution *g* which is easy to simulate from.
- Examples: if $X_i\text{'s} \sim iid\ Exp(1)$

then

$$Y = 2\sum_{j=1}^{\nu} X_j \sim \chi^2_{2\nu},$$

$$Y = \beta\sum_{j=1}^{a} X_j \sim Gamma(a,\beta),$$

$$Y = \frac{\sum_{j=1}^{a} X_j}{\sum_{j=1}^{a+b} X_j} \sim Beta(a,b).$$

Transformation method (II)

- More examples:
  - Normal distribution: Box-Muller

    generate U_1 , U_2 ~ *iid Uniform*(0,1),

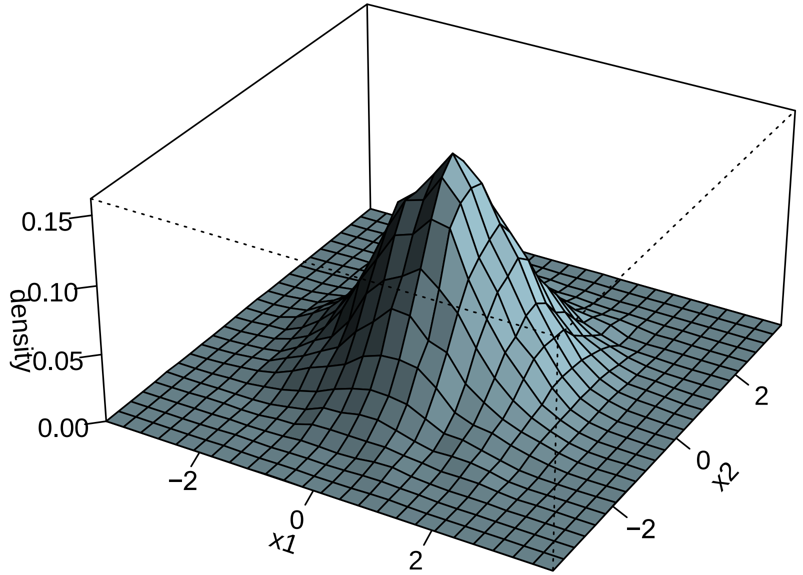
    define

$$\begin{cases} x_1 = \sqrt{-2\log(u_1)}\cos(2\pi u_2), \\ x_2 = \sqrt{-2\log(u_1)}\sin(2\pi u_2). \end{cases}$$

    then x_1 , x_2 ~ *iid* $N(0,1)$.

Example

```
u1=runif(10000); u2=runif(10000)
x1=sqrt(-2*(log(u1)))*cos(2*pi*u2)
x2=sqrt(-2*(log(u1)))*sin(2*pi*u2)
library(MASS)
a=kde2d(x1,x2)
persp(a, xlab="x1", ylab="x2", zlab="density", phi = 30,
         theta = 30, d = 5, shade = 0.75, col = "lightblue",
         expand = 0.5, ltheta = 120,ticktype = "detailed")
```



Transformation method (III)

- Discrete random variables
  - To generate $X \sim P_\theta$, calculate

    $p_0 = P_\theta(X \le 0),\ p_1 = P_\theta(X \le 1),\ p_2 = P_\theta(X \le 2),\ \ldots$

    then generate $U \sim Uniform(0,1)$ and take

    $X = k$ if $p_{k-1} < U < p_k$.
- *Beta*
  - Generate from Uniform then use order statistics.
- *Gamma*
  - From Beta and Exponential.

Fundamental theorem of simulation

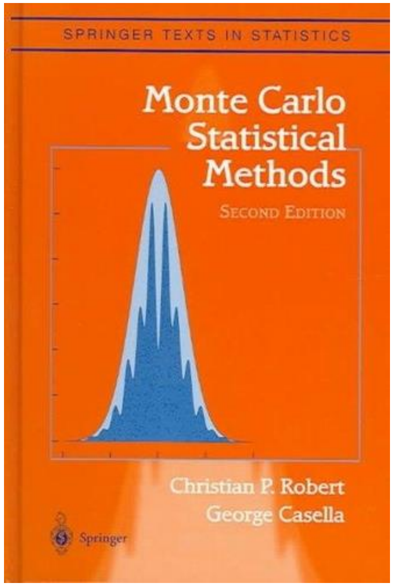
- Simulating $X \sim f(x)$ is equivalent to simulating

  $(X,U) \sim Uniform\{(x,u): 0 < u < f(x)\}$.

  f is the marginal density of the joint distribution.

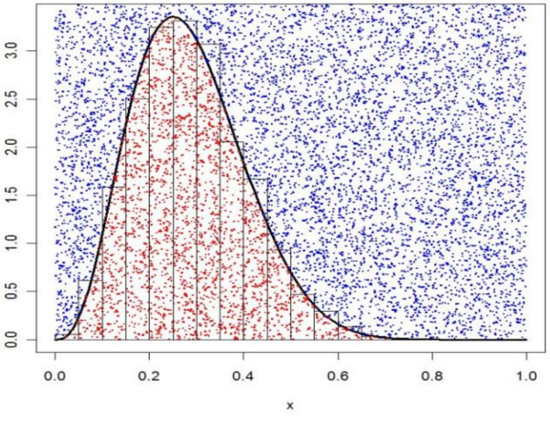
Accept-reject method

- The accept-reject method
  1. Generate $X \sim g$, $U \sim Uniform(0,1)$,
  2. Accept $Y = X$ *if* $U \leq f(X)/Mg(X)$,
  3. Repeat.



Accept-reject method example

- *Beta* (α,β), $\alpha \geq 1$, $\beta \geq 1$,
  simulate $Y \sim \mathit{Uniform}(0,1)$ and
  $U \sim \mathit{Uniform}(0,\mathrm{m})$,
  m is the max of the Beta density.
  select $X = Y$ if under curve



what is the acceptance rate?

Importance sampling

- *Importance sampling:*
  to evaluate $E_f[h(X)] = \int_{\aleph} h(x) f(x) dx$
  based on generating a sample $X_1, \cdots, X_n$ from a given distribution *g* and approximating
  $$E_f[h(X)] \approx \frac{1}{m} \sum_{j=1}^{m} \frac{f(X_j)}{g(X_j)} h(X_j)$$
  which is based on
  $$E_f[h(X)] = \int_{\aleph} h(x) \frac{f(x)}{g(x)} g(x) dx$$

Importance sampling example (I)

- Small tail probabilities:

  $Z \sim N(0,1)$, $P(Z > 4.5)$

  naïve: simulate $Z_i \sim N(0,1)$, $i=1,\ldots,M$.

  calculate

$$P(Z > 4.5) \approx \frac{1}{M}\sum_{i=1}^{M} I(Z_i > 4.5)$$

Importance sampling example (II)

Let $Y \sim TExp(4.5,1)$ with density

$$f_Y(y) = e^{-(x-4.5)} / \int_{4.5}^{\infty} e^{-x} dx.$$

Now simulated from f_Y and use importance sampling, we obtain

$$P(Z > 4.5) \approx \frac{1}{M} \sum_{i=1}^{M} \frac{\varphi(Y_i)}{f_Y(Y_i)} I(Y_i > 4.5) = .000003377 \ .$$

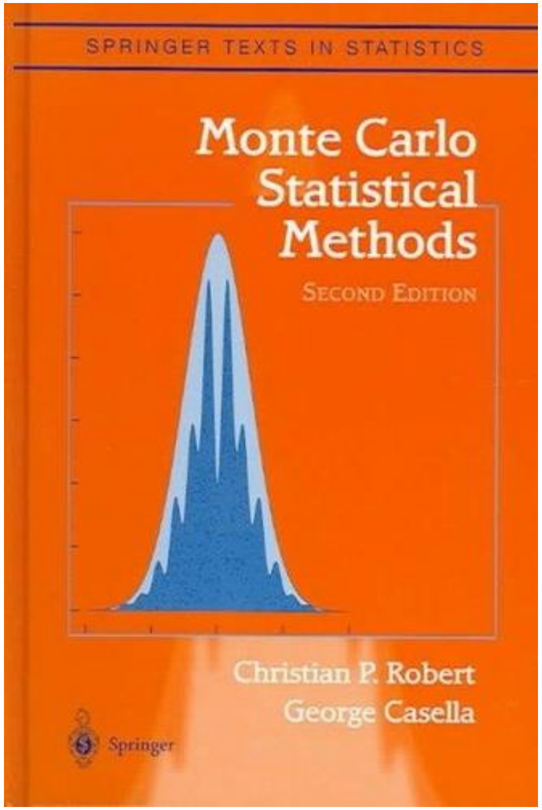
Importance sampling example

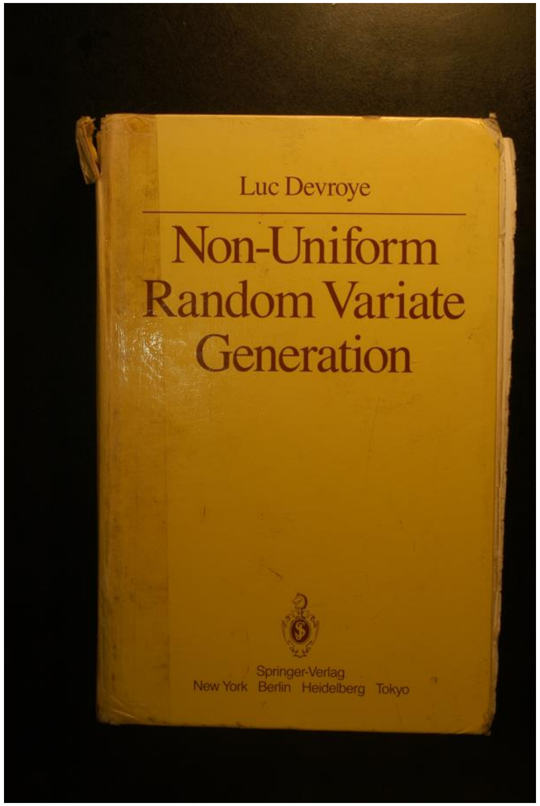
```
## theoretical value
p0=1-pnorm(4.5)
## sample directly from normal distribution
## this needs large number of samples
z=rnorm(10000000)
p1=mean(z>4.5)

## importance sampling
n0=10000
Y=rexp(n0, 1)+4.5
a=dnorm(Y)/dexp(Y-4.5)
p2=mean(a[Y>4.5])

c(p0, p1, p2) ##
[1] 3.397673e-06 2.600000e-06 3.418534e-06
```

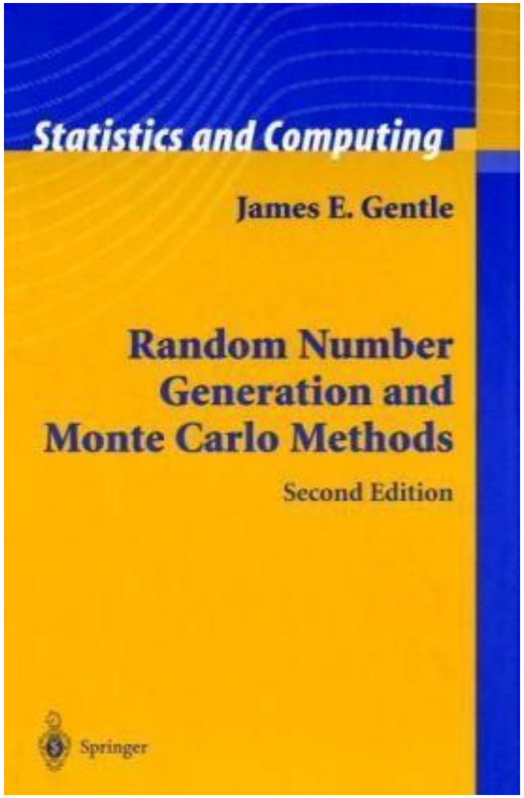
Programming

- In R
  - Lots of functions: runif, rnorm, rbeta, …
- In C/C++
  - Use numerical recipe,
  - Use NAG,
  - Other libraries.

Additional references







Online resources

- Numerical recipe
  http://www.nr.com/
- Luc Devroye's website
  http://luc.devroye.org/rng.html
- Luc Devroye's book
  http://luc.devroye.org/rnbookindex.html