

Introducing Monte Carlo Methods with R

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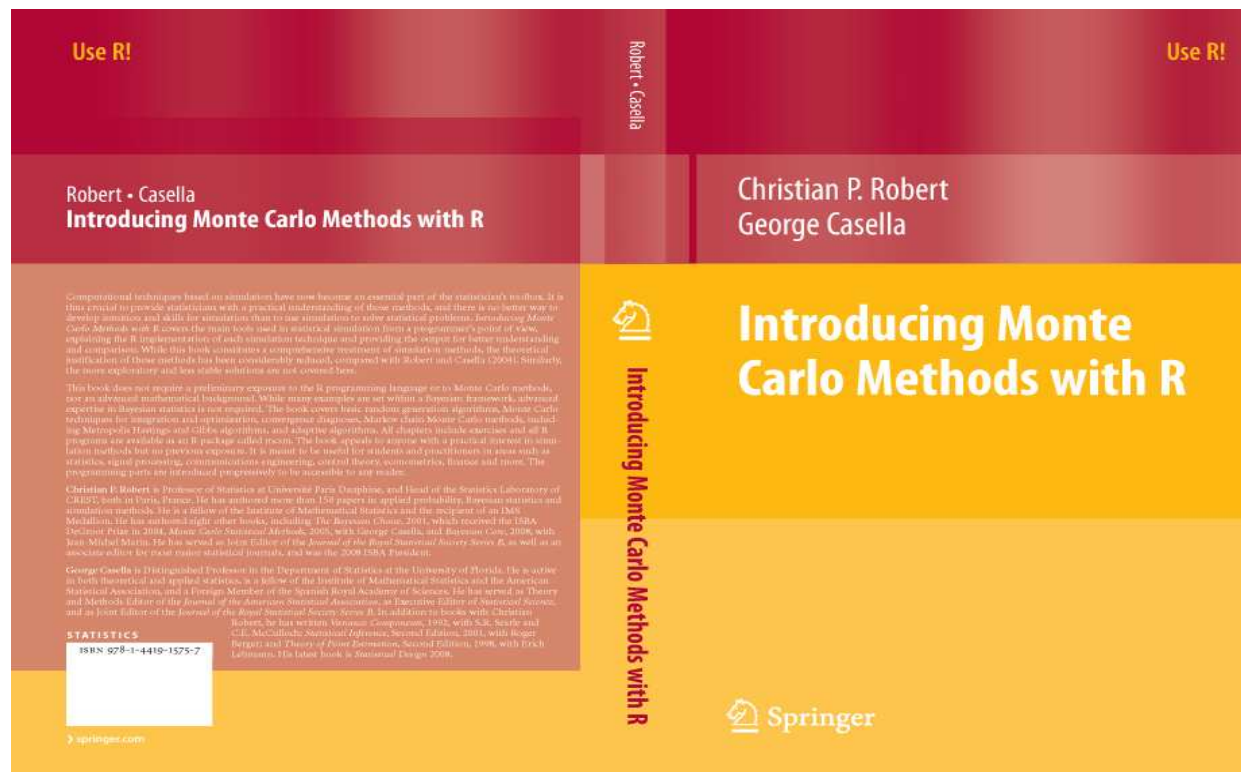
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Based on

- **Introducing Monte Carlo Methods with R**, 2009, Springer-Verlag
- Data and R programs for the course available at <http://www.stat.ufl.edu/casella/IntroMonte/>



Chapter 1: Basic R Programming

“You’re missing the big picture,” he told her. “A good album should be more than the sum of its parts.”

Ian Rankin
Exit Music

This Chapter

- ▶ We introduce the programming language R
- ▶ Input and output, data structures, and basic programming commands
- ▶ The material is both crucial and unavoidably sketchy

Basic R Programming Introduction

- ▶ This is a quick introduction to **R**
- ▶ There are entire books devoted to **R**
 - ▷ **R Reference Card**
 - ▷ available at <http://cran.r-project.org/doc/contrib/Short-refcard.pdf>
- ▶ Take Heart!
 - ▷ The syntax of **R** is simple and logical
 - ▷ The best, and in a sense the only, way to learn **R** is through trial-and-error
- ▶ Embedded help commands **help()** and **help.search()**
 - ▷ **help.start()** opens a Web browser linked to the local manual pages

Basic R Programming

Why R ?

- ▶ There exist other languages, most (all?) of them faster than **R**, like **Matlab**, and even free, like **C** or **Python**.
- ▶ The language combines a sufficiently high power (for an interpreted language) with a very clear syntax both for statistical computation and graphics.
- ▶ **R** is a flexible language that is *object-oriented* and thus allows the manipulation of complex data structures in a condensed and efficient manner.
- ▶ Its graphical abilities are also remarkable
 - ▷ Possible interfacing with \LaTeX using the package **Sweave**.

Basic R Programming

Why R ?

- ▶ R offers the additional advantages of being a free and open-source system
 - ▷ There is even an R newsletter, *R-News*
 - ▷ Numerous (free) Web-based tutorials and user's manuals
- ▶ It runs on all platforms: **Mac**, **Windows**, **Linux** and **Unix**
- ▶ R provides a powerful *interface*
 - ▷ Can integrate programs written in other languages
 - ▷ Such as **C**, **C++**, **Fortran**, **Perl**, **Python**, and **Java**.
- ▶ It is increasingly common to see people who develop new methodology simultaneously producing an R package
- ▶ Can interface with **WinBugs**

Basic R Programming

Getting started

- ▶ Type 'demo()' for some demos; `demo(image)` and `demo(graphics)`
- ▶ 'help()' for on-line help, or 'help.start()' for an HTML browser interface to help.
- ▶ Type 'q()' to quit R.
- ▶ Additional packages can be loaded via the `library` command, as in
 - > `library(combinat) # combinatorics utilities`
 - > `library(datasets) # The R Datasets Package`
 - ▷ There exist hundreds of packages available on the Web.
 - > `install.package("mcsm")`
- ▶ A `library` call is required each time R is launched

Basic R Programming

R objects

- ▶ R distinguishes between several types of *objects*
 - ▷ scalar, vector, matrix, time series, data frames, functions, or graphics.
 - ▷ An R object is mostly characterized by a *mode*
 - ▷ The different modes are
 - **null** (empty object),
 - **logical** (**TRUE** or **FALSE**),
 - **numeric** (such as **3**, **0.14159**, or **2+sqrt(3)**),
 - **complex**, (such as **3-2i** or **complex(1,4,-2)**), and
 - **character** (such as **"Blue"**, **"binomial"**, **"male"**, or **"y=a+bx"**),
- ▶ The R function **str** applied to any R object will show its structure.

Basic R Programming Interpreted

- ▶ R operates on those types as a regular function would operate on a scalar
- ▶ R is interpreted \Rightarrow Slow
- ▶ Avoid loops in favor of matrix manipulations

Basic R Programming – The `vector` class

- > `a=c(5,5.6,1,4,-5)` build the object `a` containing a numeric vector of dimension 5 with elements 5, 5.6, 1, 4, -5
- > `a[1]` display the first element of `a`
- > `b=a[2:4]` build the numeric vector `b` of dimension 3 with elements 5.6, 1, 4
- > `d=a[c(1,3,5)]` build the numeric vector `d` of dimension 3 with elements 5, 1, -5
- > `2*a` multiply each element of `a` by 2 and display the result
- > `b%%3` provides each element of `b` modulo 3

Basic R Programming

More `vector` class

- > `e=3/d` build the numeric vector `e` of dimension 3 and elements $3/5, 3, -3/5$
- > `log(d*e)` multiply the vectors `d` and `e` term by term and transform each term into its natural logarithm
- > `sum(d)` calculate the sum of `d`
- > `length(d)` display the length of `d`

Basic R Programming

Even more **vector** class

- > `t(d)` transpose **d**, the result is a row vector
- > `t(d)*e` elementwise product between two vectors with identical lengths
- > `t(d)%*%e` matrix product between two vectors with identical lengths
- > `g=c(sqrt(2),log(10))` build the numeric vector **g** of dimension 2 and elements $\sqrt{2}$, $\log(10)$
- > `e[d==5]` build the subvector of **e** that contains the components **e[i]** such that **d[i]=5**
- > `a[-3]` create the subvector of **a** that contains all components of **a** but the third.
- > `is.vector(d)` display the logical expression **TRUE** if a vector and **FALSE** else

Basic R Programming
Comments on the **vector** class

- ▶ The ability to apply scalar functions to vectors: [Major Advantage of R](#).
 - ▷ `> lgamma(c(3,5,7))`
 - ▷ returns the vector with components $(\log \Gamma(3), \log \Gamma(5), \log \Gamma(7))$.
- ▶ Functions that are specially designed for vectors include
sample, **permn**, **order**, **sort**, and **rank**
 - ▷ All manipulate the order in which the components of the vector occur.
 - ▷ **permn** is part of the **combinat** library
- ▶ The components of a vector can also be identified by names.
 - ▷ For a vector **x**, **names(x)** is a vector of characters of the same length as **x**

Basic R Programming

The `matrix`, `array`, and `factor` classes

- ▶ The `matrix` class provides the **R** representation of matrices.
- ▶ A typical entry is
 - > `x=matrix(vec,nrow=n,ncol=p)`
 - ▷ Creates an $n \times p$ matrix whose elements are of the dimension np vector `vec`
- ▶ Some manipulations on matrices
 - ▷ The standard matrix product is denoted by `%*%`,
 - ▷ while `*` represents the term-by-term product.
 - ▷ `diag` gives the vector of the diagonal elements of a matrix
 - ▷ `crossprod` replaces the product `t(x)%*%y` on either vectors or matrices
 - ▷ `crossprod(x,y)` more efficient
 - ▷ `apply` is easy to use for functions operating on matrices by row or column

Basic R Programming

Some **matrix** commands

<pre>> x1=matrix(1:20,nrow=5)</pre>	build the numeric matrix x1 of dimension 5×4 with first row 1, 6, 11, 16
<pre>> x2=matrix(1:20,nrow=5,byrow=T)</pre>	build the numeric matrix x2 of dimension 5×4 with first row 1, 2, 3, 4
<pre>> a=x1%*%t(x2)</pre>	matrix product
<pre>> c=x1*x2</pre>	term-by-term product between x1 and x2
<pre>> dim(x1)</pre>	display the dimensions of x1
<pre>> b[,2]</pre>	select the second column of b
<pre>> b[c(3,4),]</pre>	select the third and fourth rows of b
<pre>> b[-2,]</pre>	delete the second row of b
<pre>> rbind(x1,x2)</pre>	vertical merging of x1 and x2 <code>rbind(*)rbind</code>
<pre>> cbind(x1,x2)</pre>	horizontal merging of x1 and x2 <code>rbind(*)rbind</code>
<pre>> apply(x1,1,sum)</pre>	calculate the sum of each row of x1
<pre>> as.matrix(1:10)</pre>	turn the vector 1:10 into a 10×1 matrix

► Lots of other commands that we will see throughout the course

Basic R Programming
The `list` and `data.frame` classes
The Last One

- ▶ A **list** is a collection of arbitrary objects known as its *components*
 - > `li=list(num=1:5,y="color",a=T)` create a list with three arguments
- ▶ The last class we briefly mention is the **data frame**
 - ▷ A list whose elements are possibly made of differing modes and attributes
 - ▷ But have the same length

<ul style="list-style-type: none">> <code>v1=sample(1:12,30,rep=T)</code>> <code>v2=sample(LETTERS[1:10],30,rep=T)</code>> <code>v3=runif(30)</code>> <code>v4=rnorm(30)</code>> <code>xx=data.frame(v1,v2,v3,v4)</code>	<ul style="list-style-type: none">simulate 30 independent uniform $\{1, 2, \dots, 12\}$simulate 30 independent uniform $\{a, b, \dots, j\}$simulate 30 independent uniform $[0, 1]$simulate 30 independent standard normalscreate a data frame
---	---
- ▶ R **code**

Probability distributions in R

- ▶ R , or the web, has about all probability distributions
- ▶ Prefixes: **p**, **d**,**q**, **r**

Distribution	Core	Parameters	Default Values
Beta	beta	shape1, shape2	
Binomial	binom	size, prob	
Cauchy	cauchy	location, scale	0, 1
Chi-square	chisq	df	
Exponential	exp	1/mean	1
F	f	df1, df2	
Gamma	gamma	shape, 1/scale	NA, 1
Geometric	geom	prob	
Hypergeometric	hyper	m, n, k	
Log-normal	lnorm	mean, sd	0, 1
Logistic	logis	location, scale	0, 1
Normal	norm	mean, sd	0, 1
Poisson	pois	lambda	
Student	t	df	
Uniform	unif	min, max	0, 1
Weibull	weibull	shape	

Basic and not-so-basic statistics

t-test

► Testing equality of two means

```
> x=rnorm(25) #produces a N(0,1) sample of size 25  
> t.test(x)
```

One Sample *t*-test

```
data: x  
t = -0.8168, df = 24, p-value = 0.4220  
alternative hypothesis: true mean is not equal to 0  
95 percent confidence interval:  
 -0.4915103  0.2127705  
sample estimates:  
 mean of x  
-0.1393699
```

Basic and not-so-basic statistics
Correlation

► Correlation

```
> attach(faithful) #resident dataset  
> cor.test(faithful[,1],faithful[,2])
```

Pearson's product-moment correlation

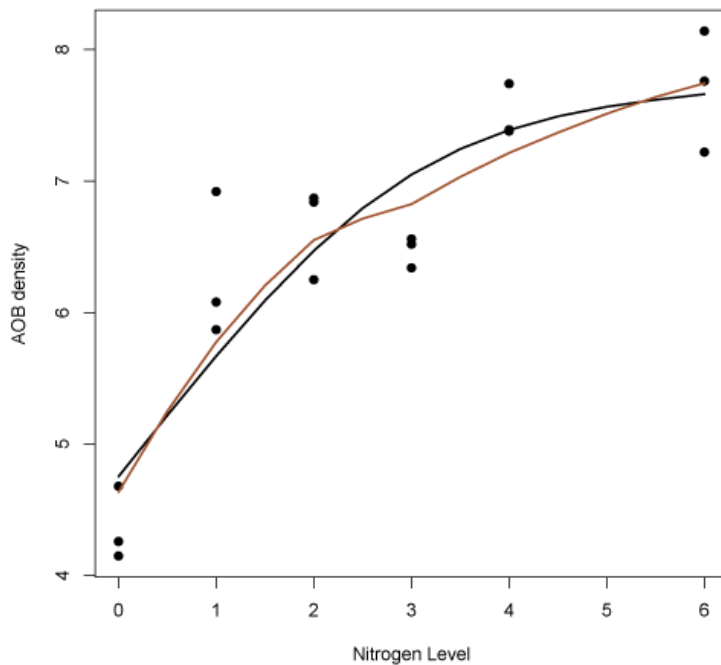
```
data: faithful[, 1] and faithful[, 2]  
t = 34.089, df = 270, p-value < 2.2e-16  
alternative hypothesis: true correlation is not equal to 0  
95 percent confidence interval:  
 0.8756964 0.9210652  
sample estimates:  
      cor  
0.9008112
```

► R [code](#)

Basic and not-so-basic statistics

Splines

- ▶ Nonparametric regression with **loess** function or using *natural splines*
- ▶ Relationship between nitrogen level in soil and abundance of a bacteria **AOB**



- ▶ Natural spline fit (*dark*)
 - ▷ With **ns=2** (linear model)
- ▶ Loess fit (*brown*) with **span=1.25**
- ▶ R **code**

Basic and not-so-basic statistics Generalized Linear Models

- ▶ Fitting a binomial (logistic) glm to the probability of suffering from diabetes for a woman within the Pima Indian population

```
> glm(formula = type ~ bmi + age, family = "binomial", data = Pima.tr)
```

Deviance Residuals:

Min	1Q	Median	3Q	Max
-1.7935	-0.8368	-0.5033	1.0211	2.2531

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	-6.49870	1.17459	-5.533	3.15e-08	***
bmi	0.10519	0.02956	3.558	0.000373	***
age	0.07104	0.01538	4.620	3.84e-06	***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 256.41 on 199 degrees of freedom

Residual deviance: 215.93 on 197 degrees of freedom

AIC: 221.93

Number of Fisher Scoring iterations: 4

Basic and not-so-basic statistics
Generalized Linear Models – Comments

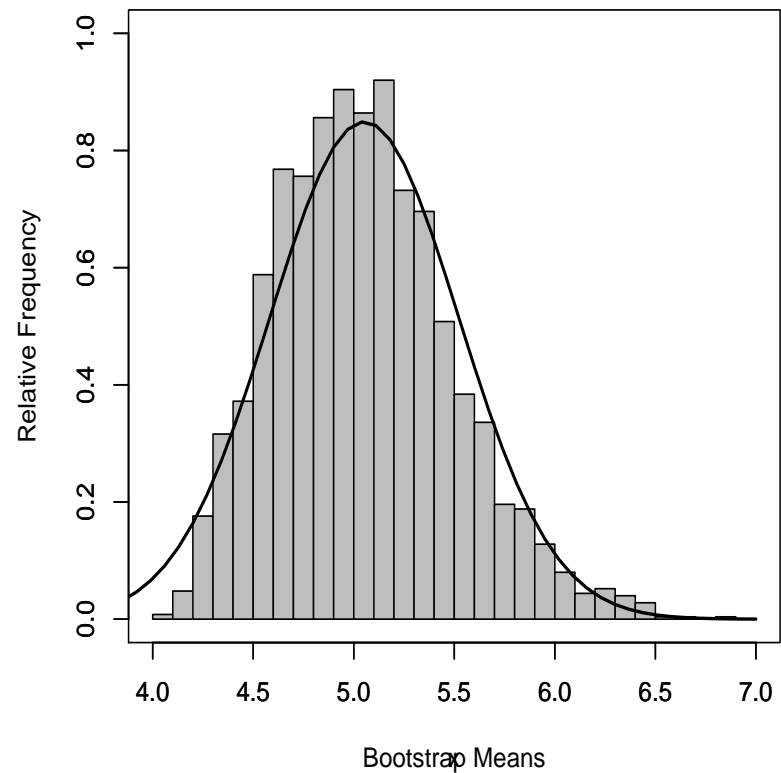
- ▶ Concluding with the significance both of the body mass index **bmi** and the age
- ▶ Other generalized linear models can be defined by using a different **family** value
 - > `glm(y ~x, family=quasi(var="mu^2", link="log"))`
 - ▷ Quasi-Likelihood also
- ▶ Many many other procedures
 - ▷ Time series, anova,...
- ▶ One last one

Basic and not-so-basic statistics
Bootstrap

- ▶ The bootstrap procedure uses the empirical distribution as a substitute for the true distribution to construct variance estimates and confidence intervals.
 - ▷ A sample X_1, \dots, X_n is **resampled** with replacement
 - ▷ The empirical distribution has a finite but large support made of n^n points

- ▶ For example, with data y , we can create a bootstrap sample y^* using the code
 - > `ystar=sample(y,replace=T)`
 - ▷ For each resample, we can calculate a mean, variance, etc

Basic and not-so-basic statistics
Simple illustration of bootstrap



- ▶ A histogram of 2500 bootstrap means
- ▶ Along with the normal approximation
- ▶ Bootstrap shows some skewness
- ▶ R `code`

Basic and not-so-basic statistics
Bootstrapping Regression

- ▶ The bootstrap is not a panacea
 - ▷ Not always clear which quantity should be bootstrapped
 - ▷ In regression, bootstrapping the residuals is preferred

- ▶ Linear regression

$$Y_{ij} = \alpha + \beta x_i + \varepsilon_{ij},$$

α and β are the unknown intercept and slope, ε_{ij} are the iid normal errors

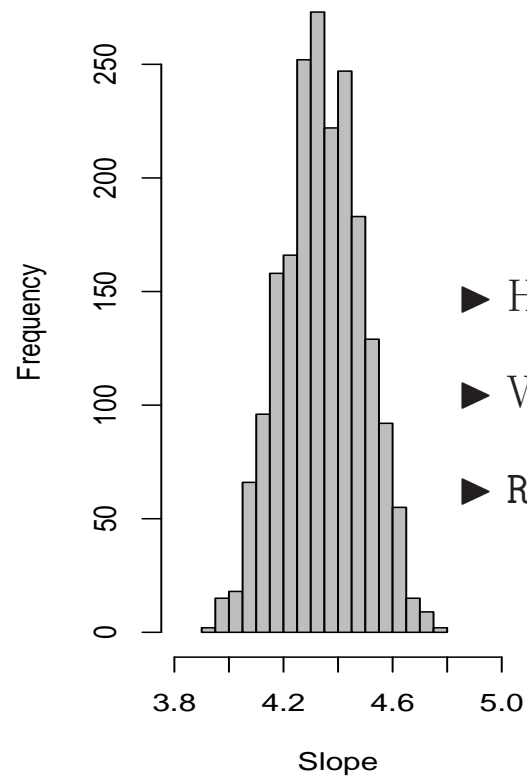
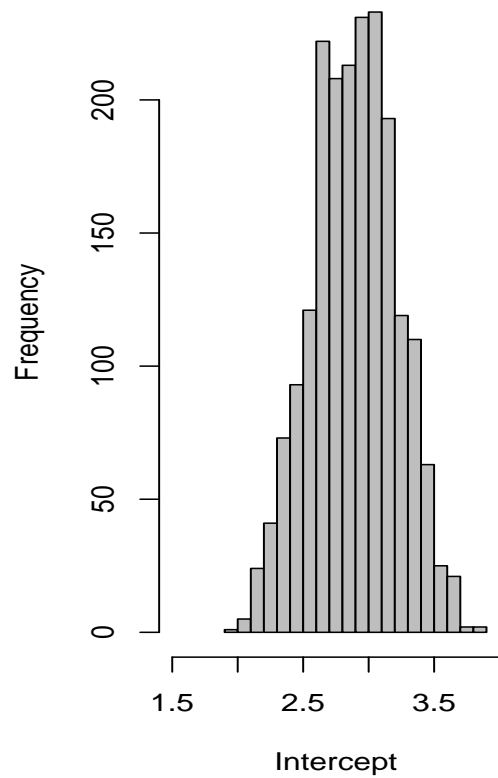
- ▶ The residuals from the least squares fit are given by

$$\hat{\varepsilon}_{ij} = y_{ij} - \hat{\alpha} - \hat{\beta}x_i,$$

- ▷ We bootstrap the residuals
- ▷ Produce a new sample $(\hat{\varepsilon}_{ij}^*)_{ij}$ by resampling from the $\hat{\varepsilon}_{ij}$'s
- ▷ The bootstrap samples are then $y_{ij}^* = y_{ij} + \hat{\varepsilon}_{ij}^*$

Basic and not-so-basic statistics

Bootstrapping Regression – 2



- ▶ Histogram of 2000 bootstrap samples
- ▶ We can also get confidence intervals
- ▶ R `code`

Basic R Programming Some Other Stuff

- ▶ Graphical facilities
 - ▷ Can do a lot; see `plot` and `par`
- ▶ Writing new R functions
 - ▷ `h=function(x) (sin(x)^2+cos(x)^3)^(3/2)`
 - ▷ We will do this a lot
- ▶ Input and output in R
 - ▷ `write.table`, `read.table`, `scan`
- ▶ Don't forget the `mcs` package

Chapter 2: Random Variable Generation

“It has long been an axiom of mine that the little things are infinitely the most important.”

Arthur Conan Doyle
A Case of Identity

This Chapter

- ▶ We present practical techniques that can produce random variables
- ▶ From both standard and nonstandard distributions
- ▶ First: Transformation methods
- ▶ Next: Indirect Methods - Accept–Reject

Introduction

- ▶ Monte Carlo methods rely on
 - ▷ The possibility of producing a supposedly endless flow of random variables
 - ▷ For well-known or new distributions.

- ▶ Such a simulation is, in turn,
 - ▷ Based on the production of uniform random variables on the interval $(0, 1)$.

- ▶ We are not concerned with the [details](#) of producing uniform random variables

- ▶ We assume the existence of such a sequence

Introduction

Using the R Generators

R has a large number of functions that will generate the standard random variables

```
> rgamma(3, 2.5, 4.5)
```

produces three independent generations from a $\mathcal{G}(5/2, 9/2)$ distribution

- ▶ It is therefore,
 - ▷ Counter-productive
 - ▷ Inefficient
 - ▷ And even dangerous,
- ▶ To generate from those standard distributions
- ▶ If it is built into R, use it
- ▶ But....we will practice on these.
- ▶ The principles are essential to deal with distributions that are not built into R.

Uniform Simulation

- ▶ The uniform generator in R is the function `runif`
- ▶ The only required entry is the number of values to be generated.
- ▶ The other optional parameters are `min` and `max`, with R [code](#)

```
> runif(100, min=2, max=5)
```

will produce 100 random variables $\mathcal{U}(2, 5)$.

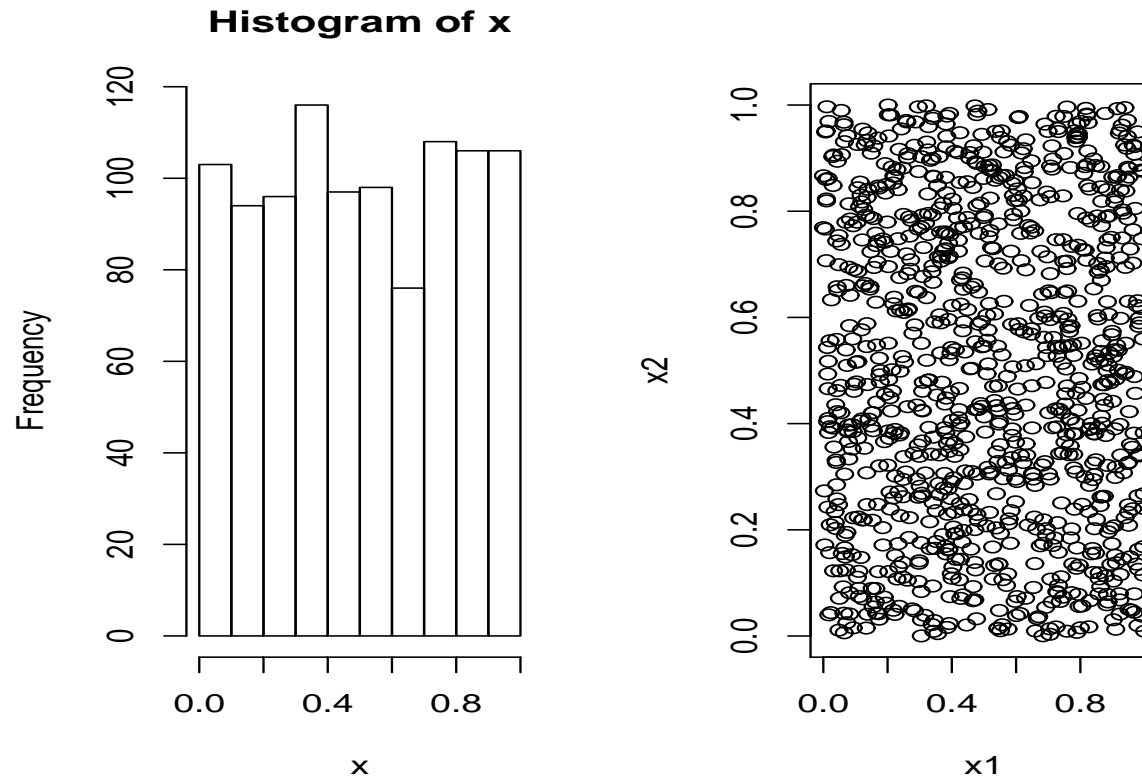
Uniform Simulation

Checking the Generator

- ▶ A quick check on the properties of this uniform generator is to
 - ▷ Look at a histogram of the X_i 's,
 - ▷ Plot the pairs (X_i, X_{i+1})
 - ▷ Look at the estimate autocorrelation function
- ▶ Look at the **R code**

```
> Nsim=10^4           #number of random numbers
> x=runif(Nsim)
> x1=x[-Nsim]        #vectors to plot
> x2=x[-1]           #adjacent pairs
> par(mfrow=c(1,3))
> hist(x)
> plot(x1,x2)
> acf(x)
```


Uniform Simulation Plots from the Generator



► Histogram (*left*), pairwise plot (*center*), and estimated autocorrelation function (*right*) of a sequence of 10^4 uniform random numbers generated by `runif`.

Uniform Simulation Some Comments

- ▶ Remember: `runif` does not involve randomness per se.
- ▶ It is a deterministic sequence based on a random starting point.
- ▶ The R function `set.seed` can produce the same sequence.

```
> set.seed(1)
```

```
> runif(5)
```

```
[1] 0.2655087 0.3721239 0.5728534 0.9082078 0.2016819
```

```
> set.seed(1)
```

```
> runif(5)
```

```
[1] 0.2655087 0.3721239 0.5728534 0.9082078 0.2016819
```

```
> set.seed(2)
```

```
> runif(5)
```

```
[1] 0.0693609 0.8177752 0.9426217 0.2693818 0.1693481
```

- ▶ Setting the seed determines all the subsequent values

The Inverse Transform

► The *Probability Integral Transform*

▷ Allows us to transform a uniform into any random variable

► For example, if X has density f and cdf F , then we have the relation

$$F(x) = \int_{-\infty}^x f(t) dt,$$

and we set $U = F(X)$ and solve for X

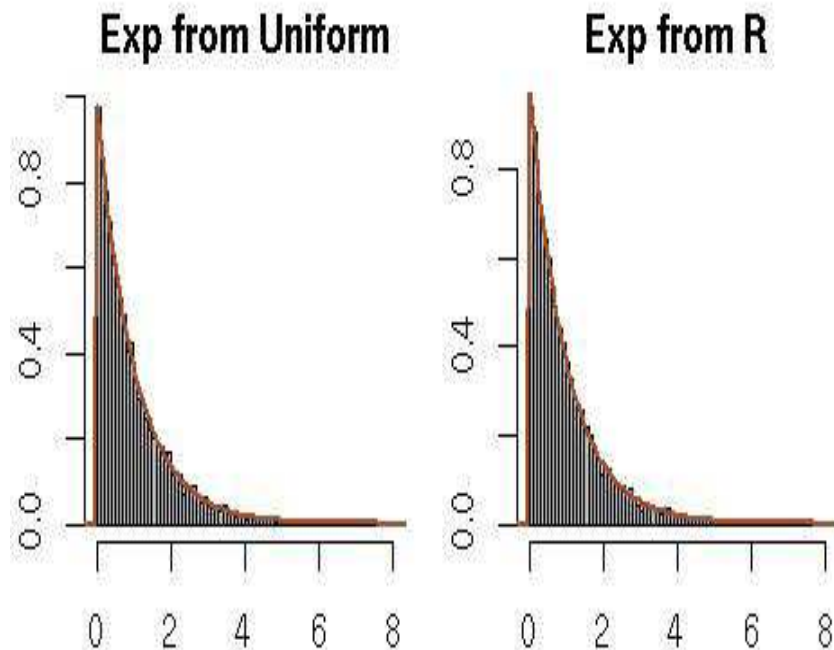
► **Example 2.1**

▷ If $X \sim \mathcal{Exp}(1)$, then $F(x) = 1 - e^{-x}$

▷ Solving for x in $u = 1 - e^{-x}$ gives $x = -\log(1 - u)$

Generating Exponentials

```
> Nsim=10^4           #number of random variables
> U=runif(Nsim)
> X=-log(U)           #transforms of uniforms
> Y=rexp(Nsim)         #exponentials from R
> par(mfrow=c(1,2))   #plots
> hist(X,freq=F,main="Exp from Uniform")
> hist(Y,freq=F,main="Exp from R")
```



- ▶ Histograms of exponential random variables
 - ▷ Inverse transform (*right*)
 - ▷ R command `rexp` (*left*)
 - ▷ $\mathcal{Exp}(1)$ density on top

Generating Other Random Variables From Uniforms

- ▶ This method is useful for other probability distributions
 - ▷ Ones obtained as a transformation of uniform random variables

- ▶ Logistic pdf: $f(x) = \frac{1}{\beta} \frac{e^{-(x-\mu)/\beta}}{[1+e^{-(x-\mu)/\beta}]^2}$, cdf: $F(x) = \frac{1}{1+e^{-(x-\mu)/\beta}}$.

- ▶ Cauchy pdf: $f(x) = \frac{1}{\pi\sigma} \frac{1}{1+(\frac{x-\mu}{\sigma})^2}$, cdf: $F(x) = \frac{1}{2} + \frac{1}{\pi} \arctan((x - \mu)/\sigma)$.

General Transformation Methods

- ▶ When a density f is linked in a relatively simple way
 - ▷ To another distribution easy to simulate
 - ▷ This relationship can be use to construct an algorithm to simulate from f
- ▶ If the X_i 's are iid $\mathcal{Exp}(1)$ random variables,
 - ▷ Three standard distributions can be derived as

$$Y = 2 \sum_{j=1}^{\nu} X_j \sim \chi_{2\nu}^2, \quad \nu \in \mathbb{N}^*,$$

$$Y = \beta \sum_{j=1}^a X_j \sim \mathcal{G}(a, \beta), \quad a \in \mathbb{N}^*,$$

$$Y = \frac{\sum_{j=1}^a X_j}{\sum_{j=1}^{a+b} X_j} \sim \mathcal{Be}(a, b), \quad a, b \in \mathbb{N}^*,$$

where $\mathbb{N}^* = \{1, 2, \dots\}$.

General Transformation Methods

χ_6^2 Random Variables

- ▶ For example, to generate χ_6^2 random variables, we could use the R code

```

> U=runif(3*10^4)
> U=matrix(data=U,nrow=3) #matrix for sums
> X=-log(U)                #uniform to exponential
> X=2* apply(X,2,sum)      #sum up to get chi squares

```

- ▶ Not nearly as efficient as calling `rchisq`, as can be checked by the R code

```

> system.time(test1());system.time(test2())
  user  system elapsed
0.104   0.000   0.107
  user  system elapsed
0.004   0.000   0.004

```

- ▶ `test1` corresponds to the R code above
- ▶ `test2` corresponds to `X=rchisq(10^4,df=6)`

General Transformation Methods Comments

- ▶ These transformations are quite simple and will be used in our illustrations.
- ▶ However, there are limits to their usefulness,
 - ▷ No odd degrees of freedom
 - ▷ No normals
- ▶ For any specific distribution, efficient algorithms have been developed.
- ▶ Thus, if **R** has a distribution built in, it is almost always worth using

General Transformation Methods A Normal Generator

▶ Box–Muller algorithm - two normals from two uniforms

▶ If U_1 and U_2 are iid $\mathcal{U}_{[0,1]}$

▶ The variables X_1 and X_2

$$X_1 = \sqrt{-2 \log(U_1)} \cos(2\pi U_2) , \quad X_2 = \sqrt{-2 \log(U_1)} \sin(2\pi U_2) ,$$

▶ Are iid $\mathcal{N}(0, 1)$ by virtue of a change of variable argument.

▶ The Box–Muller algorithm is exact, not a crude CLT-based approximation

▶ Note that this is *not* the generator implemented in R

▷ It uses the probability inverse transform

▷ With a very accurate representation of the normal cdf

General Transformation Methods Multivariate Normals

- ▶ Can simulate a multivariate normal variable using univariate normals
 - ▷ Cholesky decomposition of $\Sigma = AA'$
 - ▷ $Y \sim \mathcal{N}_p(0, I) \Rightarrow AY \sim \mathcal{N}_p(0, \Sigma)$
 - ▶ There is an R package that replicates those steps, called `rmnorm`
 - ▷ In the `mnormt` library
 - ▷ Can also calculate the probability of hypercubes with the function `sadmvn`
- ```
> sadmvn(low=c(1,2,3),upp=c(10,11,12),mean=rep(0,3),var=B)
[1] 9.012408e-05
attr(,"error")
[1] 1.729111e-08
```
- ▶ B is a positive-definite matrix
  - ▶ This is quite useful since the analytic derivation of this probability is almost always impossible.

## Discrete Distributions

- ▶ To generate discrete random variables we have an “all-purpose” algorithm.
- ▶ Based on the inverse transform principle
- ▶ To generate  $X \sim P_\theta$ , where  $P_\theta$  is supported by the integers,
  - ▷ We can calculate—the probabilities
  - ▷ Once for all, assuming we can store them

$$p_0 = P_\theta(X \leq 0), \quad p_1 = P_\theta(X \leq 1), \quad p_2 = P_\theta(X \leq 2), \quad \dots,$$

- ▷ And then generate  $U \sim \mathcal{U}_{[0,1]}$  and take

$$X = k \text{ if } p_{k-1} < U < p_k.$$

## Discrete Distributions

### Binomial

► **Example** To generate  $X \sim \mathcal{B}in(10, .3)$

▷ The probability values are obtained by `pbinom(k, 10, .3)`

$$p_0 = 0.028, \quad p_1 = 0.149, \quad p_2 = 0.382, \dots, p_{10} = 1,$$

▷ And to generate  $X \sim \mathcal{P}(7)$ , take

$$p_0 = 0.0009, \quad p_1 = 0.0073, \quad p_2 = 0.0296, \dots,$$

▷ Stopping the sequence when it reaches 1 with a given number of decimals.

▷ For instance,  $p_{20} = 0.999985$ .

► Check the **R code**

## Discrete Distributions Comments

- ▶ Specific algorithms are usually more efficient
- ▶ Improvement can come from a judicious choice of the probabilities first computed.
  
- ▶ For example, if we want to generate from a Poisson with  $\lambda = 100$ 
  - ▷ The algorithm above is woefully inefficient
  - ▷ We expect most of our observations to be in the interval  $\lambda \pm 3\sqrt{\lambda}$
  - ▷ For  $\lambda = 100$  this interval is (70, 130)
  - ▷ Thus, starting at 0 is quite wasteful
  
- ▶ A first remedy is to “ignore” what is outside of a highly likely interval
  - ▷ In the current example  $P(X < 70) + P(X > 130) = 0.00268$ .

## Discrete Distributions

### Poisson R Code

- ▶ R `code` that can be used to generate Poisson random variables for large values of lambda.
  - ▶ The sequence `t` contains the integer values in the range around the mean.
- ```
> Nsim=10^4; lambda=100
> spread=3*sqrt(lambda)
> t=round(seq(max(0,lambda-spread),lambda+spread,1))
> prob=ppois(t, lambda)
> X=rep(0,Nsim)
> for (i in 1:Nsim){
+   u=runif(1)
+   X[i]=t[1]+sum(prob<u)-1 }
```
- ▶ The last line of the program checks to see what interval the uniform random variable fell in and assigns the correct Poisson value to X .

Discrete Distributions Comments

- ▶ Another remedy is to start the cumulative probabilities at the mode of the discrete distribution
 - ▶ Then explore neighboring values until the cumulative probability is almost 1.
-
- ▶ Specific algorithms exist for almost any distribution and are often quite fast.
 - ▶ So, if **R** has it, use it.
 - ▶ But **R** does not handle every distribution that we will need,

Mixture Representations

- ▶ It is sometimes the case that a probability distribution can be naturally represented as a *mixture distribution*
- ▶ That is, we can write it in the form

$$f(x) = \int_{\mathcal{Y}} g(x|y)p(y) \, dy \quad \text{or} \quad f(x) = \sum_{i \in \mathcal{Y}} p_i f_i(x) ,$$

- ▷ The mixing distribution can be continuous or discrete.
- ▶ To generate a random variable X using such a representation,
 - ▷ we can first generate a variable Y from the mixing distribution
 - ▷ Then generate X from the selected conditional distribution

Mixture Representations

Generating the Mixture

► Continuous

$$f(x) = \int_{\mathcal{Y}} g(x|y)p(y) \, dy \Rightarrow y \sim p(y) \text{ and } X \sim f(x|y), \text{ then } X \sim f(x)$$

► Discrete

$$f(x) = \sum_{i \in \mathcal{Y}} p_i f_i(x) \Rightarrow i \sim p_i \text{ and } X \sim f_i(x), \text{ then } X \sim f(x)$$

► Discrete Normal Mixture **R code**

$$\triangleright p_1 * N(\mu_1, \sigma_1) + p_2 * N(\mu_2, \sigma_2) + p_3 * N(\mu_3, \sigma_3)$$

Mixture Representations Continuous Mixtures

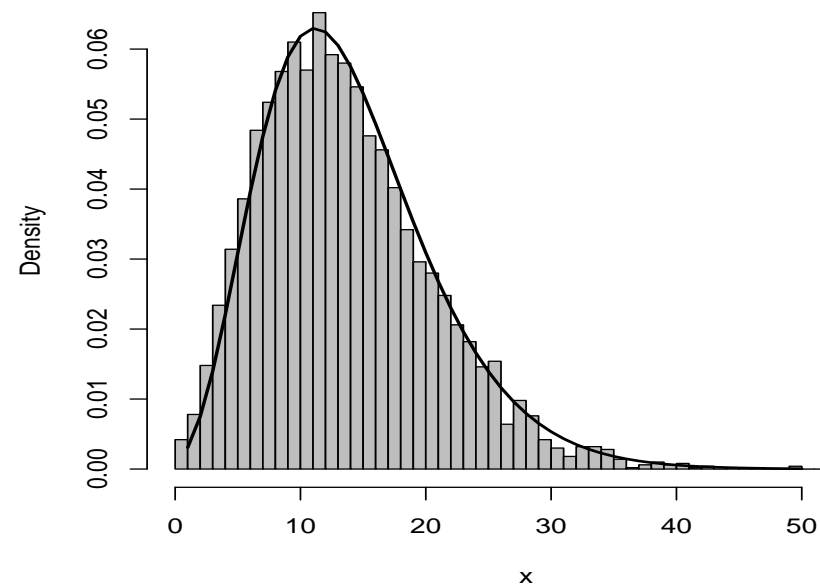
► Student's t density with ν degrees of freedom

$$X|y \sim \mathcal{N}(0, \nu/y) \quad \text{and} \quad Y \sim \chi_\nu^2.$$

- ▷ Generate from a χ_ν^2 then from the corresponding normal distribution
- ▷ Obviously, using `rt` is slightly more efficient

► If X is negative binomial $X \sim \mathcal{Neg}(n, p)$

- ▷ $X|y \sim \mathcal{P}(y)$ and $Y \sim \mathcal{G}(n, \beta)$,
- ▷ R `code` generates from this mixture



Accept–Reject Methods Introduction

- ▶ There are many distributions where transform methods fail
- ▶ For these cases, we must turn to *indirect* methods
 - ▷ We generate a candidate random variable
 - ▷ Only accept it subject to passing a test
- ▶ This class of methods is extremely powerful.
 - ▷ It will allow us to simulate from virtually any distribution.
- ▶ **Accept–Reject Methods**
 - ▷ Only require the functional form of the density f of interest
 - ▷ f = target, g =candidate
- ▶ Where it is simpler to simulate random variables from g

Accept–Reject Methods
Accept–Reject Algorithm

- ▶ The only constraints we impose on this candidate density g
 - ▷ f and g have compatible supports (i.e., $g(x) > 0$ when $f(x) > 0$).
 - ▷ There is a constant M with $f(x)/g(x) \leq M$ for all x .

- ▶ $X \sim f$ can be simulated as follows.
 - ▷ Generate $Y \sim g$ and, independently, generate $U \sim \mathcal{U}_{[0,1]}$.
 - ▷ If $U \leq \frac{1}{M} \frac{f(Y)}{g(Y)}$, set $X = Y$.
 - ▷ If the inequality is not satisfied, we then discard Y and U and start again.

- ▶ Note that $M = \sup_x \frac{f(x)}{g(x)}$

- ▶ $P(\text{Accept}) = \frac{1}{M}$, Expected Waiting Time = M

Accept–Reject Algorithm

R Implementation

Succinctly, the Accept–Reject Algorithm is

Accept–Reject Method

1. Generate $Y \sim g$, $U \sim \mathcal{U}_{[0,1]}$;
2. Accept $X = Y$ if $U \leq f(Y)/Mg(Y)$;
3. Return to 1 otherwise.

► R implementation: If `randg` generates from g

```
> u=runif(1)*M
> y=randg(1)
> while (u>f(y)/g(y))
{
  u=runif(1)*M
  y=randg(1)
}
```

► Produces a single generation y from f

Accept–Reject Algorithm
Normals from Double Exponentials

▶ **Candidate** $Y \sim \frac{1}{2} \exp(-|y|)$

▶ **Target** $X \sim \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$

$$\frac{\frac{1}{\sqrt{2\pi}} \exp(-y^2/2)}{\frac{1}{2} \exp(-|y|)} \leq \frac{2}{\sqrt{2\pi}} \exp(1/2)$$

▷ Maximum at $y = 1$

▶ Accept Y if $U \leq \exp(-.5Y^2 + |Y| - .5)$

▶ Look at R **code**

Accept–Reject Algorithm Theory

- ▶ Why does this method work?
- ▶ A straightforward probability calculation shows

$$P(Y \leq x | \text{Accept}) = P(Y \leq x | U \leq f(Y)/\{Mg(Y)\}) = P(X \leq x)$$

▷ Simulating from g , the output of this algorithm is exactly distributed from f .

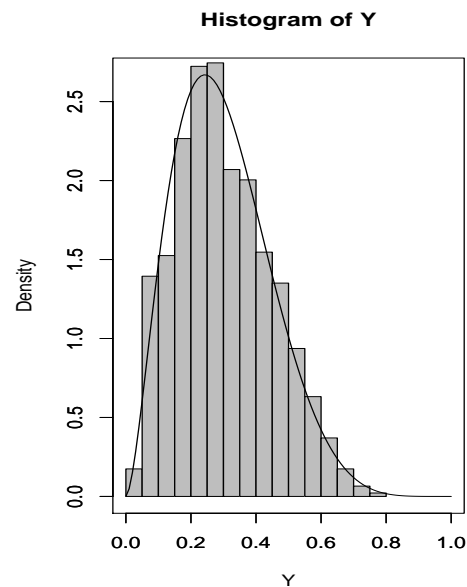
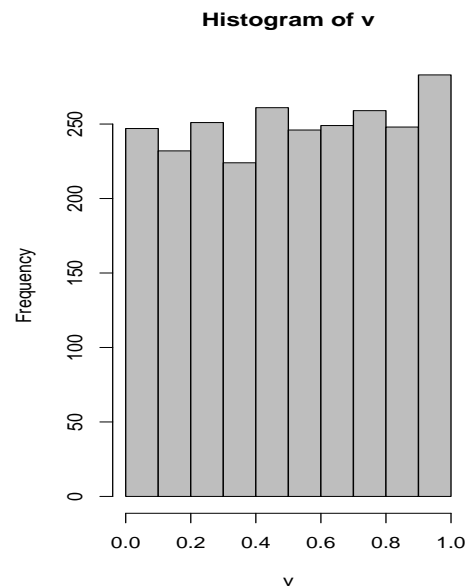
⚡

- ▶ The Accept–Reject method is applicable in any dimension
- ▶ As long as g is a density over the same space as f .

- ▶ Only need to know f/g up to a constant
- ▶ Only need an upper bound on M

Accept-Reject Algorithm Betas from Uniforms

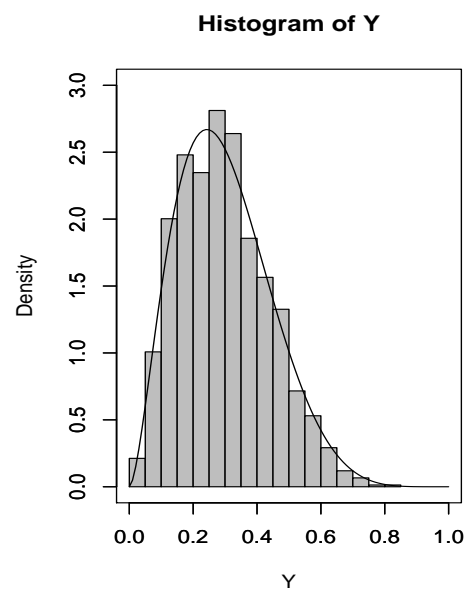
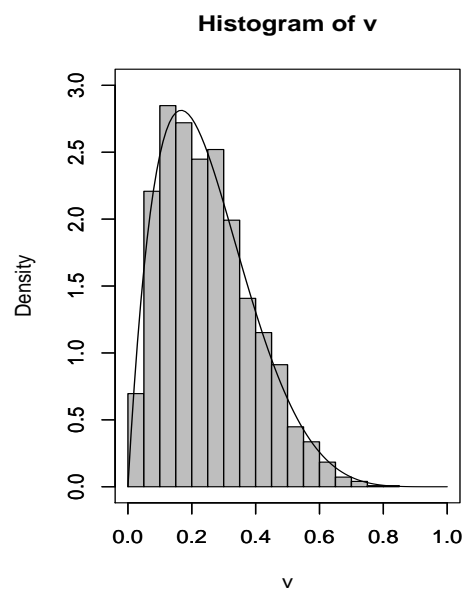
- Generate $X \sim \text{beta}(a, b)$.
- No direct method if a and b are not integers.
- Use a uniform candidate
- For $a = 2.7$ and $b = 6.3$



► Acceptance Rate = 37%

Accept-Reject Algorithm Betas from Betas

- Generate $X \sim \text{beta}(a, b)$.
- No direct method if a and b are not integers.
- Use a beta candidate
- For $a = 2.7$ and $b = 6.3$, $Y \sim \text{beta}(2, 6)$



► Acceptance Rate = 60%

Accept–Reject Algorithm
Betas from Betas-Details

- ▶ Beta density $\propto x^a(1 - x)^b$
- ▶ Can generate if a and b integers
- ▶ If not, use candidate with a_1 and b_1 integers

$$\frac{y^a(1 - y)^b}{y^{a_1}(1 - y)^{b_1}} \text{ maximized at } y = \frac{a - a_1}{a - a_1 + b - b_1}$$

- ▷ Need $a_1 < a$ and $b_1 < b$
- ▶ Efficiency \uparrow as the candidate gets closer to the target
- ▶ Look at R `code`

Accept–Reject Algorithm Comments

↯ Some key properties of the Accept–Reject algorithm::

1. Only the ratio f/M is needed

▷ So the algorithm does not depend on the normalizing constant.

2. The bound $f \leq Mg$ need not be tight

▷ Accept–Reject is valid, but less efficient, if M is replaced with a larger constant.

3. The probability of acceptance is $1/M$

▷ So M should be as small as possible for a given computational effort.

Chapter 3: Monte Carlo Integration

“Every time I think I know what’s going on, suddenly there’s another layer of complications. I just want this damn thing solved.”

John Scalzi
The Last Colony

This Chapter

- ▶ This chapter introduces the major concepts of Monte Carlo methods
- ▶ The validity of Monte Carlo approximations relies on the Law of Large Numbers
- ▶ The versatility of the representation of an integral as an expectation

Monte Carlo Integration Introduction

- ▶ We will be concerned with evaluating integrals of the form

$$\int_{\mathcal{X}} h(x) f(x) dx,$$

- ▶ f is a density
- ▶ We can produce an almost infinite number of random variables from f
- ▶ **We apply probabilistic results**
 - ▶ Law of Large Numbers
 - ▶ Central Limit Theorem
- ▶ **The Alternative - Deterministic Numerical Integration**
 - ▶ R functions `area` and `integrate`
 - ▶ OK in low (one) dimensions
 - ▶ Usually needs some knowledge of the function

Classical Monte Carlo Integration

The Monte Carlo Method

- ▶ The generic problem: Evaluate

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

- ▷ X takes its values in \mathcal{X}

- ▶ [The Monte Carlo Method](#)

- ▷ Generate a sample (X_1, \dots, X_n) from the density f
- ▷ Approximate the integral with

$$\bar{h}_n = \frac{1}{n} \sum_{j=1}^n h(x_j) ,$$

Classical Monte Carlo Integration
Validating the Monte Carlo Method

► The Convergence

$$\bar{h}_n = \frac{1}{n} \sum_{j=1}^n h(x_j) \rightarrow \int_{\mathcal{X}} h(x) f(x) dx = \mathbb{E}_f[h(X)]$$

▷ Is valid by the Strong Law of Large Numbers

► When $h^2(X)$ has a finite expectation under f ,

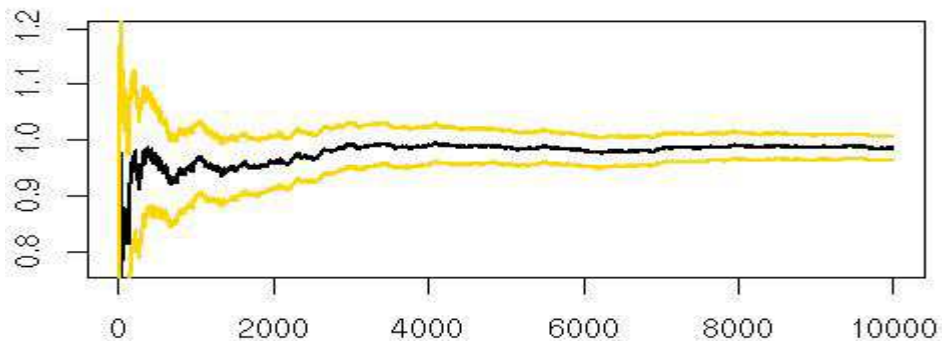
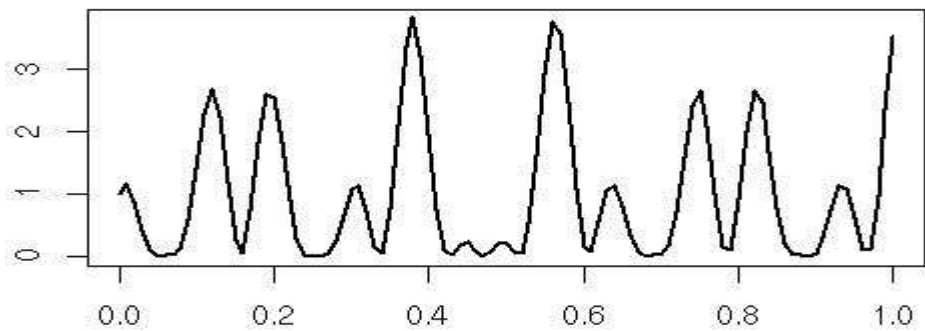
$$\frac{\bar{h}_n - \mathbb{E}_f[h(X)]}{\sqrt{v_n}} \rightarrow \mathcal{N}(0, 1)$$

▷ Follows from the Central Limit Theorem

▷ $v_n = \frac{1}{n^2} \sum_{j=1}^n [h(x_j) - \bar{h}_n]^2.$

Classical Monte Carlo Integration A First Example

► Look at the function

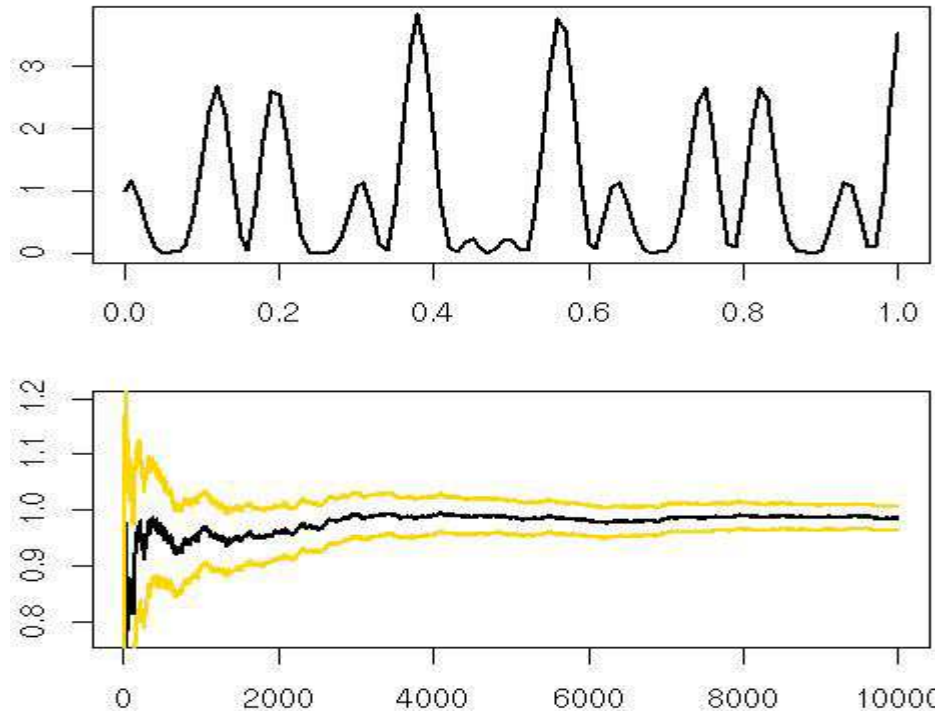


► $h(x) = [\cos(50x) + \sin(20x)]^2$

► Monitoring Convergence

► R `code`

Classical Monte Carlo Integration A Caution



► The confidence band produced in this figure is not a 95% confidence band in the classical sense

► They are **Confidence Intervals** were you to stop at a chosen number of iterations

Classical Monte Carlo Integration Comments

⚡

- ▶ The evaluation of the Monte Carlo error is a bonus
- ▶ It assumes that v_n is a **proper** estimate of the variance of \bar{h}_n
- ▶ If v_n does not converge, converges too slowly, a CLT may not apply

Classical Monte Carlo Integration

Another Example

► Normal Probability

$$\hat{\Phi}(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{I}_{x_i \leq t} \rightarrow \Phi(t) = \int_{-\infty}^t \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy$$

▷ The exact variance $\Phi(t)[1 - \Phi(t)]/n$

▷ Conservative: $\text{Var} \approx 1/4n$

▷ For a precision of four decimals

▷ Want $2 \times \sqrt{1/4n} \leq 10^{-4}$ simulations

▷ Take $n = (10^4)^2 = 10^8$

► This method breaks for tail probabilities

Importance Sampling

Introduction

- [Importance sampling](#) is based on an alternative formulation of the SLLN

$$\mathbb{E}_f[h(X)] = \int_{\mathcal{X}} h(x) \frac{f(x)}{g(x)} g(x) \, dx = \mathbb{E}_g \left[\frac{h(X)f(X)}{g(X)} \right] ;$$

- ▷ f is the target density
- ▷ g is the candidate density

- ▷ Sound Familiar?

Importance Sampling Introduction

- ▶ Importance sampling is based on an alternative formulation of the SLLN

$$\mathbb{E}_f[h(X)] = \int_{\mathcal{X}} h(x) \frac{f(x)}{g(x)} g(x) \, dx = \mathbb{E}_g \left[\frac{h(X)f(X)}{g(X)} \right] ;$$

- ▷ f is the target density
- ▷ g is the candidate density
- ▷ **Sound Familiar? – Just like Accept–Reject**

- ▶ So

$$\frac{1}{n} \sum_{j=1}^n \frac{f(X_j)}{g(X_j)} h(X_j) \rightarrow \mathbb{E}_f[h(X)]$$

- ▶ As long as

- ▷ $\text{Var}(h(X)f(X)/g(X)) < \infty$
- ▷ $\text{supp}(g) \supset \text{supp}(h \times f)$

Importance Sampling Revisiting Normal Tail Probabilities

- ▶ $Z \sim \mathcal{N}(0, 1)$ and we are interested in the probability $P(Z > 4.5)$
- ▶

```
> pnorm(-4.5, log=T)
[1] -12.59242
```
- ▶ Simulating $Z^{(i)} \sim \mathcal{N}(0, 1)$ only produces a hit once in about 3 million iterations!
 - ▷ Very rare event for the normal
 - ▷ Not-so-rare for a distribution sitting out there!
- ▶ Take $g = \mathcal{E}xp(1)$ truncated at 4.5:

$$g(y) = \frac{e^{-y}}{\int_{4.5}^{\infty} e^{-x} dx} = e^{-(y-4.5)},$$

- ▶ The IS estimator is

$$\frac{1}{n} \sum_{i=1}^n \frac{f(Y^{(i)})}{g(Y^{(i)})} = \frac{1}{n} \sum_{i=1}^n \frac{e^{-Y_i^2/2 + Y_i - 4.5}}{\sqrt{2\pi}}$$

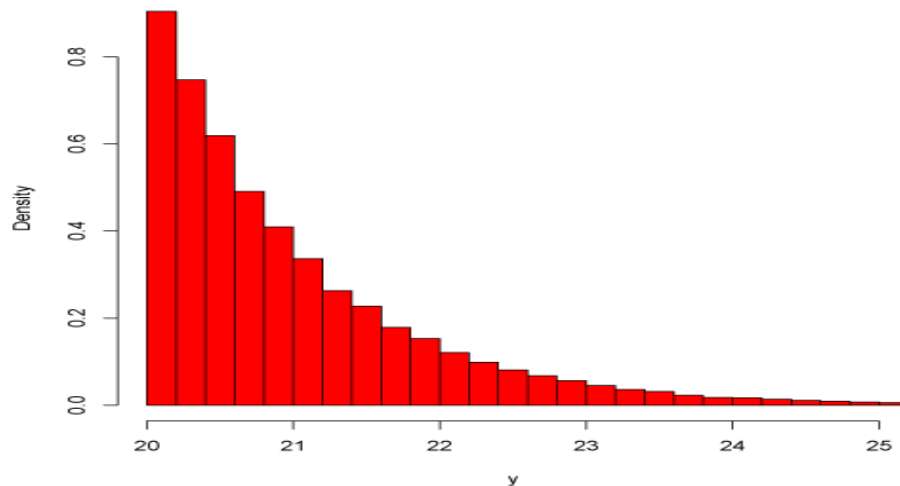
R code

Importance Sampling
Normal Tail Variables

- ▶ The Importance sampler does not give us a sample \Rightarrow Can use Accept–Reject
- ▶ Sample $Z \sim \mathcal{N}(0, 1)$, $Z > a \Rightarrow$ Use Exponential Candidate

$$\frac{\frac{1}{\sqrt{2\pi}} \exp(-.5x^2)}{\exp(-(x - a))} = \frac{1}{\sqrt{2\pi}} \exp(-.5x^2 + x + a) \leq \frac{1}{\sqrt{2\pi}} \exp(-.5a^{*2} + a^* + a)$$

▷ Where $a^* = \max\{a, 1\}$



- ▶ Normals > 20
- ▶ The Twilight Zone
- ▶ R `code`

Importance Sampling Comments

- ⚡ Importance sampling has little restriction on the choice of the candidate
 - ▶ g can be chosen from distributions that are easy to simulate
 - ▷ Or efficient in the approximation of the integral.
 - ▶ Moreover, the same sample (generated from g) can be used repeatedly
 - ▷ Not only for different functions h but also for different densities f .

Importance Sampling
Easy Model - Difficult Distribution

Example: Beta posterior importance approximation

- ▶ Have an observation x from a beta $\mathcal{B}(\alpha, \beta)$ distribution,

$$x \sim \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1} \mathbb{I}_{[0,1]}(x)$$

- ▶ There exists a family of conjugate priors on (α, β) of the form

$$\pi(\alpha, \beta) \propto \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{\lambda} x_0^{\alpha} y_0^{\beta},$$

where λ, x_0, y_0 are hyperparameters,

- ▶ The posterior is then equal to

$$\pi(\alpha, \beta | x) \propto \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{\lambda+1} [xx_0]^{\alpha} [(1-x)y_0]^{\beta}.$$

Importance Sampling

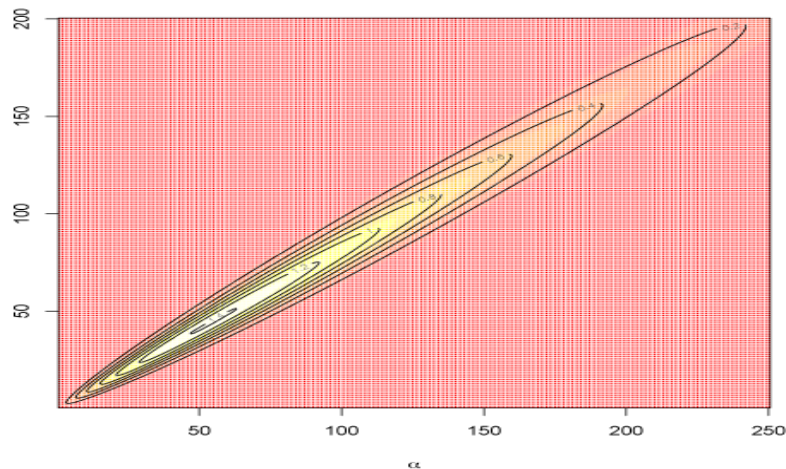
Easy Model - Difficult Distribution -2

- ▶ The posterior distribution is intractable

$$\pi(\alpha, \beta | x) \propto \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{\lambda+1} [xx_0]^\alpha [(1-x)y_0]^\beta.$$

- ▷ Difficult to deal with the gamma functions
- ▷ Simulating directly from $\pi(\alpha, \beta | x)$ is impossible.

- ▶ What candidate to use?



- ▶ Contour Plot
- ▶ Suggest a candidate?
- ▶ R `code`

Importance Sampling
Easy Model - Difficult Distribution – 3

- ▶ Try a Bivariate Student's T (or Normal)
- ▶ Trial and error
 - ▷ Student's $\mathcal{T}(3, \mu, \Sigma)$ distribution with $\mu = (50, 45)$ and

$$\Sigma = \begin{pmatrix} 220 & 190 \\ 190 & 180 \end{pmatrix}$$

- ▷ Produce a reasonable fit
 - ▷ R `code`
- ▶ Note that we are using the fact that

$$X \sim f(x) \Rightarrow \Sigma^{1/2}X + \mu \sim f((x - \mu)' \Sigma^{-1}(x - \mu))$$

Importance Sampling

Easy Model - Difficult Distribution – Posterior Means

- ▶ The posterior mean of α is

$$\int \int \alpha \pi(\alpha, \beta | x) d\alpha d\beta = \int \int \left[\alpha \frac{\pi(\alpha, \beta | x)}{g(\alpha, \beta)} \right] g(\alpha, \beta) d\alpha d\beta \approx \frac{1}{M} \sum_{i=1}^M \alpha_i \frac{\pi(\alpha_i, \beta_i | x)}{g(\alpha_i, \beta_i)}$$

where

$$\triangleright \pi(\alpha, \beta | x) \propto \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{\lambda+1} [xx_0]^\alpha [(1-x)y_0]^\beta$$

$$\triangleright g(\alpha, \beta) = \mathcal{T}(3, \mu, \Sigma)$$

- ▶ Note that $\pi(\alpha, \beta | x)$ is not normalized, so we have to calculate

$$\frac{\int \int \alpha \pi(\alpha, \beta | x) d\alpha d\beta}{\int \int \pi(\alpha, \beta | x) d\alpha d\beta} \approx \frac{\sum_{i=1}^M \alpha_i \frac{\pi(\alpha_i, \beta_i | x)}{g(\alpha_i, \beta_i)}}{\sum_{i=1}^M \frac{\pi(\alpha_i, \beta_i | x)}{g(\alpha_i, \beta_i)}}$$

- ▶ The same samples can be used for every posterior expectation
- ▶ R code

Importance Sampling Probit Analysis

Example: Probit posterior importance sampling approximation

- ▶ y are binary variables, and we have covariates $x \in \mathbb{R}^p$ such that

$$\Pr(y = 1|x) = 1 - \Pr(y = 0|x) = \Phi(x^T \beta), \quad \beta \in \mathbb{R}^p.$$

- ▶ We return to the dataset `Pima.tr`, x =BMI
- ▶ A GLM estimation of the model is (using centered x)

```
>glm(formula = y ~ x, family = binomial(link = "probit"))
```

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	-0.44957	0.09497	-4.734	2.20e-06	***
x	0.06479	0.01615	4.011	6.05e-05	***

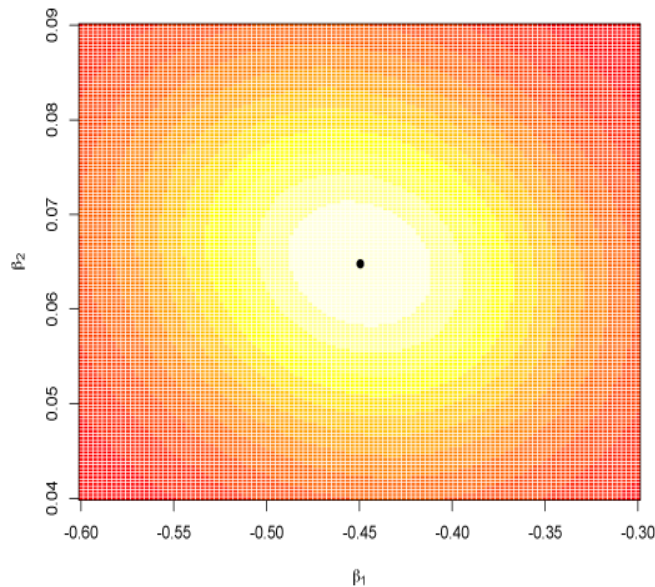
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

So BMI has a significant impact on the possible presence of diabetes.

Importance Sampling Bayesian Probit Analysis

- ▶ From a Bayesian perspective, we use a vague prior
 - ▷ $\beta = (\beta_1, \beta_2)$, each having a $\mathcal{N}(0, 100)$ distribution
- ▶ With Φ the normal cdf, the posterior is proportional to

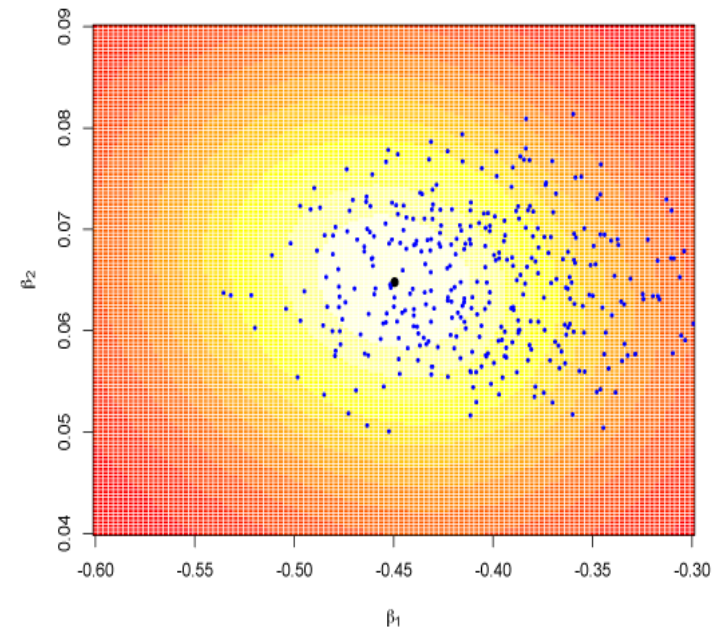
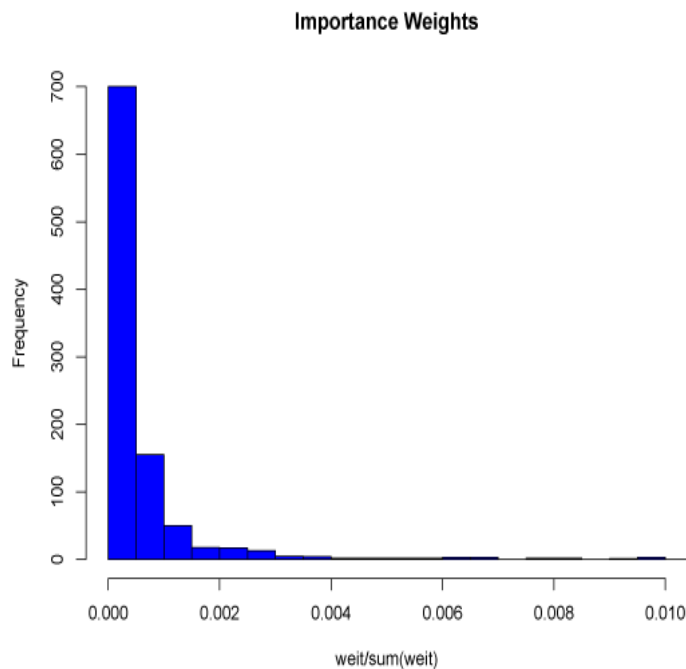
$$\prod_{i=1}^n [\Phi(\beta_1 + (x_i - \bar{x})\beta_2)]^{y_i} [\Phi(-\beta_1 - (x_i - \bar{x})\beta_2)]^{1-y_i} \times e^{-\frac{\beta_1^2 + \beta_2^2}{2 \times 100}}$$



- ▶ Level curves of posterior
- ▶ MLE in the center
- ▶ R [code](#)

Importance Sampling Probit Analysis Importance Weights

- ▶ Normal candidate centered at the MLE - no finite variance guarantee
- ▶ The importance weights are rather uneven, if not degenerate



- ▶ Right side = reweighted candidate sample (**R** code)
- ▶ Somewhat of a failure

Chapter 5: Monte Carlo Optimization

“He invented a game that allowed players to predict the outcome?”

Susanna Gregory

To Kill or Cure

This Chapter

- ▶ Two uses of computer-generated random variables to solve optimization problems.
- ▶ **The first use** is to produce stochastic search techniques
 - ▷ To reach the maximum (or minimum) of a function
 - ▷ Avoid being trapped in local maxima (or minima)
 - ▷ Are sufficiently attracted by the global maximum (or minimum).
- ▶ **The second** use of simulation is to approximate the function to be optimized.