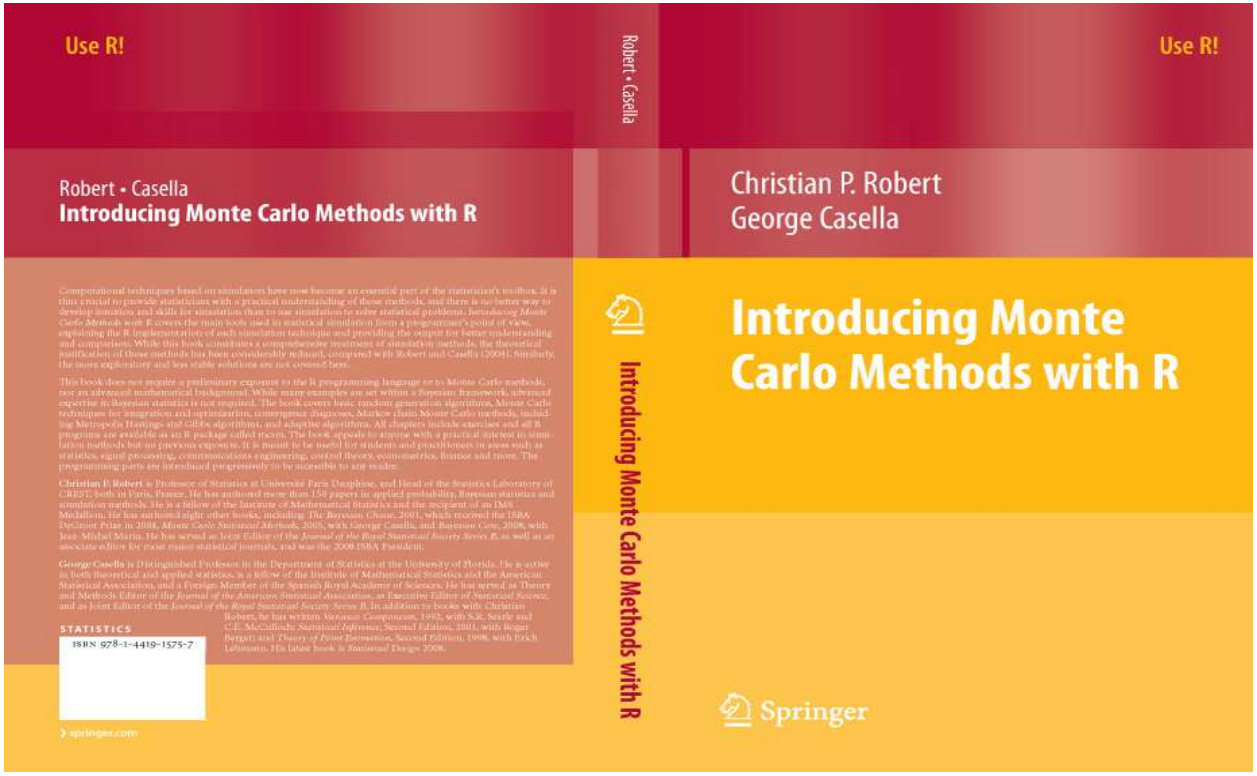
Introducing Monte Carlo Methods with R

Christian P. Robert
Université Paris Dauphine
xian@ceremade.dauphine.fr

George Casella
University of Florida
casella@ufl.edu

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 LaTeXusing 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 mainpulations

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

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

`> v1=sample(1:12,30,rep=T)`	simulate 30 independent uniform $\{1, 2, \ldots, 12\}$
`> v2=sample(LETTERS[1:10],30,rep=T)`	simulate 30 independent uniform $\{a, b, ..., j\}$
`> v3=runif(30)`	simulate 30 independent uniform $[0, 1]$
`> v4=rnorm(30)`	simulate 30 independent standard normals
`> xx=data.frame(v1,v2,v3,v4)`	create 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])

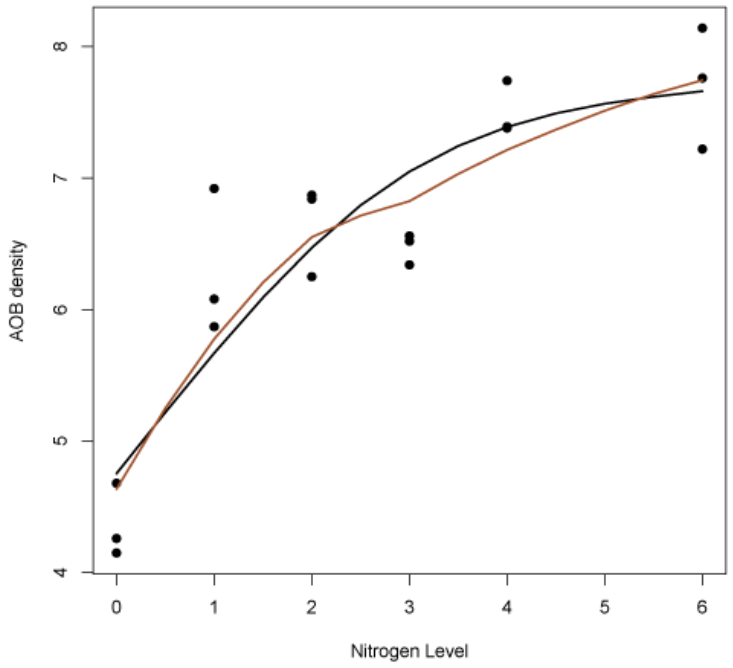
        Pearson's product-moment correlation

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

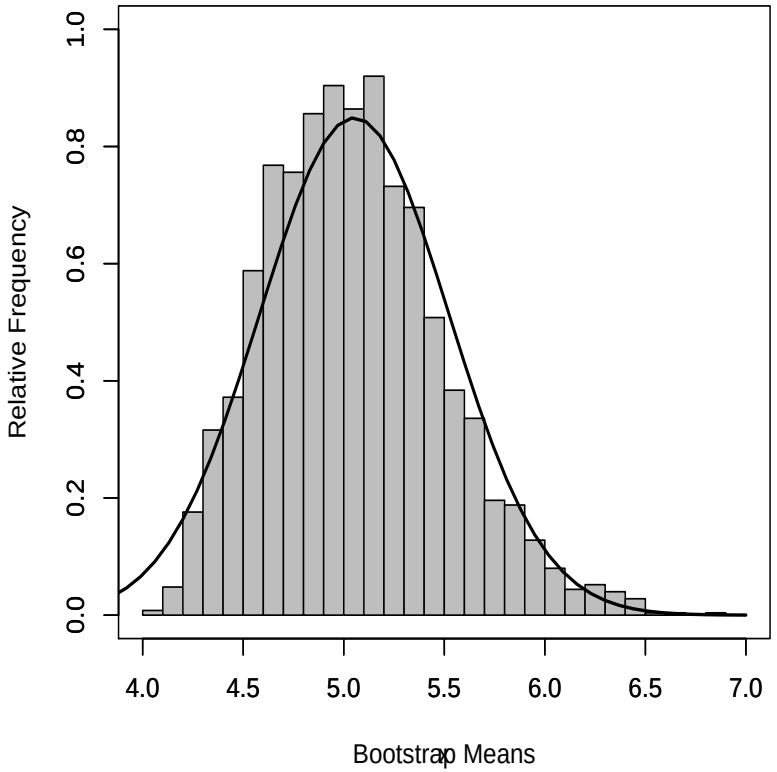
- The bootstrap procedure uses the empirical distribution as a substitute for the true distribution to construct variance estimates and confidence intervals.
  - A sample $X_1, \ldots, X_n$ is resampled with replacement
  - The empirical distribution has a finite but large support made of n^n points

- 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



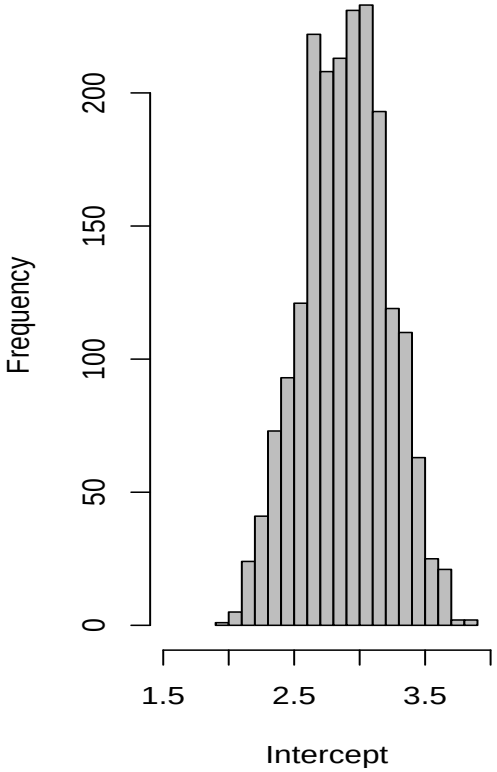
- A histogram of 2500 bootstrap means
- Along with the normal approximation
- Bootstrap shows some skewness
- R code

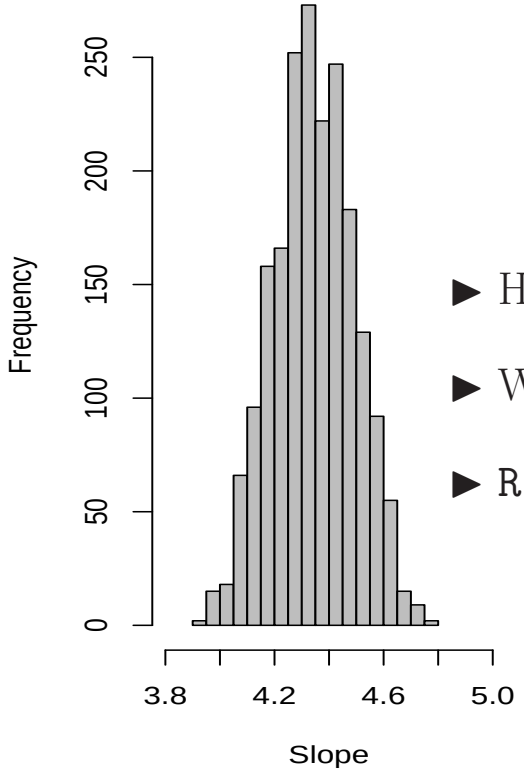
Basic and not-so-basic statistics
Bootstrapping Regression

- 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 `mcsm` 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)
```

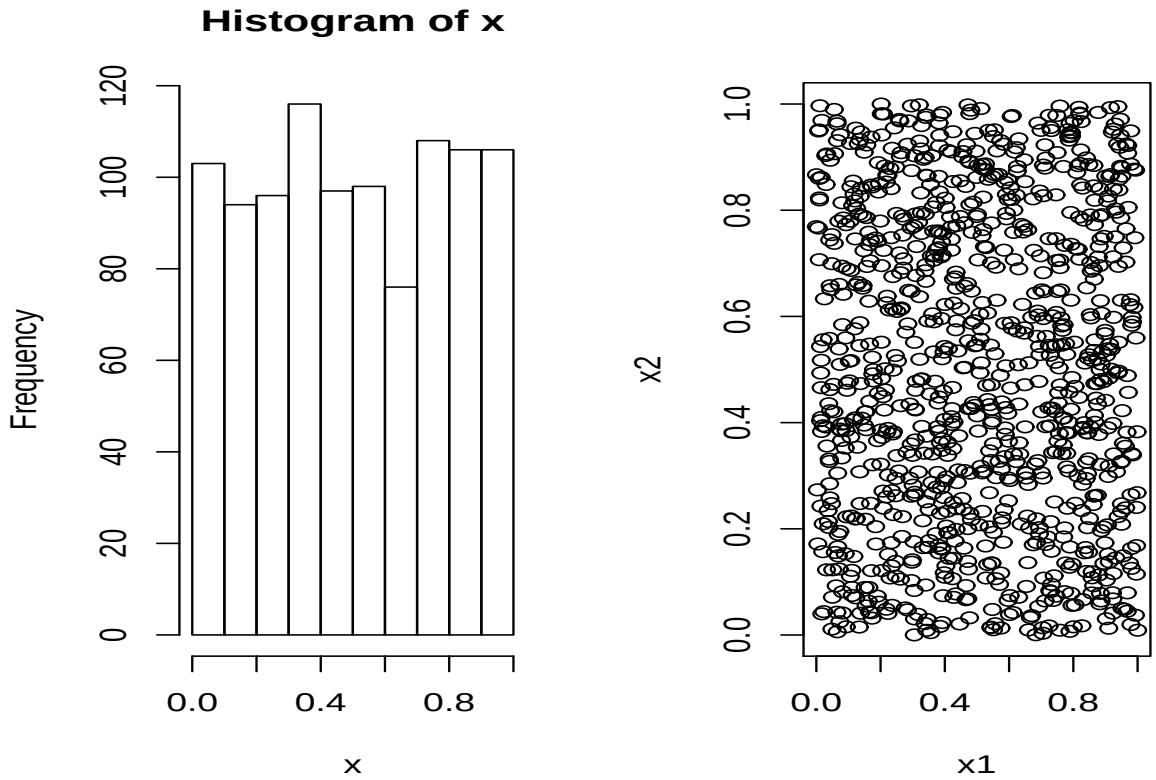
will produce 100 random variables $\mathcal{U}(2, 5)$.

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

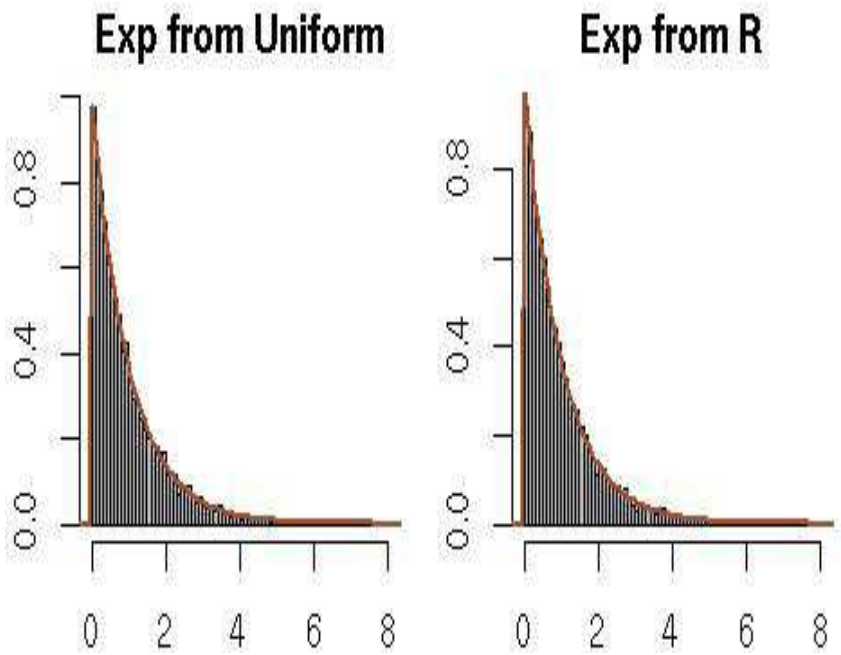
$$F(x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t,$$

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

- Example 2.1
  - If $X \sim \mathcal{E}xp(1)$, 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)*
  - $\mathcal{E}xp(1)$ 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: $f(x) = \frac{1}{\pi\sigma}\frac{1}{1+\left(\frac{x-\mu}{\sigma}\right)^2}$, 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 $\mathcal{E}xp(1)$ random variables,
  - Three standard distributions can be derived as

$$Y = 2\sum_{j=1}^{\nu} X_j \sim \chi^2_{2\nu}\,, \qquad \nu \in \mathbb{N}^*\,,$$

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

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

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

General Transformation Methods
χ^2_6 Random Variables

- For example, to generate χ^2_6 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

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

- 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_θ is supported by the integers,
  - ▷ We can calculate—the probabilities
  - ▷ Once for all, assuming we can store them

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

  - ▷ 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)`

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

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

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

  - 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

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

  - 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

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

- 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

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

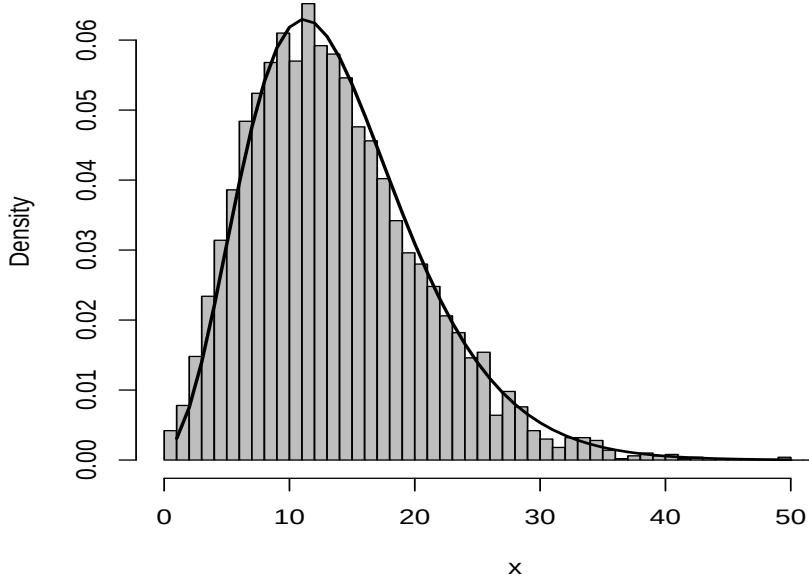
Mixture Representations
Continuous Mixtures

- Student's t density with ν degrees of freedom

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

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

- If X is negative binomial $X \sim \mathcal{N}eg(n, p)$
  - $X|y \sim \mathcal{P}(y) \quad \text{and} \quad Y \sim \mathcal{G}(n, \beta)$,
  - `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

$$P(Y \le x| \text{ Accept }) = P\left(Y \le x | U \le \frac{f(Y)}{Mg(Y)}\right) = P(X \le x)$$

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

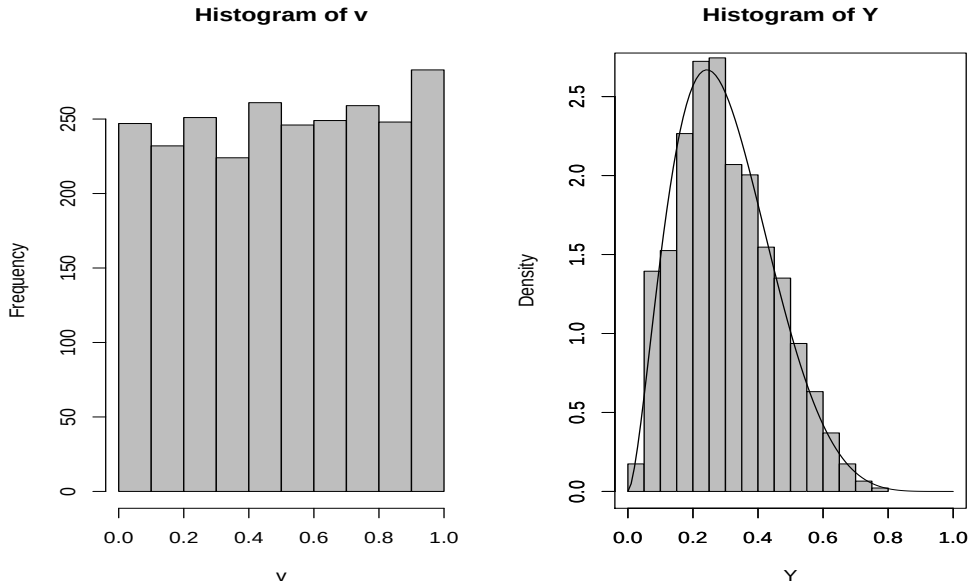
ϟ

- 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

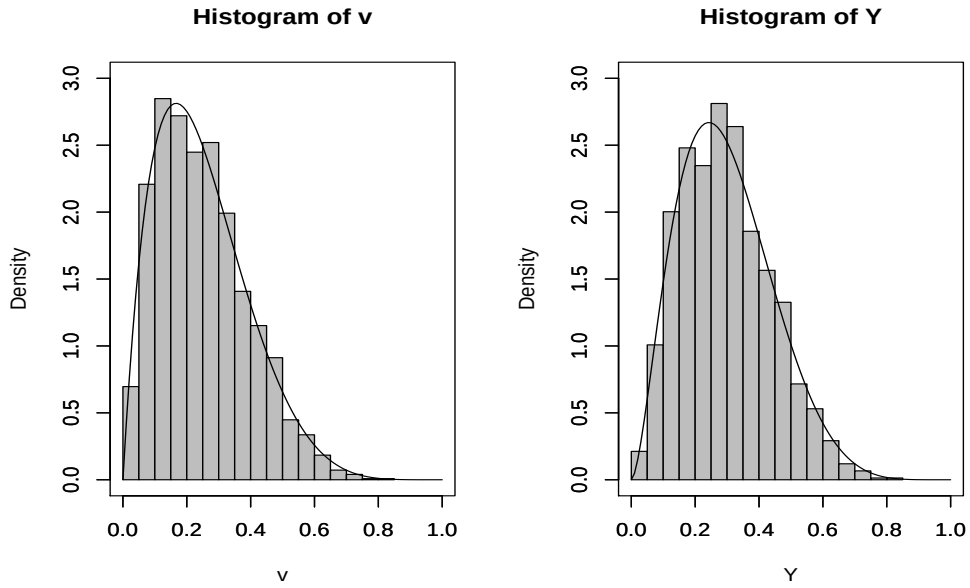
- Generate $X \sim \text{beta}(a, b)$.
- No direct method if a and b are not integers.
- Use a uniform candidate
- For $a = 2.7$ and $b = 6.3$



▶ 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 ↑ as the candidate gets closer to the target
- Look at `R` code

Accept–Reject Algorithm
Comments

ϟSome 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

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

  - 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

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

  - X takes its values in $\mathcal{X}$

- The Monte Carlo Method
  - Generate a sample $(X_1, \ldots, X_n)$ from the density f
  - Approximate the integral with

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

Classical Monte Carlo Integration
Validating the Monte Carlo Method

- The Convergence

$$\overline{h}_n = \frac{1}{n} \sum_{j=1}^{n} h(x_j) \to \int_{\mathcal{X}} h(x)\, f(x)\, \mathrm{d}x = \mathbb{E}_f[h(X)]$$

  - Is valid by the Strong Law of Large Numbers

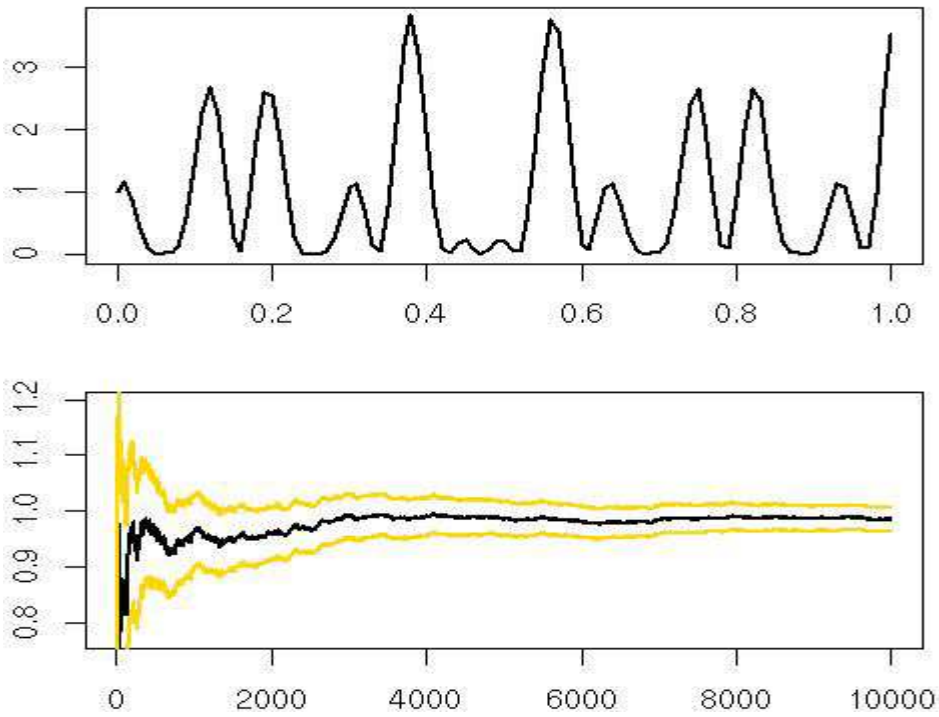
- When $h^2(X)$ has a finite expectation under f,

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

  - Follows from the Central Limit Theorem
  - $v_n = \frac{1}{n^2} \sum_{j=1}^{n} [h(x_j) - \overline{h}_n]^2$.

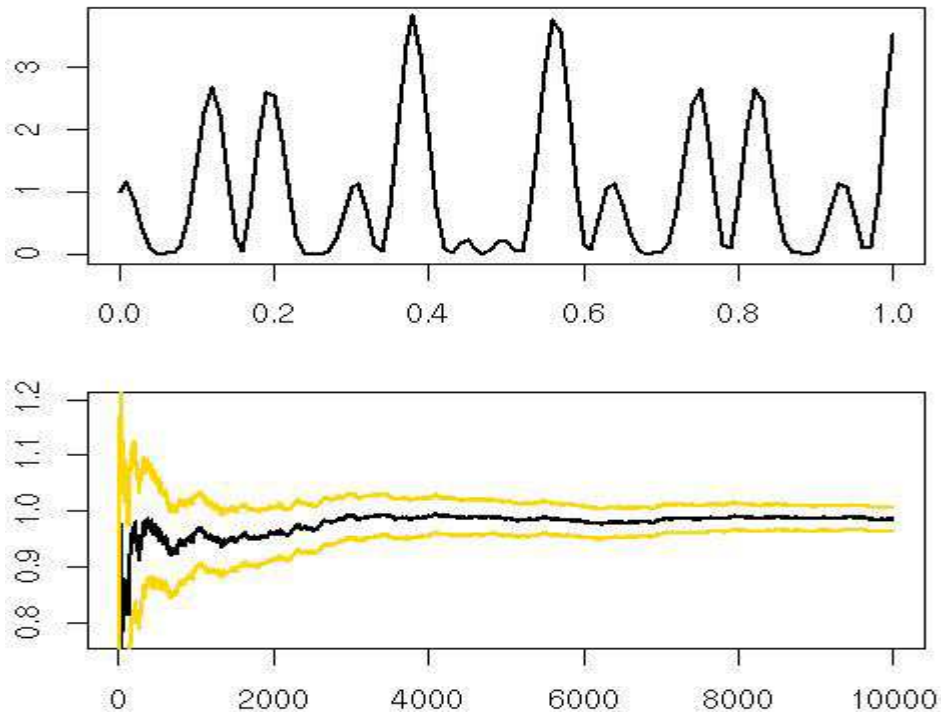
Classical Monte Carlo Integration
A First Example

- 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

ϟ

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

Classical Monte Carlo Integration
Another Example

- Normal Probability

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

  - The exact variance $\Phi(t)[1 - \Phi(t)]/n$
  - Conservative: 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 down for tail probabilities

Importance Sampling
Introduction

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

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

▷ 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

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

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

- So

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

- As long as
  - $\mathrm{Var}\,(h(X)f(X)/g(X)) < \infty$
  - $\mathrm{supp}(g) \supset \mathrm{supp}(h \times f)$

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:

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

- The IS estimator is

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

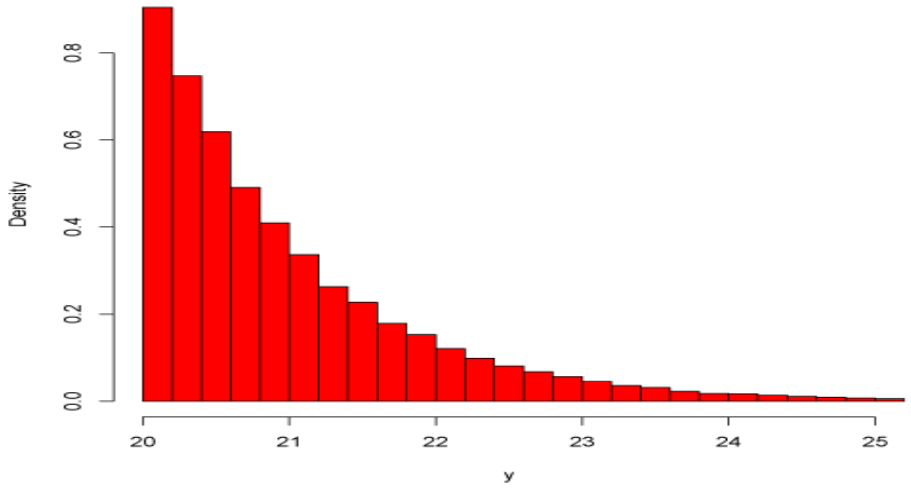
R code
  ```

Importance Sampling
Normal Tail Variables

- The Importance sampler does not give us a sample ⇒ 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

ϟ 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

$$\pi(\alpha,\beta|x) \propto \left\{\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\right\}^{\lambda+1} [x x_0]^{\alpha}[(1-x)y_0]^{\beta}\,.$$

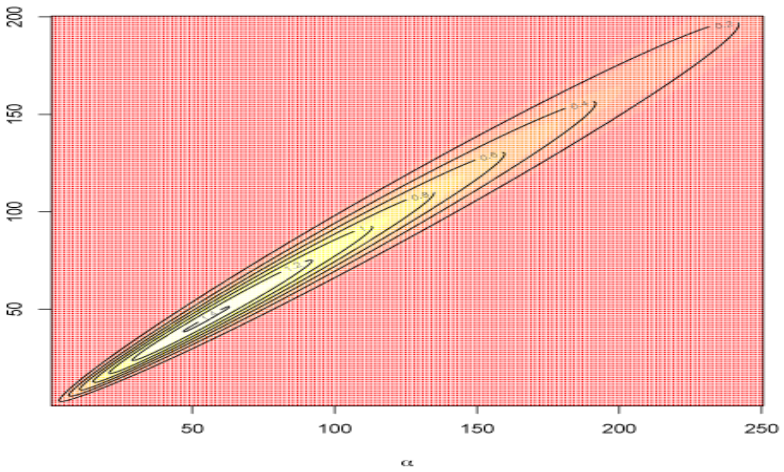
Importance Sampling
Easy Model - Difficult Distribution -2

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

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

  - $\pi(\alpha,\beta|x) \propto \left\{\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\right\}^{\lambda+1} [xx_0]^{\alpha}[(1-x)y_0]^{\beta}$
  - $g(\alpha,\beta) = \mathcal{T}(3,\mu,\Sigma)$

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

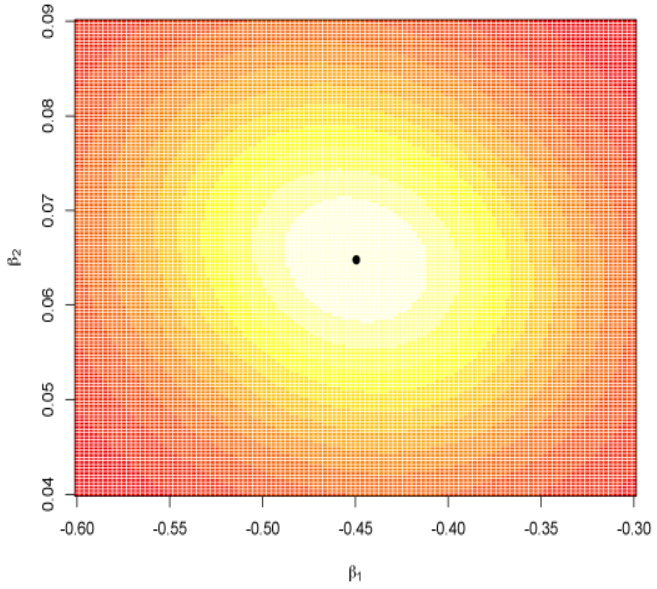
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.44957    0.09497  -4.734 2.20e-06 ***
x            0.06479    0.01615   4.011 6.05e-05 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

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

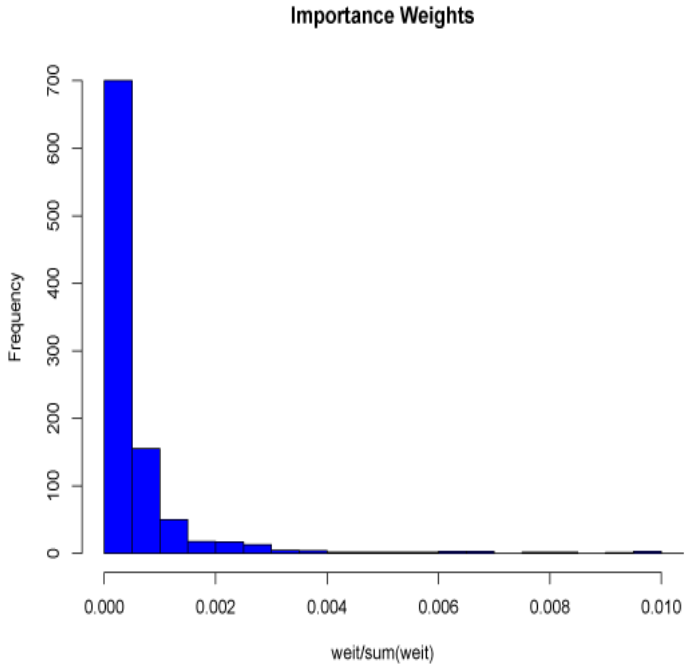
$$\prod_{i=1}^{n} [\Phi(\beta_1 + (x_i - \bar{x})\beta_2]^{y_i} [\Phi(-\beta_1 - (x_i - \bar{x})\beta_2]^{1-y_i} \times e^{-\frac{\beta_1^2+\beta_2^2}{2\times 100}}$$

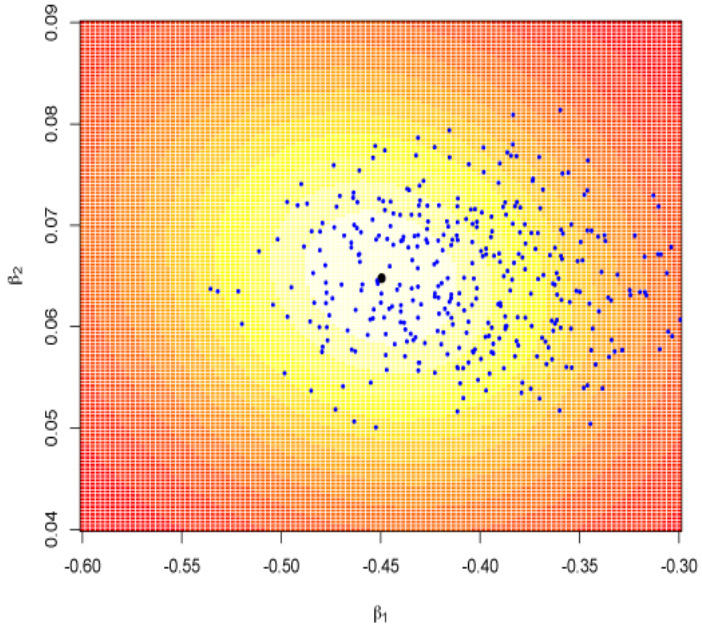


- Level curves of posterior
- MLE in the center
- R code

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.

Monte Carlo Optimization
Introduction

- Optimization problems can mostly be seen as one of two kinds:
  - Find the extrema of a function $h(\theta)$ over a domain Θ
  - Find the solution(s) to an implicit equation $g(\theta) = 0$ over a domain Θ.
- The problems are exchangeable
  - The second one is a minimization problem for a function like $h(\theta) = g^2(\theta)$
  - while the first one is equivalent to solving $\partial h(\theta)/\partial\theta = 0$
- We only focus on the maximization problem

Monte Carlo Optimization
Deterministic or Stochastic

- Similar to integration, optimization can be deterministic or stochastic
- Deterministic: performance dependent on properties of the function
  - such as convexity, boundedness, and smoothness
- Stochastic (simulation)
  - Properties of h play a lesser role in simulation-based approaches.
- Therefore, if h is complex or Θ is irregular, chose the stochastic approach.

Monte Carlo Optimization
Numerical Optimization

- R has several embedded functions to solve optimization problems
  - The simplest one is `optimize` (one dimensional)

Example: Maximizing a Cauchy likelihood $\mathcal{C}(\theta, 1)$

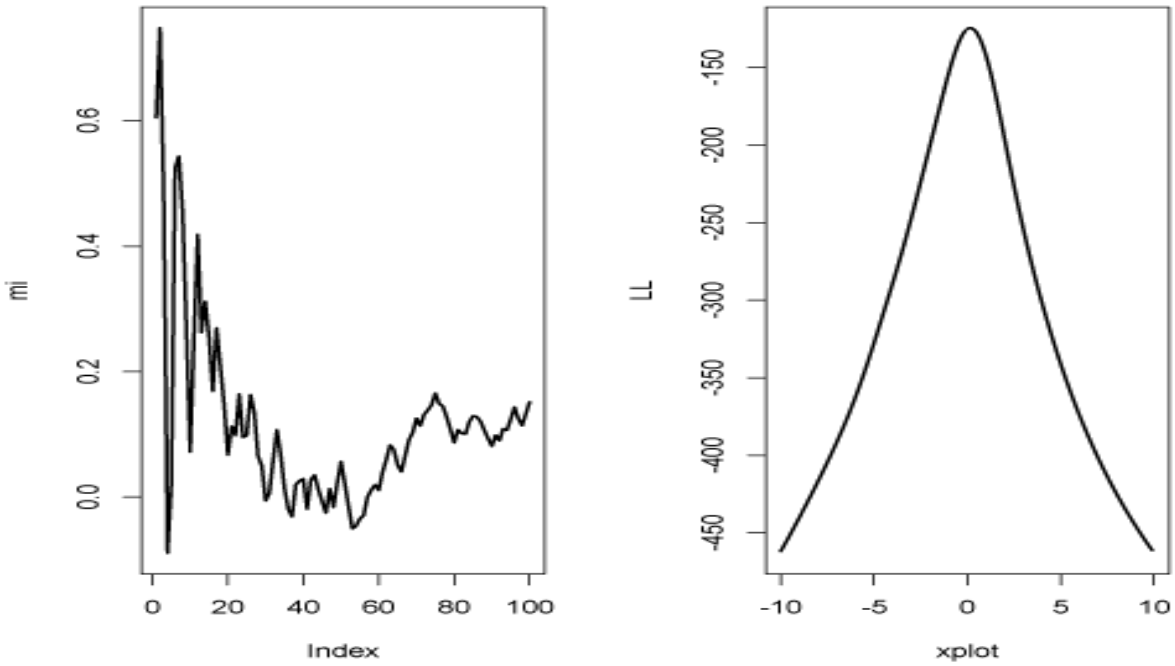
- When maximizing the likelihood of a Cauchy $\mathcal{C}(\theta, 1)$ sample,

$$\ell(\theta|x_1, \ldots, x_n) = \prod_{i=1}^{n} \frac{1}{1 + (x_i - \theta)^2},$$

- The sequence of maxima (MLEs) $\to \theta^* = 0$ when $n \to \infty$.
- But the journey is not a smooth one...

Monte Carlo Optimization

Cauchy Likelihood



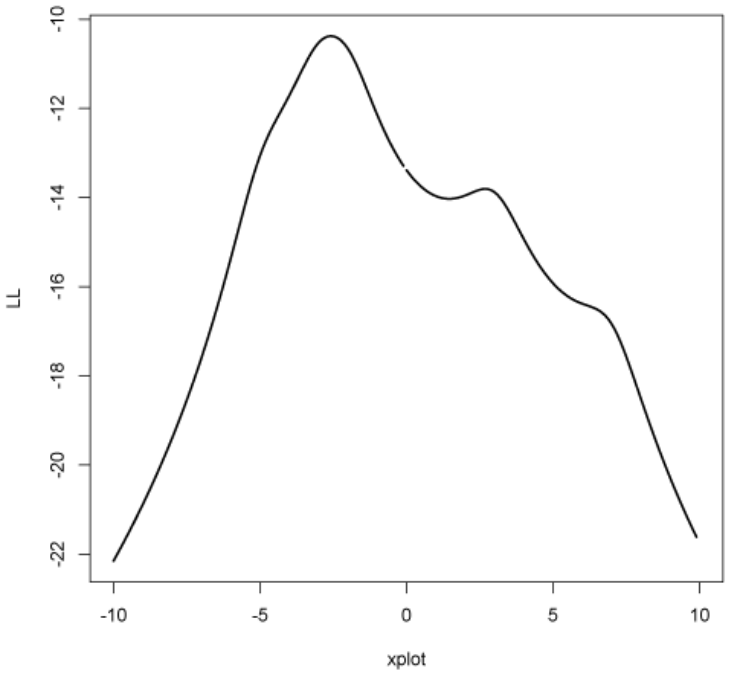
- MLEs *(left)* at each sample size, $n = 1,500$, and plot of final likelihood *(right)*.
  - Why are the MLEs so wiggly?
  - The likelihood is not as well-behaved as it seems

Monte Carlo Optimization

Cauchy Likelihood-2

- The likelihood $\ell(\theta|x_1,\ldots,x_n) = \prod_{i=1}^{n} \frac{1}{1+(x_i-\theta)^2}$

- Is like a polynomial of degree $2n$
- The derivative has $2n$ zeros
- Hard to see if $n = 500$
- Here is $n = 5$
- R code



Monte Carlo Optimization
Newton-Raphson

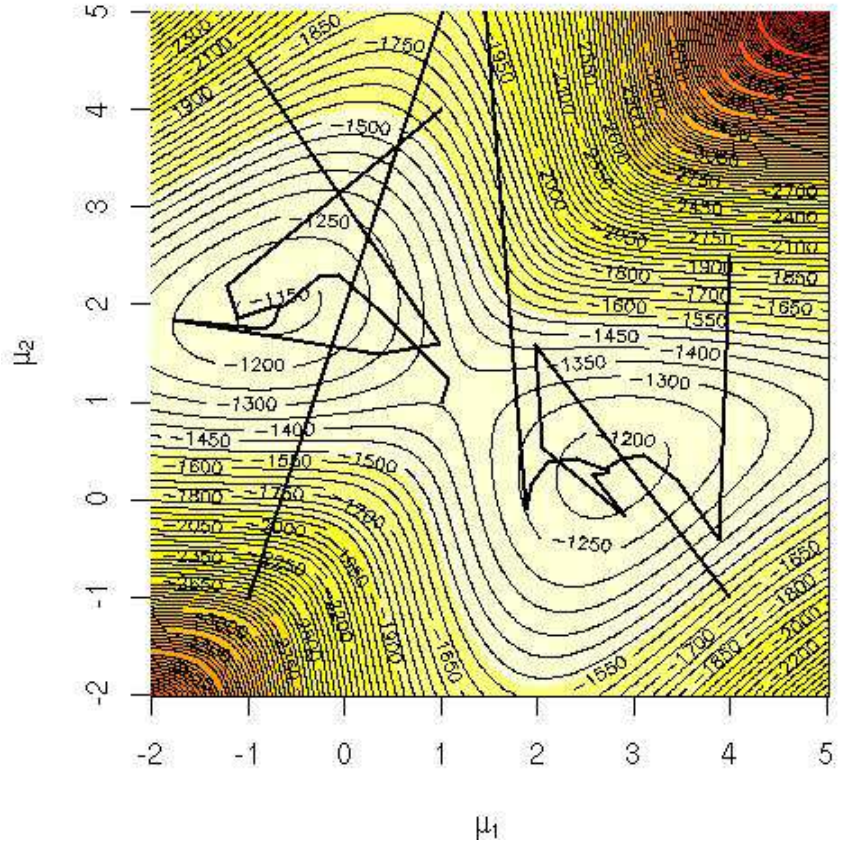
- Similarly, `nlm` is a generic `R` function using the Newton–Raphson method
- Based on the recurrence relation

$$\theta_{i+1} = \theta_i - \left[\frac{\partial^2 h}{\partial\theta\partial\theta^{\mathrm{T}}}(\theta_i)\right]^{-1} \frac{\partial h}{\partial\theta}(\theta_i)$$

- Where the matrix of the second derivatives is called the *Hessian*
  - This method is perfect when h is quadratic
    - But may also deteriorate when h is highly nonlinear
  - It also obviously depends on the starting point θ_0 when h has several minima.

Monte Carlo Optimization
Newton-Raphson; Mixture Model Likelihood

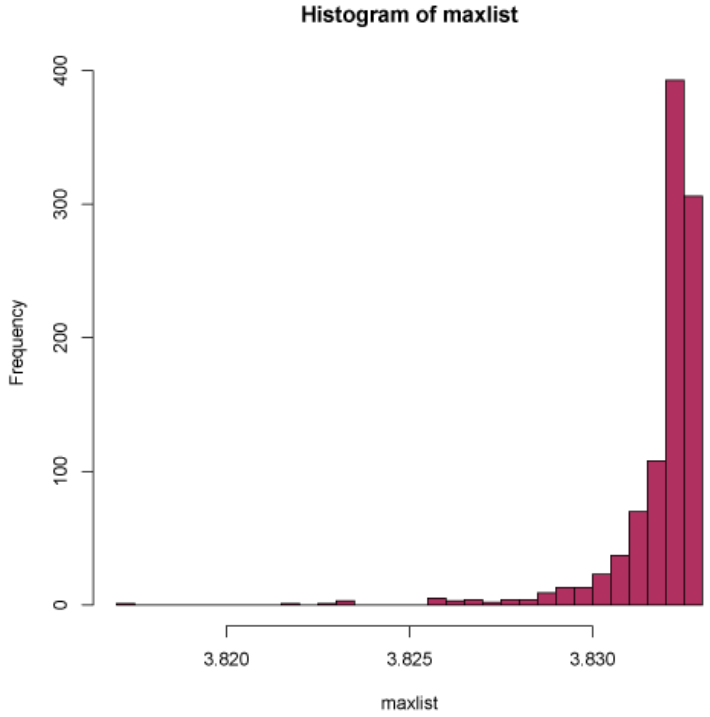
- Bimodal Mixture Model Likelihood $\frac{1}{4}\mathcal{N}(\mu_1, 1) + \frac{3}{4}\mathcal{N}(\mu_2, 1)$

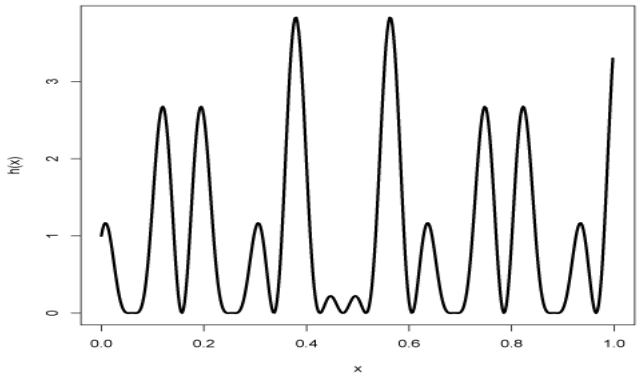


- Sequences go to the closest mode
- Starting point $(-1, -1)$ has a steep gradient
  - ▷ Bypasses the main mode $(-0.68, 1.98)$
  - ▷ Goes to other mode (lower likelihood)

Stochastic search
A Basic Solution

- A natural if rudimentary way of using simulation to find $\max_\theta h(\theta)$
  - Simulate points over Θ according to an arbitrary distribution f positive on Θ
  - Until a high value of $h(\theta)$ is observed





- Recall $h(x) = [\cos(50x) + \sin(20x)]^2$
- Max=3.8325
- Histogram of 1000 runs

Stochastic search
Stochastic Gradient Methods

- Generating direct simulations from the target can be difficult.
- Different stochastic approach to maximization
  - Explore the surface in a local manner.
  - Can use $\theta_{j+1} = \theta_j + \epsilon_j$
  - A Markov Chain
  - The random component ϵ_j can be arbitrary
- Can also use features of the function: Newton-Raphson Variation

$$\theta_{j+1} = \theta_j + \alpha_j \nabla h(\theta_j)\,, \qquad \alpha_j > 0\,,$$

  - Where $\nabla h(\theta_j)$ is the gradient
  - α_j the step size

Stochastic search
Stochastic Gradient Methods-2

- In difficult problems
  - The gradient sequence will most likely get stuck in a local extremum of h.
- Stochastic Variation

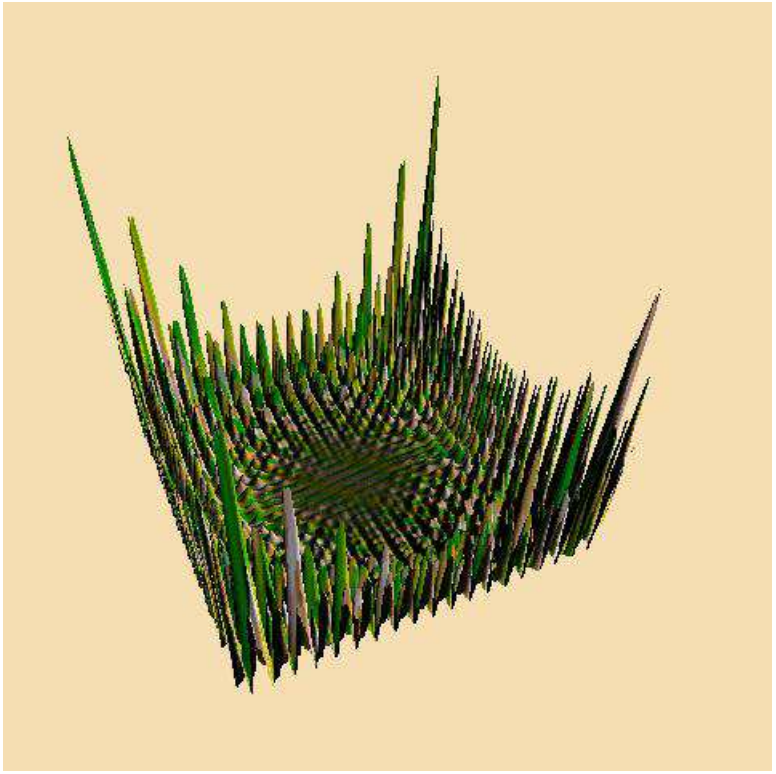
$$\nabla h(\theta_j) \approx \frac{h(\theta_j + \beta_j\zeta_j) - h(\theta_j + \beta_j\zeta_j)}{2\beta_j}\,\zeta_j = \frac{\Delta h(\theta_j, \beta_j\zeta_j)}{2\beta_j}\,\zeta_j\,,$$

  - (β_j) is a second decreasing sequence
  - ζ_j is uniform on the unit sphere $||\zeta|| = 1$.
- We then use

$$\theta_{j+1} = \theta_j + \frac{\alpha_j}{2\beta_j}\,\Delta h(\theta_j, \beta_j\zeta_j)\,\zeta_j$$

Stochastic Search

A Difficult Minimization

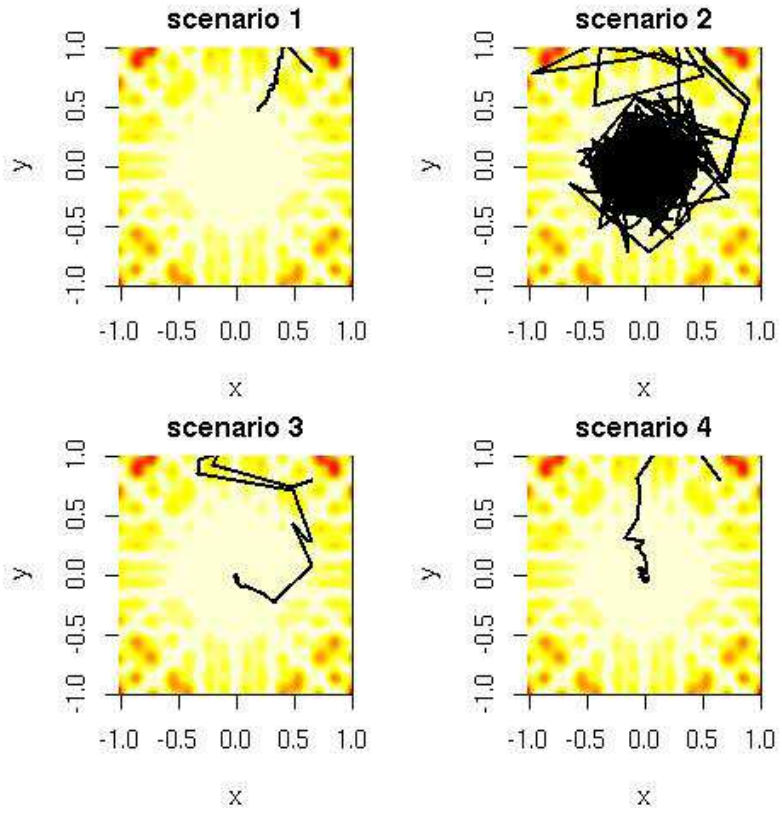


- Many Local Minima
- Global Min at $(0, 0)$
- Code in the text

Stochastic Search

A Difficult Minimization – 2

Scenario	1	2	3	4
α_j	$1/\log(j+1)$	$1/100\log(j+1)$	$1/(j+1)$	$1/(j+1)$
β_j	$1/\log(j+1)^{.1}$	$1/\log(j+1)^{.1}$	$1/(j+1)^{.5}$	$1/(j+1)^{.1}$



- $\alpha \downarrow 0$ slowly, $\sum_j \alpha_j = \infty$
- $\beta \downarrow 0$ more slowly, $\sum_j (\alpha_j/\beta_j)^2 < \infty$
- Scenarios 1-2: Not enough energy
- Scenarios 3-4: Good

Simulated Annealing
Introduction

- This name is borrowed from Metallurgy:
- A metal manufactured by a slow decrease of temperature (*annealing*)
  - Is stronger than a metal manufactured by a fast decrease of temperature.
- The fundamental idea of simulated annealing methods
  - A change of scale, or temperature
  - Allows for faster moves on the surface of the function h to maximize.
  - Rescaling partially avoids the trapping attraction of local maxima.
- As T decreases toward 0, the values simulated from this distribution become concentrated in a narrower and narrower neighborhood of the local maxima of h

Simulated Annealing

Metropolis Algorithm/Simulated Annealing

- Simulation method proposed by Metropolis *et al.* (1953)
- Starting from θ_0, ζ is generated from

$$\zeta \sim \text{Uniform in a neighborhood of } \theta_0.$$

- The new value of θ is generated as

$$\theta_1 = \begin{cases} \zeta & \text{with probability } \rho = \exp(\Delta h/T) \wedge 1 \\ \theta_0 & \text{with probability } 1-\rho, \end{cases}$$

  - $\Delta h = h(\zeta) - h(\theta_0)$
  - If $h(\zeta) \geq h(\theta_0)$, ζ is accepted
  - If $h(\zeta) < h(\theta_0)$, ζ may still be accepted
  - This allows escape from local maxima

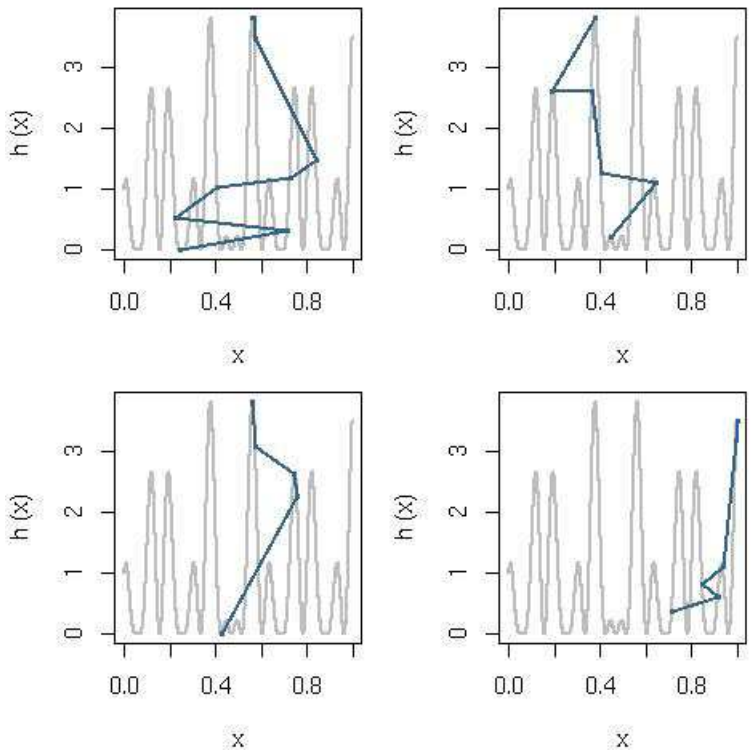
Simulated Annealing
Metropolis Algorithm - Comments

- Simulated annealing typically modifies the temperature T at each iteration
- It has the form

1. Simulate ζ from an instrumental distribution with density $g(|\zeta - \theta_i|)$;
2. Accept $\theta_{i+1} = \zeta$ with probability
$$\rho_i = \exp\{\Delta h_i / T_i\} \wedge 1;$$
take $\theta_{i+1} = \theta_i$ otherwise.
3. Update T_i to T_{i+1}.

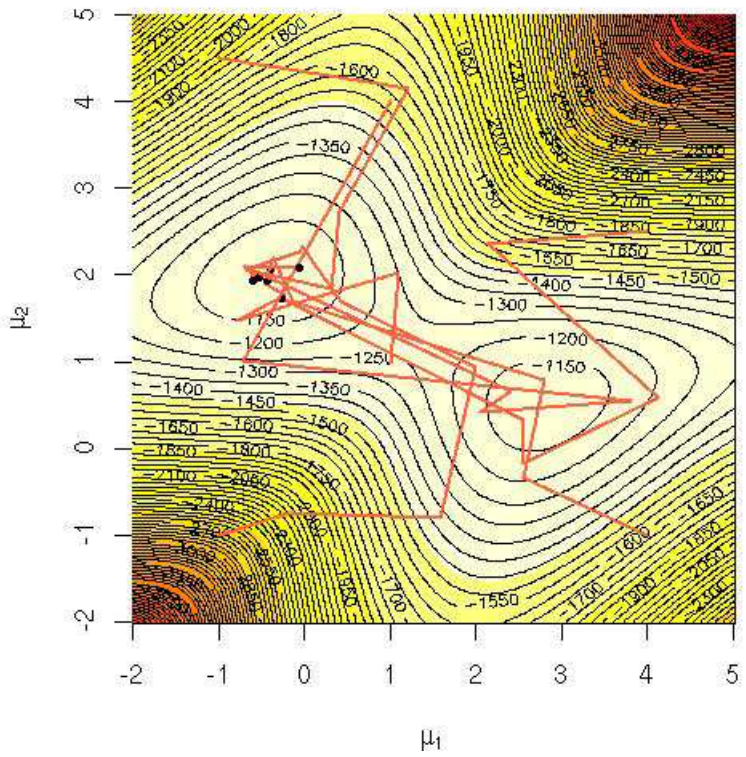
- All positive moves accepted
- As $T \downarrow 0$
  - Harder to accept downward moves
  - No big downward moves
- Not a Markov Chain - difficult to analyze

Simulated Annealing
Simple Example



- Trajectory: $T_i = \frac{1}{(1+i)^2}$
- Log trajectory also works
- Can Guarantee Finding Global Max
- R code

Simulated Annealing
Normal Mixture



- Previous normal mixture
- Most sequences find max
- They visit both modes

Stochastic Approximation
Introduction

- We now consider methods that work with the objective function h
  - Rather than being concerned with fast exploration of the domain Θ.
- Unfortunately, the use of those methods results in an additional level of error
  - Due to this approximation of h.
- But, the objective function in many statistical problems can be expressed as
  - $h(x) = \mathbb{E}[H(x, Z)]$
  - This is the setting of so-called missing-data models

Stochastic Approximation
Optimizing Monte Carlo Approximations

- If $h(x) = \mathbb{E}[H(x, Z)]$, a Monte Carlo approximation is

$$\hat{h}(x) = \frac{1}{m} \sum_{i=1}^{m} H(x, z_i),$$

  - Z_i's are generated from the conditional distribution $f(z|x)$.

- This approximation yields a convergent estimator of $h(x)$ for every value of x

  - This is a *pointwise convergent estimator*
  - Its use in optimization setups is not recommended
  - Changing sample of Z_i's $\Rightarrow$ unstable sequence of evaluations
  - And a rather noisy approximation to $\arg\max h(x)$

Stochastic Approximation
Bayesian Probit

Example: Bayesian analysis of a simple probit model

- $Y \in \{0, 1\}$ has a distribution depending on a covariate X:

$$P_\theta(Y = 1|X = x) = 1 - P_\theta(Y = 0|X = x) = \Phi(\theta_0 + \theta_1 x)\,,$$

  - Illustrate with `Pima.tr` dataset, Y= diabetes indicator, X=BMI

- Typically infer from the marginal posterior

$$\arg\max_{\theta_0} \int \prod_{i=1} \Phi(\theta_0 + \theta_1 x_n)^{y_i} \Phi(-\theta_0 - \theta_1 x_n)^{1-y_i}\, \mathrm{d}\theta_1 = \arg\max_{\theta_0} h(\theta_0)$$

  - For a flat prior on θ and a sample $(x_1, \ldots, x_n)$.

Stochastic Approximation
Bayesian Probit – Importance Sampling

- No analytic expression for h
- The conditional distribution of θ_1 given θ_0 is also nonstandard
  - Use importance sampling with a t distribution with 5 df
  - Take $\mu = 0.1$ and $\sigma = 0.03$ (MLEs)
- Importance Sampling Approximation

$$\widehat{h}_0(\theta_0) = \frac{1}{M}\sum_{m=1}^{M}\prod_{i=1}\Phi(\theta_0+\theta_1^m x_n)^{y_i}\Phi(-\theta_0-\theta_1^m x_n)^{1-y_i}\mathfrak{t}_5(\theta_1^m;\mu,\sigma)^{-1}\,,$$

Stochastic Approximation
Importance Sampling Evaluation

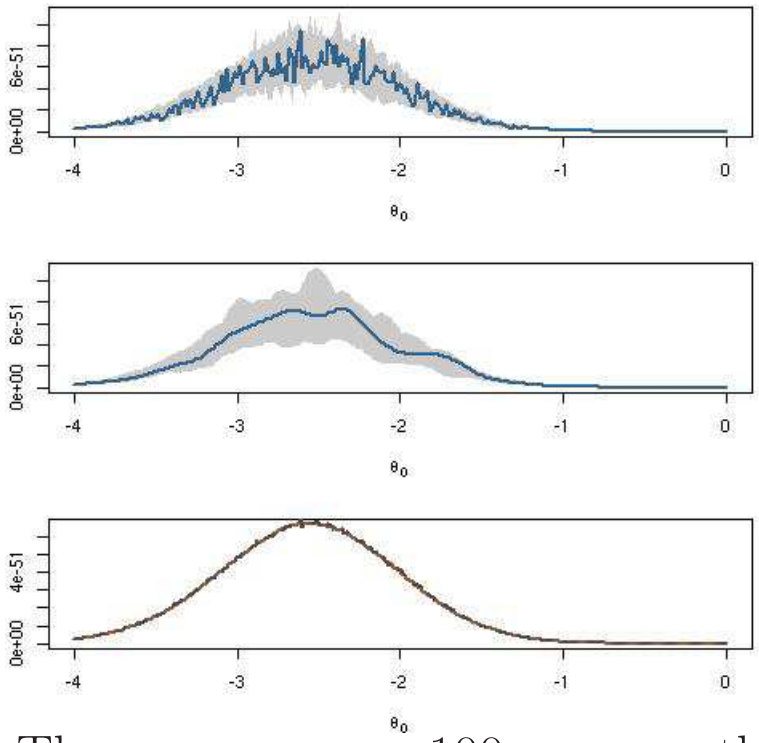
- Plotting this approximation of h with t samples simulated for each value of θ_0
  - The maximization of the represented $\widehat{h}$ function is not to be trusted as an approximation to the maximization of h.

- But, if we use the same t sample for all values of θ_0
  - We obtain a much smoother function

- We use importance sampling based on a *single* sample of Z_i's
  - Simulated from an importance function $g(z)$ for *all* values of x
  - Estimate h with

$$\hat{h}_m(x) = \frac{1}{m} \sum_{i=1}^{m} \frac{f(z_i|x)}{g(z_i)} H(x, z_i).$$

Stochastic Approximation
Importance Sampling Likelihood Representation



- Top: 100 runs, different samples
- Middle: 100 runs, same sample
- Bottom: averages over 100 runs

- The averages over 100 runs are the same - but we will not do 100 runs
- `R` code: Run `pimax(25)` from `mcsm`

Stochastic Approximation
Comments

- This approach is not absolutely fool-proof
  - The precision of $\hat{h}_m(x)$ has no reason to be independent of x
  - The number m of simulations has to reflect the most varying case.

- As in every importance sampling experiment
  - The choice of the candidate g is influential
  - In obtaining a good (or a disastrous) approximation of $h(x)$.

- Checking for the finite variance of the ratio $f(z_i|x)H(x,z_i)/g(z_i)$
  - Is a minimal requirement in the choice of g

Missing-Data Models and Demarginalization
Introduction

- Missing data models are special cases of the representation $h(x) = \mathbb{E}[H(x, Z)]$
- These are models where the density of the observations can be expressed as

$$g(x|\theta) = \int_{\mathcal{Z}} f(x, z|\theta)\, \mathrm{d}z\,.$$

- This representation occurs in many statistical settings
  - Censoring models and mixtures
  - Latent variable models (tobit, probit, arch, stochastic volatility, etc.)
  - Genetics: Missing SNP calls

Missing-Data Models and Demarginalization
Mixture Model

Example: Normal mixture model as a missing-data model

- Start with a sample $(x_1, \ldots, x_n)$
- Introduce a vector $(z_1, \ldots, z_n) \in \{1, 2\}^n$ such that

$$P_\theta(Z_i = 1) = 1 - P_\theta(Z_i = 2) = 1/4\,, \quad X_i | Z_i = z \sim \mathcal{N}(\mu_z, 1)\,,$$

- The (observed) likelihood is then obtained as $\mathbb{E}[H(\mathbf{x}, \mathbf{Z})]$ for

$$H(\mathbf{x}, \mathbf{z}) \propto \prod_{i;\, z_i=1} \frac{1}{4} \exp\left\{-(x_i - \mu_1)^2/2\right\} \prod_{i;\, z_i=2} \frac{3}{4} \exp\left\{-(x_i - \mu_2)^2/2\right\}\,,$$

- We recover the mixture model

$$\frac{1}{4}\mathcal{N}(\mu_1, 1) + \frac{3}{4}\mathcal{N}(\mu_2, 1)$$

  - As the marginal distribution of X_i.

Missing-Data Models and Demarginalization
Censored–Data Likelihood

Example: Censored–data likelihood

- Censored data may come from experiments
  - Where some potential observations are replaced with a lower bound
  - Because they take too long to observe.

- Suppose that we observe $Y_1, \ldots, Y_m$, iid, from $f(y-\theta)$
  - And the $(n-m)$ remaining $(Y_{m+1}, \ldots, Y_n)$ are censored at the threshold a.

- The corresponding likelihood function is

$$L(\theta|\mathbf{y}) = [1 - F(a-\theta)]^{n-m} \prod_{i=1}^{m} f(y_i - \theta),$$

  - F is the cdf associated with f

Missing-Data Models and Demarginalization
Recovering the Observed Data Likelihood

- If we had observed the last $n - m$ values
  - Say $\mathbf{z} = (z_{m+1}, \ldots, z_n)$, with $z_i \geq a$ $(i = m+1, \ldots, n)$,
  - We could have constructed the (complete data) likelihood

$$L^c(\theta|\mathbf{y}, \mathbf{z}) = \prod_{i=1}^{m} f(y_i - \theta) \prod_{i=m+1}^{n} f(z_i - \theta)\,.$$

- Note that

$$L(\theta|\mathbf{y}) = \mathbb{E}[L^c(\theta|\mathbf{y}, \mathbf{Z})] = \int_{\mathcal{Z}} L^c(\theta|\mathbf{y}, \mathbf{z}) k(\mathbf{z}|\mathbf{y}, \theta)\, \mathrm{d}\mathbf{z},$$

  - Where $k(\mathbf{z}|\mathbf{y}, \theta)$ is the density of the missing data
  - Conditional on the observed data
  - The product of the $f(z_i - \theta)/[1 - F(a - \theta)]$'s
  - $f(z - \theta)$ restricted to $(a, +\infty)$.

Missing-Data Models and Demarginalization
Comments

- When we have the relationship
$$g(x|\theta) = \int_{\mathcal{Z}} f(x, z|\theta)\, \mathrm{d}z\,.$$
  - ▷ $\mathbf{Z}$ merely serves to simplify calculations
  - ▷ it does not necessarily have a specific meaning
- We have the complete-data likelihood $L^c(\theta|\mathbf{x}, \mathbf{z})) = f(\mathbf{x}, \mathbf{z}|\theta)$
  - ▷ The likelihood we would obtain
  - ▷ Were we to observe $(\mathbf{x}, \mathbf{z})$,the complete data
- REMEMBER:
$$g(x|\theta) = \int_{\mathcal{Z}} f(x, z|\theta)\, \mathrm{d}z\,.$$

The EM Algorithm
Introduction

- The EM algorithm is a deterministic optimization technique
  - Dempster, Laird and Rubin 1977
- Takes advantage of the missing data representation
  - Builds a sequence of easier maximization problems
  - Whose limit is the answer to the original problem

- We assume that we observe $X_1, \ldots, X_n \sim g(\mathbf{x}|\theta)$ that satisfies

$$g(\mathbf{x}|\theta) = \int_{\mathcal{Z}} f(\mathbf{x}, \mathbf{z}|\theta)\, \mathrm{d}\mathbf{z},$$

  - And we want to compute $\hat{\theta} = \arg\max L(\theta|\mathbf{x}) = \arg\max g(\mathbf{x}|\theta)$.

The EM Algorithm
First Details

- With the relationship $g(\mathbf{x}|\theta) = \int_{\mathcal{Z}} f(\mathbf{x}, \mathbf{z}|\theta)\, \mathrm{d}\mathbf{z}$,
  - $(\mathbf{X}, \mathbf{Z}) \sim f(\mathbf{x}, \mathbf{z}|\theta)$
- The conditional distribution of the missing data $\mathbf{Z}$
  - Given the observed data $\mathbf{x}$ is

$$k(\mathbf{z}|\theta, \mathbf{x}) = f(\mathbf{x}, \mathbf{z}|\theta) \big/ g(\mathbf{x}|\theta)\,.$$

- Taking the logarithm of this expression leads to the following relationship

$$\underbrace{\log L(\theta|\mathbf{x})}_{\text{Obs. Data}} = \underbrace{\mathbb{E}_{\theta_0}[\log L^c(\theta|\mathbf{x}, \mathbf{Z})]}_{\text{Complete Data}} - \underbrace{\mathbb{E}_{\theta_0}[\log k(\mathbf{Z}|\theta, \mathbf{x})]}_{\text{Missing Data}},$$

- Where the expectation is with respect to $k(\mathbf{z}|\theta_0, \mathbf{x})$.
- In maximizing $\log L(\theta|\mathbf{x})$, we can ignore the last term

The EM Algorithm
Iterations

- Denoting
$$Q(\theta|\theta_0, \mathbf{x}) = \mathbb{E}_{\theta_0}[\log L^c(\theta|\mathbf{x}, \mathbf{Z})],$$
- EM algorithm indeed proceeds by maximizing $Q(\theta|\theta_0, \mathbf{x})$ at each iteration
  - If $\hat{\theta}_{(1)} = \text{argmax}Q(\theta|\theta_0, \mathbf{x})$, $\hat{\theta}_{(0)} \to \hat{\theta}_{(1)}$
- Sequence of estimators $\{\hat{\theta}_{(j)}\}$, where
$$\hat{\theta}_{(j)} = \text{argmax}Q(\theta|\hat{\theta}_{(j-1)})$$
- This iterative scheme
  - Contains both an expectation step
  - And a maximization step
  - Giving the algorithm its name.

The EM Algorithm

The Algorithm

Pick a starting value $\hat{\theta}_{(0)}$ and set $m = 0$.

Repeat

1. Compute (*the E-step*)

$$Q(\theta|\hat{\theta}_{(m)}, \mathbf{x}) = \mathbb{E}_{\hat{\theta}_{(m)}}[\log L^c(\theta|\mathbf{x}, \mathbf{Z})]\,,$$

where the expectation is with respect to $k(\mathbf{z}|\hat{\theta}_{(m)}, \mathbf{x})$.

2. Maximize $Q(\theta|\hat{\theta}_{(m)}, \mathbf{x})$ in θ and take (*the M-step*)

$$\hat{\theta}_{(m+1)} = \arg\max_{\theta} Q(\theta|\hat{\theta}_{(m)}, \mathbf{x})$$

and set $m = m + 1$

until a fixed point is reached; i.e., $\hat{\theta}_{(m+1)} = \hat{\theta}_{(m)}$.fixed point

The EM Algorithm
Properties

- Jensen's inequality $\Rightarrow$ The likelihood increases at each step of the EM algorithm

$$L(\hat{\theta}_{(j+1)}|\mathbf{x}) \geq L(\hat{\theta}_{(j)}|\mathbf{x}),$$

  - ▷ Equality holding if and only if $Q(\hat{\theta}_{(j+1)}|\hat{\theta}_{(j)}, \mathbf{x}) = Q(\hat{\theta}_{(j)}|\hat{\theta}_{(j)}, \mathbf{x})$.

- Every limit point of an EM sequence $\{\hat{\theta}_{(j)}\}$ is a stationary point of $L(\theta|\mathbf{x})$
  - ▷ Not necessarily the maximum likelihood estimator
  - ▷ In practice, we run EM several times with different starting points.

- Implementing the EM algorithm thus means being able to

  (a) Compute the function $Q(\theta'|\theta, \mathbf{x})$

  (b) Maximize this function.

The EM Algorithm
Censored Data Example

- The complete-data likelihood is

$$L^c(\theta|\mathbf{y},\mathbf{z}) \propto \prod_{i=1}^{m} \exp\{-(y_i-\theta)^2/2\} \prod_{i=m+1}^{n} \exp\{-(z_i-\theta)^2/2\}\,,$$

- With expected complete-data log-likelihood

$$Q(\theta|\theta_0,\mathbf{y}) = -\frac{1}{2}\sum_{i=1}^{m}(y_i-\theta)^2 - \frac{1}{2}\sum_{i=m+1}^{n}\mathbb{E}_{\theta_0}[(Z_i-\theta)^2]\,,$$

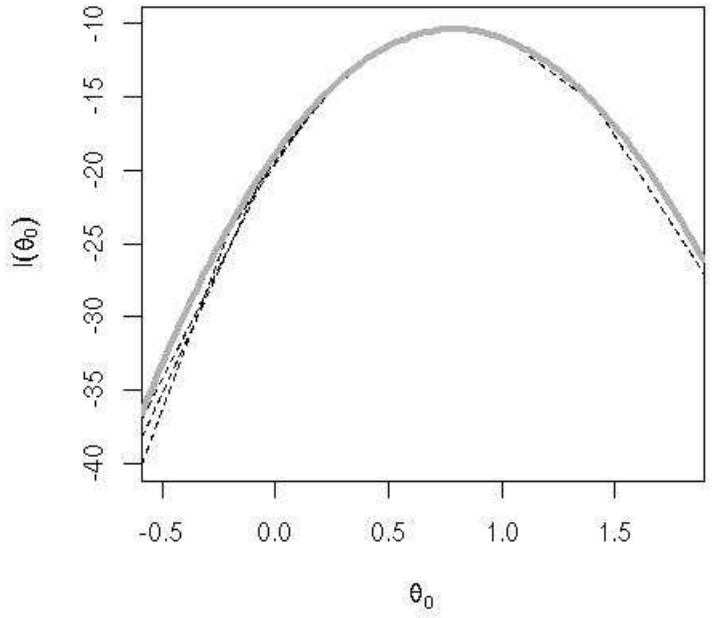
  ▷ the Z_i are distributed from a normal $\mathcal{N}(\theta,1)$ distribution truncated at a.

- M-step (differentiating $Q(\theta|\theta_0,\mathbf{y})$ in θ and setting it equal to 0 gives

$$\hat{\theta} = \frac{m\bar{y} + (n-m)\mathbb{E}_{\theta'}[Z_1]}{n}.$$

  ▷ With $\mathbb{E}_\theta[Z_1] = \theta + \frac{\varphi(a-\theta)}{1-\Phi(a-\theta)}$,

The EM Algorithm
Censored Data MLEs



- EM sequence

$$\hat{\theta}^{(j+1)} = \frac{m}{n}\bar{y} + \frac{n-m}{n}\left[\hat{\theta}^{(j)} + \frac{\varphi(a-\hat{\theta}^{(j)})}{1-\Phi(a-\hat{\theta}^{(j)})}\right]$$

- Climbing the Likelihood
- R code

The EM Algorithm

Normal Mixture

▶ Normal Mixture Bimodal Likelihood

$$Q(\theta'|\theta,\mathbf{x}) = -\frac{1}{2}\sum_{i=1}^{n}\mathbb{E}_\theta\left[Z_i(x_i-\mu_1)^2 + (1-Z_i)(x_i-\mu_2)^2\Big|\,\mathbf{x}\right].$$

Solving the M-step then provides the closed-form expressions

$$\mu_1' = \mathbb{E}_\theta\left[\sum_{i=1}^{n} Z_i x_i|\mathbf{x}\right] \Big/ \mathbb{E}_\theta\left[\sum_{i=1}^{n} Z_i|\mathbf{x}\right]$$

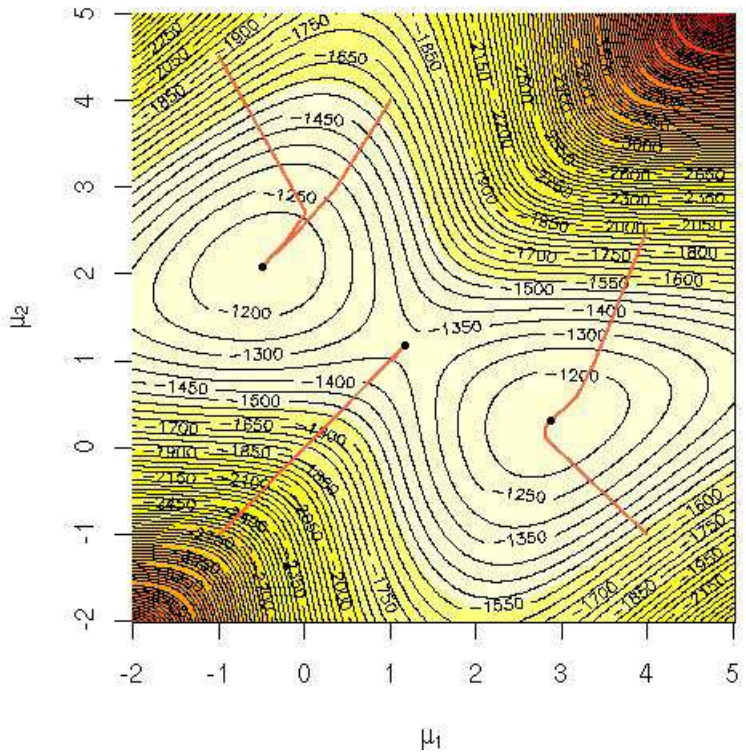
and

$$\mu_2' = \mathbb{E}_\theta\left[\sum_{i=1}^{n}(1-Z_i) x_i|\mathbf{x}\right] \Big/ \mathbb{E}_\theta\left[\sum_{i=1}^{n}(1-Z_i)|\mathbf{x}\right].$$

Since

$$\mathbb{E}_\theta\left[Z_i|\mathbf{x}\right] = \frac{\varphi(x_i-\mu_1)}{\varphi(x_i-\mu_1)+3\varphi(x_i-\mu_2)},$$

The EM Algorithm
Normal Mixture MLEs



- EM five times with various starting points
- Two out of five sequences → higher mode
- Others → lower mode

Monte Carlo EM
Introduction

- If computation $Q(\theta|\theta_0, \mathbf{x})$ is difficult, can use Monte Carlo
- For $\mathbf{Z}_1, \ldots, \mathbf{Z}_T \sim k(\mathbf{z}|\mathbf{x}, \hat{\theta}_{(m)})$, maximize

$$\hat{Q}(\theta|\theta_0, \mathbf{x}) = \frac{1}{T}\sum_{i=1}^{T} \log L^c(\theta|\mathbf{x}, \mathbf{z}_i)$$

- Better: Use importance sampling
  - Since

$$\arg\max_\theta L(\theta|\mathbf{x}) = \arg\max_\theta \log \frac{g(\mathbf{x}|\theta)}{g(\mathbf{x}|\theta_{(0)})} = \arg\max_\theta \log \mathbb{E}_{\theta_{(0)}}\left[\frac{f(\mathbf{x}, \mathbf{z}|\theta)}{f(\mathbf{x}, \mathbf{z}|\theta_{(0)})}\middle| \mathbf{x}\right],$$

  - Use the approximation to the log-likelihood

$$\log L(\theta|\mathbf{x}) \approx \frac{1}{T}\sum_{i=1}^{T} \frac{L^c(\theta|\mathbf{x}, \mathbf{z}_i)}{L^c(\theta_{(0)}|\mathbf{x}, \mathbf{z}_i)},$$

Monte Carlo EM
Genetics Data

Example: Genetic linkage.

- A classic example of the EM algorithm
- Observations (x_1, x_2, x_3, x_4) are gathered from the multinomial distribution

$$\mathcal{M}\left(n; \frac{1}{2} + \frac{\theta}{4}, \frac{1}{4}(1-\theta), \frac{1}{4}(1-\theta), \frac{\theta}{4}\right).$$

- Estimation is easier if the x_1 cell is split into two cells
  - We create the augmented model

$$(z_1, z_2, x_2, x_3, x_4) \sim \mathcal{M}\left(n; \frac{1}{2}, \frac{\theta}{4}, \frac{1}{4}(1-\theta), \frac{1}{4}(1-\theta), \frac{\theta}{4}\right)$$

  with $x_1 = z_1 + z_2$.

  - Complete-data likelihood: $\theta^{z_2+x_4}(1-\theta)^{x_2+x_3}$
  - Observed-data likelihood: $(2+\theta)^{x_1}\theta^{x_4}(1-\theta)^{x_2+x_3}$

Monte Carlo EM
Genetics Linkage Calculations

- The expected complete log-likelihood function is

$$\mathbb{E}_{\theta_0}[(Z_2 + x_4)\log\theta + (x_2 + x_3)\log(1-\theta)] = \left(\frac{\theta_0}{2+\theta_0}x_1 + x_4\right)\log\theta + (x_2 + x_3)\log(1-\theta),$$

  - which can easily be maximized in θ, leading to the EM step

$$\hat{\theta}_1 = \left\{\frac{\theta_0\, x_1}{2+\theta_0}\right\} \Big/ \left\{\frac{\theta_0\, x_1}{2+\theta_0} + x_2 + x_3 + x_4\right\}.$$

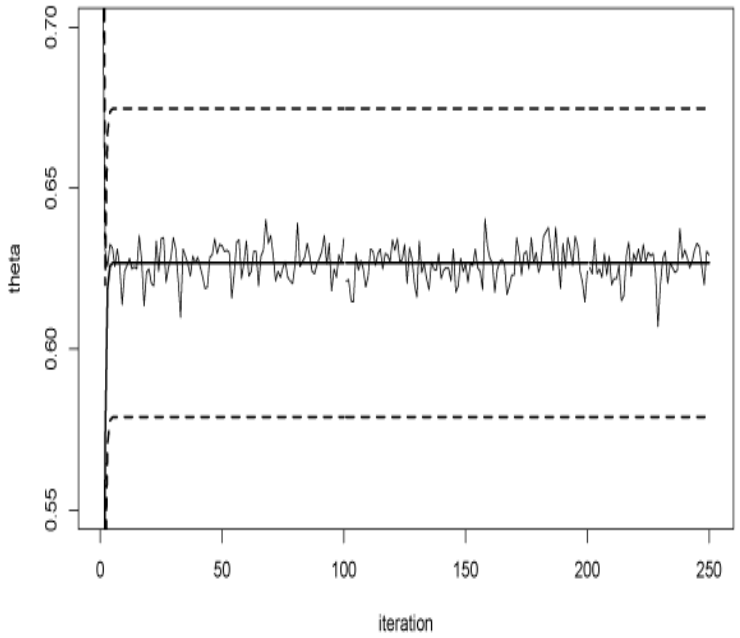
- Monte Carlo EM: Replace the expectation with
  - $\overline{z}_m = \frac{1}{m}\sum_{i=1}^{m} z_i$, $z_i \sim \mathcal{B}(x_1, \theta_0/(2+\theta_0))$

- The MCEM step would then be

$$\widehat{\widehat{\theta}}_1 = \frac{\overline{z}_m}{\overline{z}_m + x_2 + x_3 + x_4},$$

  which converges to $\hat{\theta}_1$ as m grows to infinity.

Monte Carlo EM
Genetics Linkage MLEs



- Note variation in MCEM sequence
- Can control with ↑ simulations
- R code

Monte Carlo EM
Random effect logit model

Example: Random effect logit model

- Random effect logit model,
  - y_{ij} is distributed conditionally on one covariate x_{ij} as a logit model

$$P(y_{ij} = 1|x_{ij}, u_i, \beta) = \frac{\exp\{\beta x_{ij} + u_i\}}{1 + \exp\{\beta x_{ij} + u_i\}},$$

  - $u_i \sim \mathcal{N}(0, \sigma^2)$ is an unobserved random effect.
  - $(U_1, \ldots, U_n)$ therefore corresponds to the missing data $\mathbf{Z}$

Monte Carlo EM
Random effect logit model likelihood

- For the complete data likelihood with $\theta = (\beta, \sigma)$,

$$\begin{aligned} Q(\theta'|\theta, \mathbf{x}, \mathbf{y}) = &\sum_{i,j} y_{ij} \mathbb{E}[\beta' x_{ij} + U_i | \beta, \sigma, \mathbf{x}, \mathbf{y}] \\ &- \sum_{i,j} \mathbb{E}[\log 1 + \exp\{\beta' x_{ij} + U_i\} | \beta, \sigma, \mathbf{x}, \mathbf{y}] \\ &- \sum_{i} \mathbb{E}[U_i^2 | \beta, \sigma, \mathbf{x}, \mathbf{y}]/2\sigma'^2 - n \log \sigma' \,, \end{aligned}$$

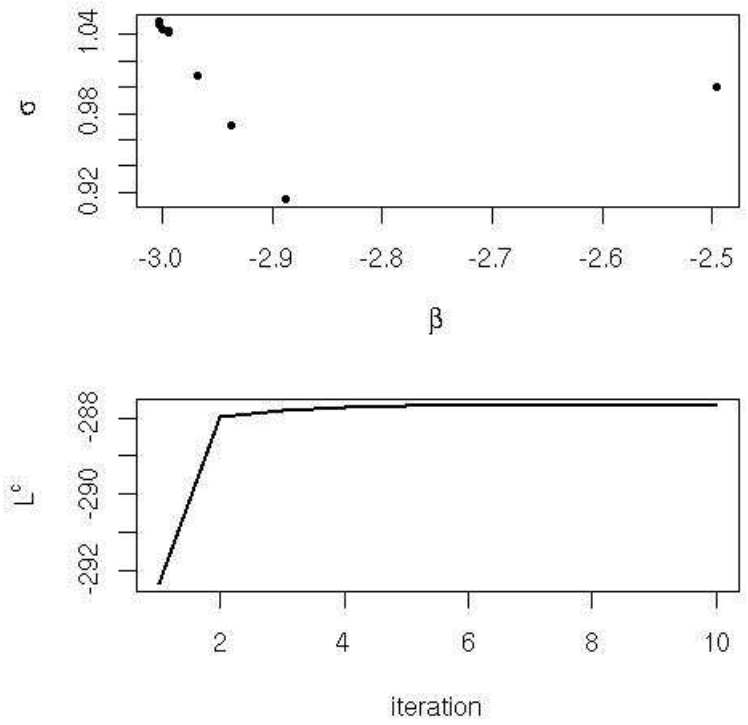
  - ▷ it is impossible to compute the expectations in U_i.

- Were those available, the M-step would be difficult but feasible

- MCEM: Simulate the U_i's conditional on $\beta, \sigma, \mathbf{x}, \mathbf{y}$ from

$$\pi(u_i|\beta, \sigma, \mathbf{x}, \mathbf{y}) \propto \frac{\exp\left\{\sum_j y_{ij} u_i - u_i^2/2\sigma^2\right\}}{\prod_j \left[1 + \exp\left\{\beta x_{ij} + u_i\right\}\right]}$$

Monte Carlo EM
Random effect logit MLEs



- Top: Sequence of β's from the MCEM algorithm
- Bottom: Sequence of completed likelihoods

- MCEM sequence
  - Increases the number of Monte Carlo steps at each iteration
- MCEM algorithm
  - Does not have EM monotonicity property

Chapter 6: Metropolis–Hastings Algorithms

"How absurdly simple!", I cried.
"Quite so!", said he, a little nettled. "Every problem becomes very childish when once it is explained to you."

Arthur Conan Doyle
The Adventure of the Dancing Men

This Chapter

- The first of a of two on simulation methods based on *Markov chains*
- The Metropolis–Hastings algorithm is one of the most general MCMC algorithms
  - And one of the simplest.
- There is a quick refresher on Markov chains, just the basics.
- We focus on the most common versions of the Metropolis–Hastings algorithm.
- We also look at calibration of the algorithm via its acceptance rate

Metropolis–Hastings Algorithms
Introduction

- We now make a fundamental shift in the choice of our simulation strategy.
  - Up to now we have typically generated *iid* variables
  - The Metropolis–Hastings algorithm generates *correlated* variables
    - From a Markov chain

- The use of Markov chains broadens our scope of applications
  - The requirements on the target f are quite minimal
  - Efficient decompositions of high-dimensional problems
    - Into a sequence of smaller problems.

- This has been part of a Paradigm Shift in Statistics

Metropolis–Hastings Algorithms
A Peek at Markov Chain Theory

- A minimalist refresher on Markov chains
- Basically to define terms
- See Robert and Casella (2004, Chapter 6) for more of the story

- A Markov chain $\{X^{(t)}\}$ is a sequence of dependent random variables
$$X^{(0)}, X^{(1)}, X^{(2)}, \ldots, X^{(t)}, \ldots$$
where the probability distribution of $X^{(t)}$ depends only on $X^{(t-1)}$.
- The conditional distribution of $X^{(t)}|X^{(t-1)}$ is a *transition kernel* K,
$$X^{(t+1)} \mid X^{(0)}, X^{(1)}, X^{(2)}, \ldots, X^{(t)} \sim K(X^{(t)}, X^{(t+1)}) .$$

Markov Chains
Basics

- For example, a simple *random walk* Markov chain satisfies

$$X^{(t+1)} = X^{(t)} + \epsilon_t\,, \qquad \epsilon_t \sim \mathcal{N}(0,1)\,,$$

  - The Markov kernel $K(X^{(t)}, X^{(t+1)})$ corresponds to a $\mathcal{N}(X^{(t)}, 1)$ density.

- Markov chain Monte Carlo (MCMC) Markov chains typically have a very strong stability property.

- They have a a *stationary probability distribution*

  - A *probability distribution* f such that if $X^{(t)} \sim f$, then $X^{(t+1)} \sim f$, so we have the equation

$$\int_{\mathcal{X}} K(x,y) f(x) \mathrm{d}x = f(y).$$

Markov Chains
Properties

- MCMC Markov chains are also *irreducible*, or else they are useless
  - The kernel K allows for free moves all over the state-space
  - For any $X^{(0)}$, the sequence $\{X^{(t)}\}$ has a positive probability of eventually reaching any region of the state-space
- MCMC Markov chains are also *recurrent*, or else they are useless
  - They will return to any arbitrary nonnegligible set an infinite number of times

Markov Chains
AR(1) Process

- AR(1) models provide a simple illustration of continuous Markov chains
- Here
$$X_n = \theta X_{n-1} + \varepsilon_n \ , \qquad \theta \in \Re,$$
with $\varepsilon_n \sim N(0, \sigma^2)$
- If the ε_n's are independent
  - X_n is independent from $X_{n-2}, X_{n-3}, \ldots$ conditionally on X_{n-1}.
- The stationary distribution $\phi(x|\mu, \tau^2)$ is
$$\mathcal{N}\left(0, \frac{\sigma^2}{1-\theta^2}\right),$$
  - which requires $|\theta| < 1$.

Markov Chains
Statistical Language

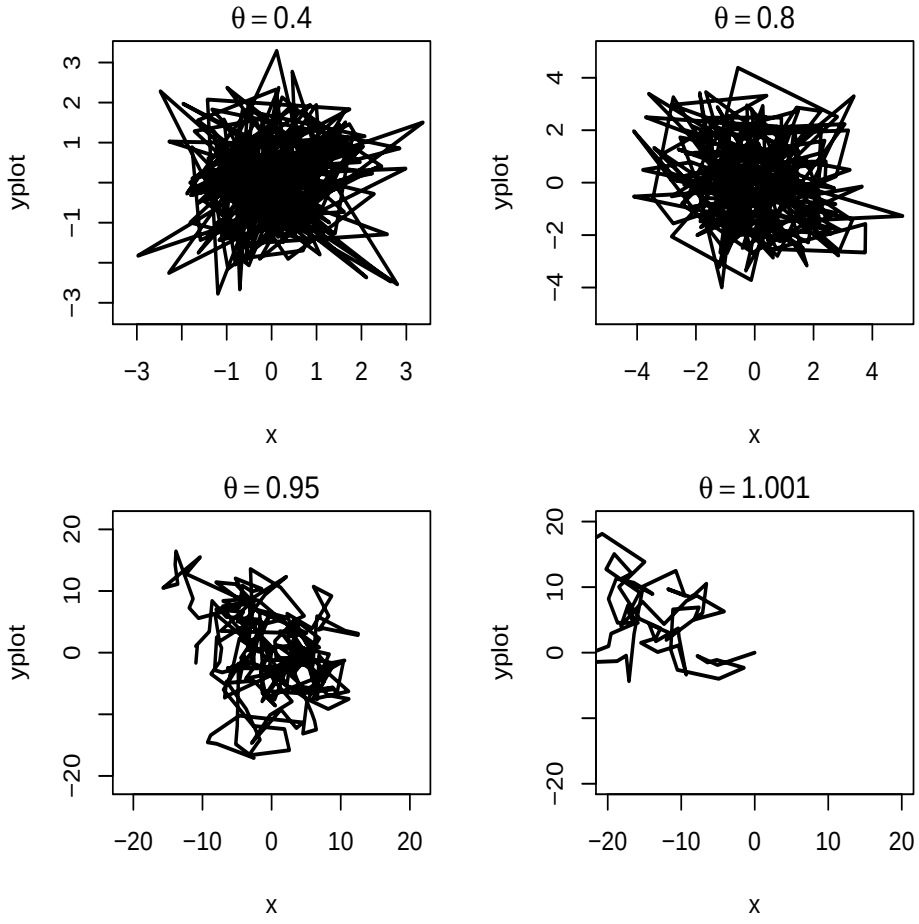
- We associate the probabilistic language of Markov chains
  - ▷ With the statistical language of data analysis.

Statistics		Markov Chain
marginal distribution	$\Leftrightarrow$	invariant distribution
proper marginals	$\Leftrightarrow$	positive recurrent

- If the marginals are not proper, or if they do not exist
  - ▷ Then the chain is not positive recurrent.
  - ▷ It is either null recurrent or transient, and both are bad.

Markov Chains
Pictures of the AR(1) Process

- AR(1) Recurrent and Transient -Note the Scale



- R code

Markov Chains
Ergodicity

- In recurrent chains, the stationary distribution is also a *limiting distribution*
- If f is the limiting distribution

$$X^{(t)} \to X \sim f, \text{ for any initial value } X^{(0)}$$

  - This property is also called *ergodicity*

- For integrable functions h, the standard average

$$\frac{1}{T}\sum_{t=1}^{T} h(X^{(t)}) \longrightarrow \mathbb{E}_f[h(X)]\,,$$

  - The Law of Large Numbers
  - Sometimes called the *Ergodic Theorem*

Markov Chains
In Bayesian Analysis

- There is one case where convergence never occurs
- When, in a Bayesian analysis, the posterior distribution is not proper
- The use of improper priors $f(x)$ is quite common in complex models,
  - ▷ Sometimes the posterior is proper, and MCMC works (recurrent)
  - ▷ Sometimes the posterior is improper, and MCMC fails (transient)
- These transient Markov chains may present all the outer signs of stability
  - ▷ More later

Basic Metropolis–Hastings algorithms
Introduction

- The working principle of Markov chain Monte Carlo methods is straightforward
- Given a target density f
  - We build a Markov kernel K with stationary distribution f
  - Then generate a Markov chain $(X^{(t)}) \to X \sim f$
  - Integrals can be approximated by to the Ergodic Theorem
- The Metropolis–Hastings algorithm is an example of those methods.
  - Given the target density f, we simulate from a candidate $q(y|x)$
  - Only need that the ratio $f(y)/q(y|x)$ is known up to a constant

Basic Metropolis–Hastings algorithms
A First Metropolis–Hastings Algorithm

Metropolis–Hastings **Given** $x^{(t)}$,

1. **Generate** $Y_t \sim q(y|x^{(t)})$.
2. **Take**

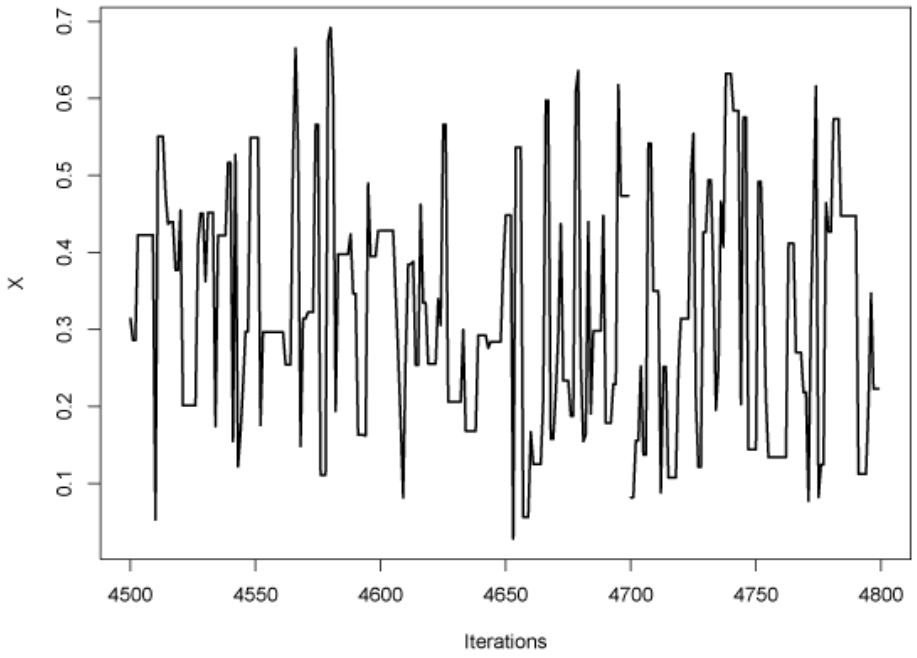
$$X^{(t+1)} = \begin{cases} Y_t & \text{with probability } \rho(x^{(t)}, Y_t), \\ x^{(t)} & \text{with probability } 1 - \rho(x^{(t)}, Y_t), \end{cases}$$

where

$$\rho(x, y) = \min\left\{ \frac{f(y)}{f(x)} \frac{q(x|y)}{q(y|x)}, 1 \right\}.$$

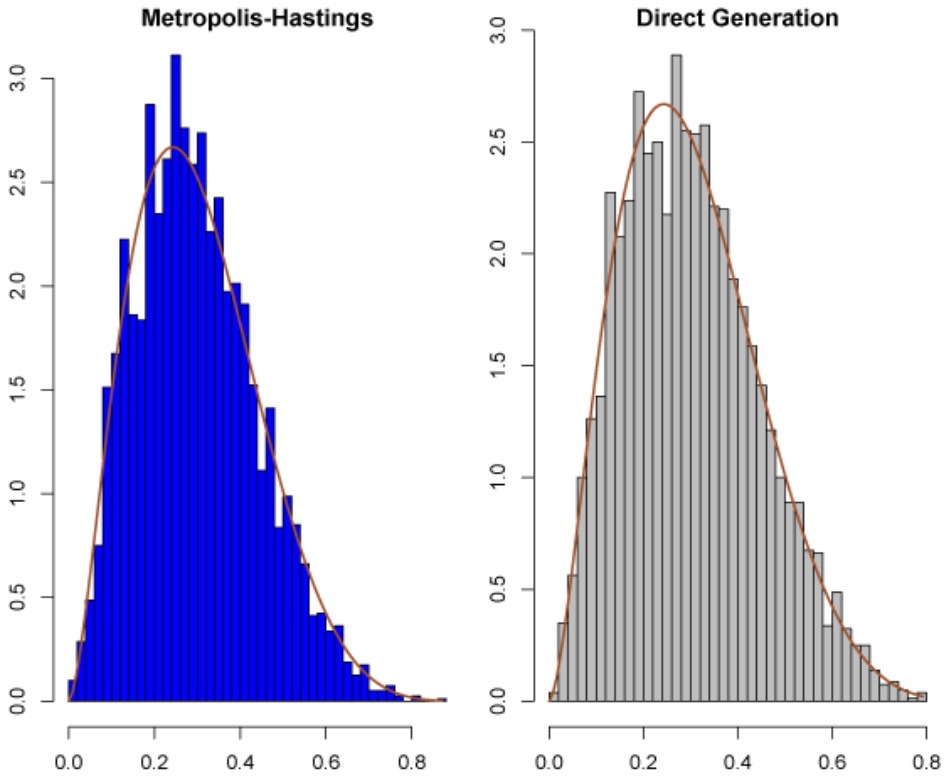
- q is called the instrumental or proposal or candidate distribution
- $\rho(x, y)$ is the Metropolis–Hastings acceptance probability
- Looks like Simulated Annealing - but constant temperature
  - ▷ Metropolis–Hastings explores rather than maximizes

Basic Metropolis–Hastings algorithms
Generating Beta Random Variables



- Target density f is the $\mathcal{B}e(2.7, 6.3)$
- Candidate q is uniform
- Notice the repeats
- Repeats must be kept!

Basic Metropolis–Hastings algorithms
Comparing Beta densities



- Comparison with independent sampling
- Histograms indistinguishable
  - Moments match
  - K-S test accepts
- R code

Basic Metropolis–Hastings algorithms
A Caution

- The MCMC and exact sampling outcomes look identical, but
  - Markov chain Monte Carlo sample has correlation, the iid sample does not
  - This means that the quality of the sample is necessarily degraded
  - We need more simulations to achieve the same precision
- This is formalized by the *effective sample size* for Markov chains - later

Basic Metropolis–Hastings algorithms
Some Comments

- In the symmetric case $q(x|y) = q(y|x)$,

$$\rho(x_t, y_t) = \min\left\{\frac{f(y_t)}{f(x_t)}\,, 1\right\}\,.$$

  - The acceptance probability is independent of q

- Metropolis–Hastings always accept values of y_t such that

$$f(y_t)/q(y_t|x^{(t)}) > f(x^{(t)})/q(x^{(t)}|y_t)$$

- Values y_t that decrease the ratio may also be accepted

- Metropolis–Hastings only depends on the ratios

$$f(y_t)/f(x^{(t)}) \qquad \text{and} \qquad q(x^{(t)}|y_t)/q(y_t|x^{(t)})\,.$$

  - Independent of normalizing constants

Basic Metropolis–Hastings algorithms
The Independent Metropolis–Hastings algorithm

- The Metropolis–Hastings algorithm allows $q(y|x)$
  - We can use $q(y|x) = g(y)$, a special case

Independent Metropolis–Hastings

Given $x^{(t)}$

1. Generate $Y_t \sim g(y)$.
2. Take

$$X^{(t+1)} = \begin{cases} Y_t & \text{with probability } \min\left\{\dfrac{f(Y_t)\, g(x^{(t)})}{f(x^{(t)})\, g(Y_t)}, 1\right\} \\ x^{(t)} & \text{otherwise.} \end{cases}$$

Basic Metropolis–Hastings algorithms
Properties of the Independent Metropolis–Hastings algorithm

- Straightforward generalization of the Accept–Reject method
- Candidates are independent, but still a Markov chain
  - The Accept–Reject sample is iid, but the Metropolis–Hastings sample is not
  - The Accept–Reject acceptance step requires calculating M
  - Metropolis–Hastings is Accept–Reject "for the lazy person"

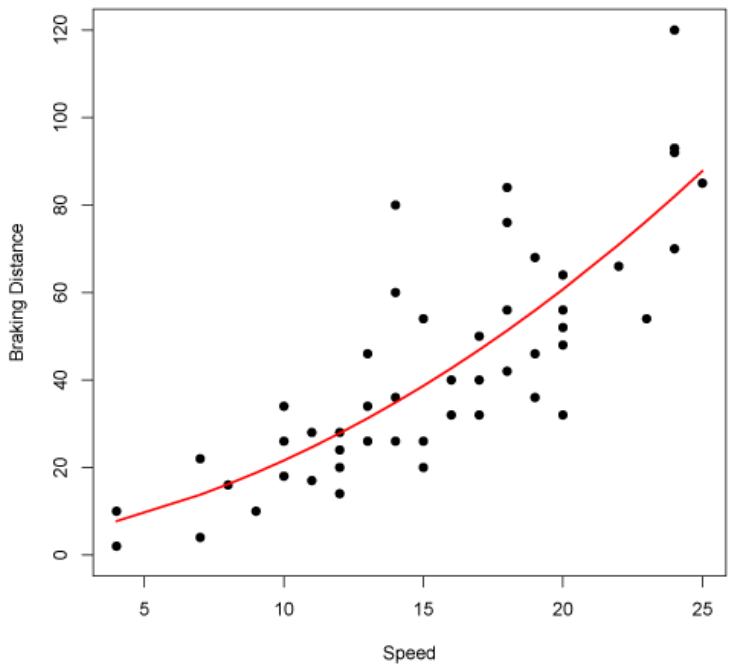
Basic Metropolis–Hastings algorithms
Application of the Independent Metropolis–Hastings algorithm

- We now look at a somewhat more realistic statistical example
  - ▷ Get preliminary parameter estimates from a model
  - ▷ Use an independent proposal with those parameter estimates.

- For example, to simulate from a posterior distribution $\pi(\theta|x) \propto \pi(\theta)f(x|\theta)$
  - ▷ Take a normal or a t distribution centered at the MLE $\hat{\theta}$
  - ▷ Covariance matrix equal to the inverse of Fisher's information matrix.

Independent Metropolis–Hastings algorithm
Braking Data

▶ The `cars` dataset relates braking distance (y) to speed (x) in a sample of cars.



▶ Model

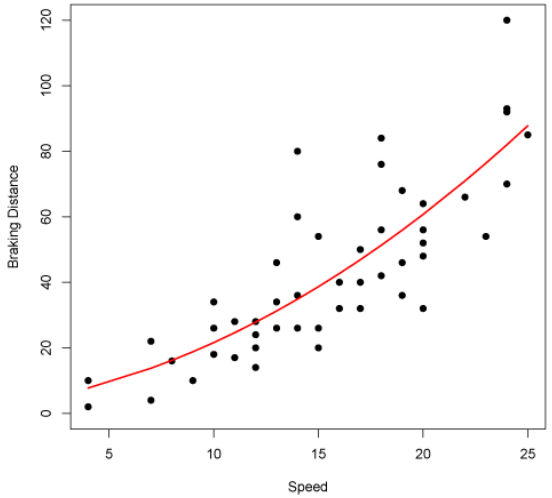
$$y_{ij} = a + bx_i + cx_i^2 + \varepsilon_{ij}$$

▶ The likelihood function is

$$\left(\frac{1}{\sigma^2}\right)^{N/2} \exp\left\{\frac{-1}{2\sigma^2}\sum_{ij}(y_{ij} - a - bx_i - cx_i^2)^2\right\},$$

where $N = \sum_i n_i$

Independent Metropolis–Hastings algorithm
Braking Data Least Squares Fit

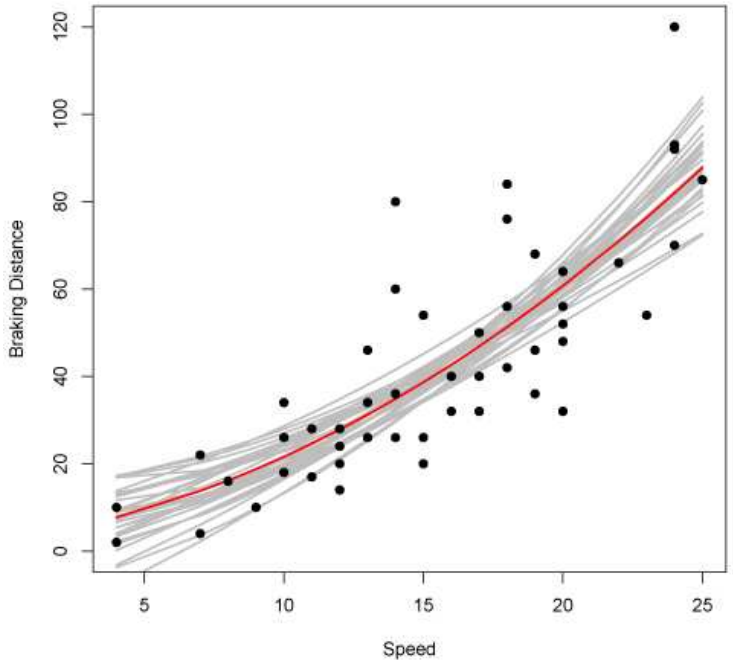


- Candidate from Least Squares

R command: `x2=x^2; summary(lm(y~x+x2))`

```
Coefficients:
             Estimate  Std. Error  t value  Pr(>|t|)
(Intercept)  2.63328   14.80693    0.178    0.860
x            0.88770   2.03282     0.437    0.664
x2           0.10068   0.06592     1.527    0.133
Residual standard error:  15.17 on 47 degrees of freedom
```

Independent Metropolis–Hastings algorithm
Braking Data Metropolis Algorithm



- Candidate: normal centered at the MLEs,

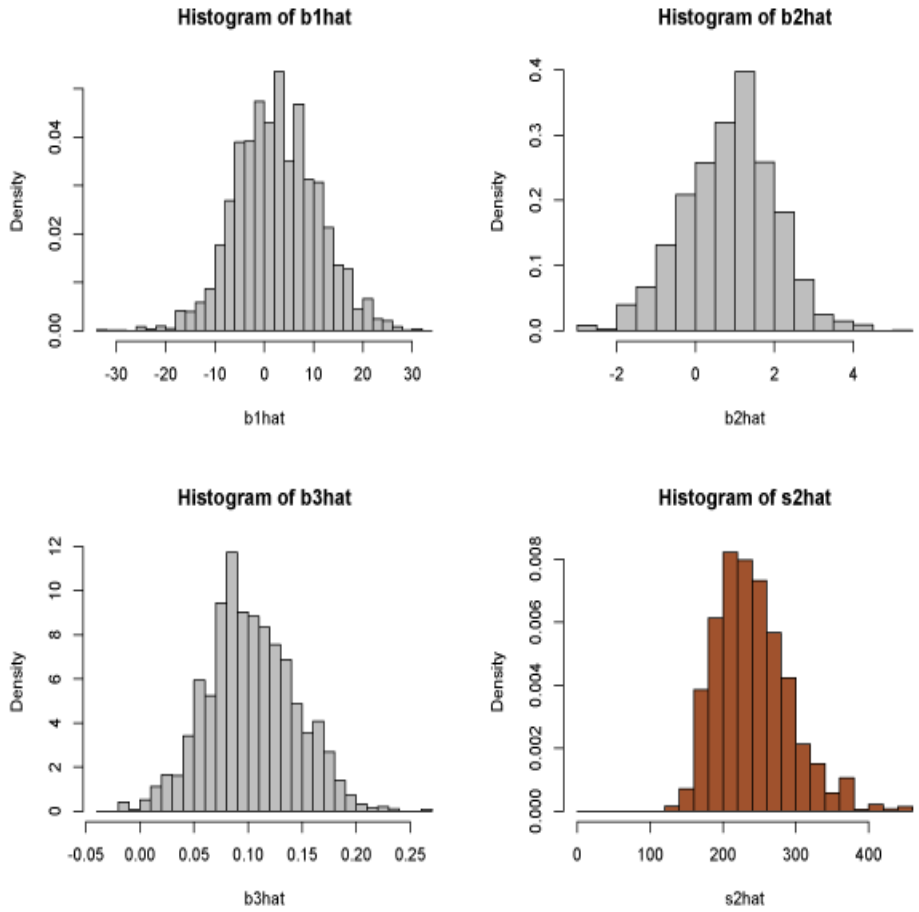
$$a \sim \mathcal{N}(2.63, (14.8)^2),$$
$$b \sim \mathcal{N}(.887, (2.03)^2),$$
$$c \sim \mathcal{N}(.100, (0.065)^2),$$

- Inverted gamma

$$\sigma^{-2} \sim \mathcal{G}(n/2, (n-3)(15.17)^2)$$

- See the variability of the curves associated with the simulation.

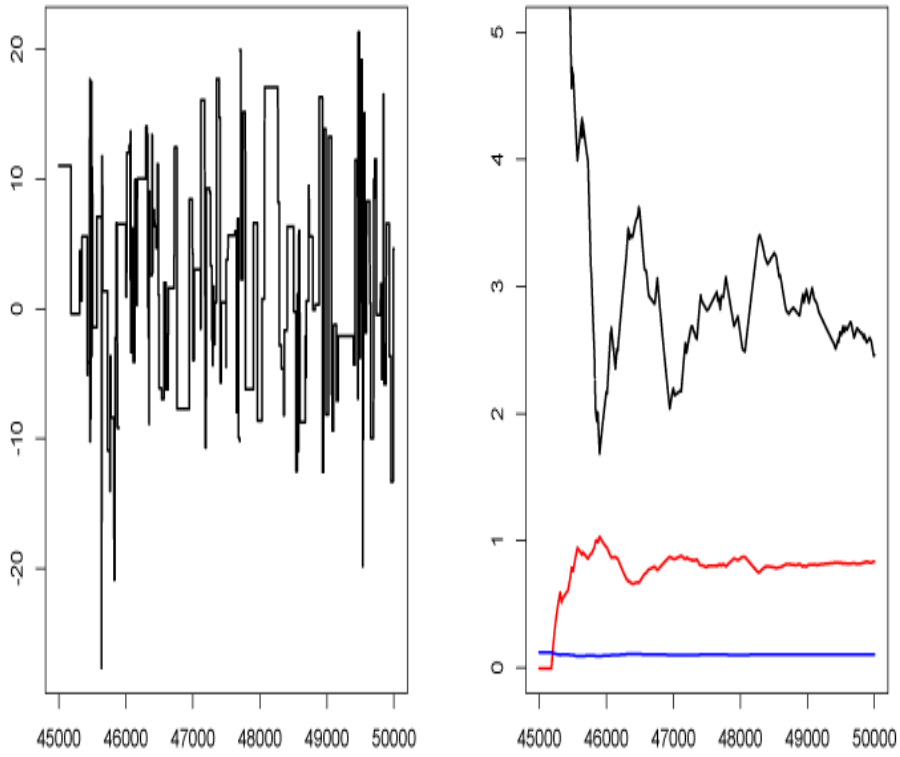
Independent Metropolis–Hastings algorithm
Braking Data Coefficients



- Distributions of estimates
- Credible intervals
- See the skewness

- Note that these are marginal distributions

Independent Metropolis–Hastings algorithm
Braking Data Assessment



- 50,000 iterations
- See the repeats
- Intercept may not have converged

- R code

Random Walk Metropolis–Hastings
Introduction

- Implementation of independent Metropolis–Hastings can sometimes be difficult
  - ▷ Construction of the proposal may be complicated
  - ▷ They ignore local information
- An alternative is to gather information stepwise
  - ▷ Exploring the neighborhood of the current value of the chain
- Can take into account the value previously simulated to generate the next value
  - ▷ Gives a more local exploration of the neighborhood of the current value

Random Walk Metropolis–Hastings
Some Details

- The implementation of this idea is to simulate Y_t according to

$$Y_t = X^{(t)} + \varepsilon_t,$$

  - ε_t is a random perturbation
  - with distribution g, independent of $X^{(t)}$
  - Uniform, normal, etc...

- The proposal density $q(y|x)$ is now of the form $g(y - x)$

  - Typically, g is symmetric around zero, satisfying $g(-t) = g(t)$
  - The Markov chain associated with q is a *random walk*

Random Walk Metropolis–Hastings
The Algorithm

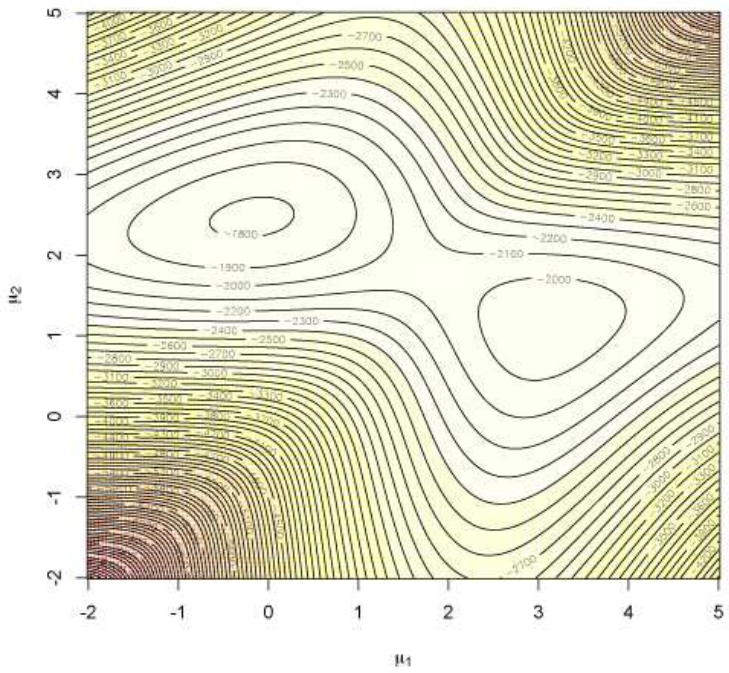
Given $x^{(t)}$,

1. Generate $Y_t \sim g(y - x^{(t)})$.
2. Take

$$X^{(t+1)} = \begin{cases} Y_t & \text{with probability } \min\left\{1, \dfrac{f(Y_t)}{f(x^{(t)})}\right\}, \\ x^{(t)} & \text{otherwise.} \end{cases}$$

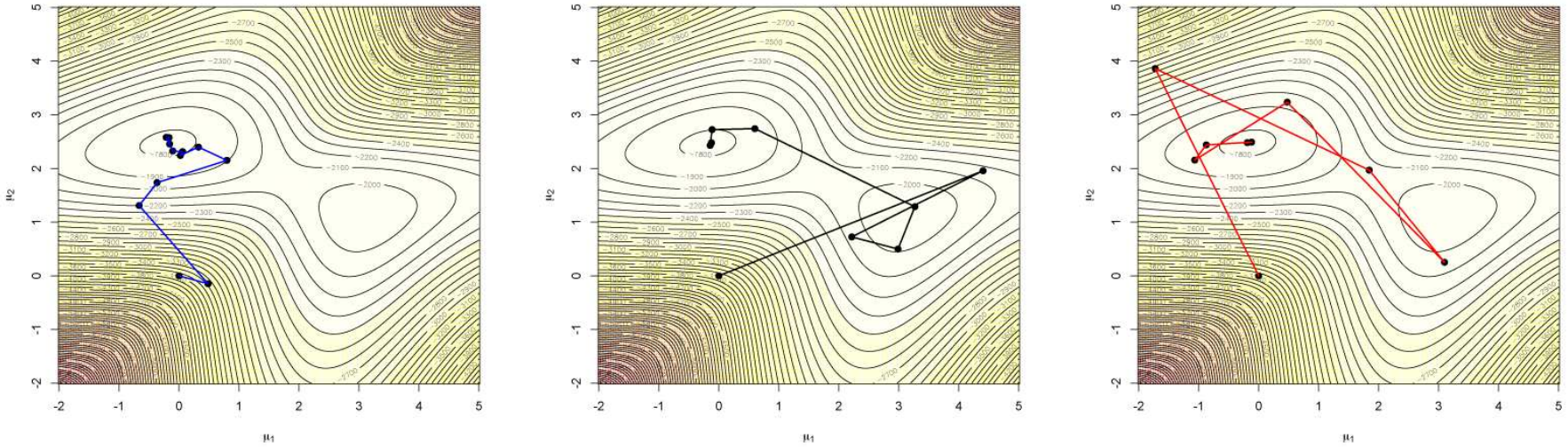
- The g chain is a random walk
  - Due to the Metropolis–Hastings acceptance step, the $\{X^{(t)}\}$ chain is not
- The acceptance probability does not depend on g
  - But different gs result in different ranges and different acceptance rates
- Calibrating the scale of the random walk is for good exploration

Random Walk Metropolis–Hastings
Normal Mixtures



- Explore likelihood with random walk
- Similar to Simulated Annealing
  - But constant temperature (scale)
- Multimodal ⇒ Scale is important
  - Too small ⇒ get stuck
  - Too big ⇒ miss modes

Random Walk Metropolis–Hastings
Normal Mixtures - Different Scales



- Left → Right: Scale=1, Scale=2, Scale=3
  - Scale=1: Too small, gets stuck
  - Scale=2: Just right, finds both modes
  - Scale=3: Too big, misses mode
- R code

Random Walk Metropolis–Hastings
Model Selection or Model Choice

- Random walk Metropolis–Hastings algorithms also apply to discrete targets.
- As an illustration, we consider a regression
  - The `swiss` dataset in `R`
  - y= logarithm of the fertility in 47 districts of Switzerland $\approx$ 1888
  - The covariate matrix X involves five explanatory variables

```
> names(swiss)
[1] "Fertility"  "Agriculture"  "Examination"  "Education"
[5] "Catholic"   "Infant.Mortality"
```

- Compare the $2^5 = 32$ models corresponding to all possible subsets of covariates.
  - If we include squares and twoway interactions
  - $2^{20} = 1048576$ models, same `R` code

Random Walk Metropolis–Hastings
Model Selection using Marginals

- Given an ordinary linear regression with n observations,

$$\mathbf{y}|\beta,\sigma^2,X \sim \mathcal{N}_n(X\beta,\sigma^2 I_n)\,, X \text{ is an } (n,p) \text{ matrix}$$

- The likelihood is

$$\ell\left(\beta,\sigma^2|\mathbf{y},X\right) = \left(2\pi\sigma^2\right)^{-n/2} \exp\left[-\frac{1}{2\sigma^2}(\mathbf{y}-X\beta)^{\mathrm{T}}(\mathbf{y}-X\beta)\right]$$

- Using Zellner's g-prior, with the constant $g = n$

$$\beta|\sigma^2,X \sim \mathcal{N}_{k+1}(\tilde{\beta}, n\sigma^2(X^{\mathrm{T}}X)^{-1}) \quad \text{and} \quad \pi(\sigma^2|X) \propto \sigma^{-2}$$

  - The marginal distribution of $\mathbf{y}$ is a multivariate t distribution,

$$m(\mathbf{y}|X) \propto \left[\mathbf{y}'\left(I - \frac{n}{n+1}X(X'X)^{-1}X'\right)\mathbf{y} - \frac{1}{n+1}\tilde{\beta}'X'X\tilde{\beta}\right]^{-n/2}.$$

- Find the model with maximum marginal probability

Random Walk Metropolis–Hastings
Random Walk on Model Space

- To go from $\gamma^{(t)} \longrightarrow \gamma^{(t+1)}$
  - ▷ First get a candidate γ^*

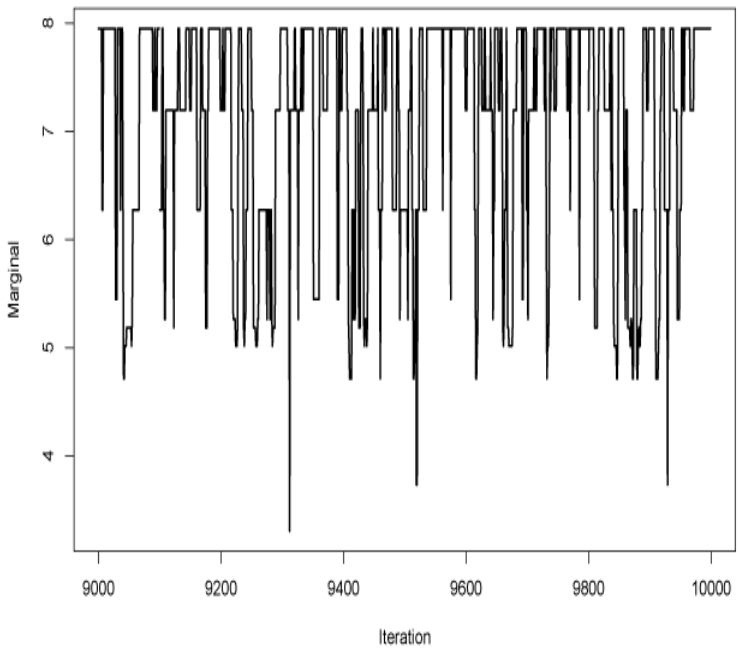
$$\gamma^{(t)} = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \rightarrow \gamma^* = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

  - ▷ Choose a component of $\gamma^{(t)}$ at random, and flip $1 \longrightarrow 0$ or $0 \longrightarrow 1$
  - ▷ Accept the proposed model $\gamma^\star$ with probability

$$\min\left\{\frac{m(\mathbf{y}|X,\gamma^\star)}{m(\mathbf{y}|X,\gamma^{(t)})}, 1\right\}$$

- The candidate is symmetric
- Note: This is not the Metropolis–Hastings algorithm in the book - it is simpler

Random Walk Metropolis–Hastings
Results from the Random Walk on Model Space



- Last iterations of the MH search
- The chain goes down often

- Top Five Models

Marg.	γ				
7.95	1	0	1	1	1
7.19	0	0	1	1	1
6.27	1	1	1	1	1
5.44	1	0	1	1	0
5.45	1	0	1	1	0

- Best model excludes the variable Examination
  - $\gamma = (1, 0, 1, 1, 1)$

- Inclusion rates:

Agri	Exam	Educ	Cath	Inf.Mort
0.661	0.194	1.000	0.904	0.949

Metropolis–Hastings Algorithms
Acceptance Rates

- Infinite number of choices for the candidate q in a Metropolis–Hastings algorithm
- Is there and "optimal" choice?
  - The choice of $q = f$, the target distribution? Not practical.
- A criterion for comparison is the acceptance rate
  - It can be easily computed with the empirical frequency of acceptance
- In contrast to the Accept–Reject algorithm
  - Maximizing the acceptance rate will is not necessarily best
  - Especially for random walks
- Also look at autocovariance

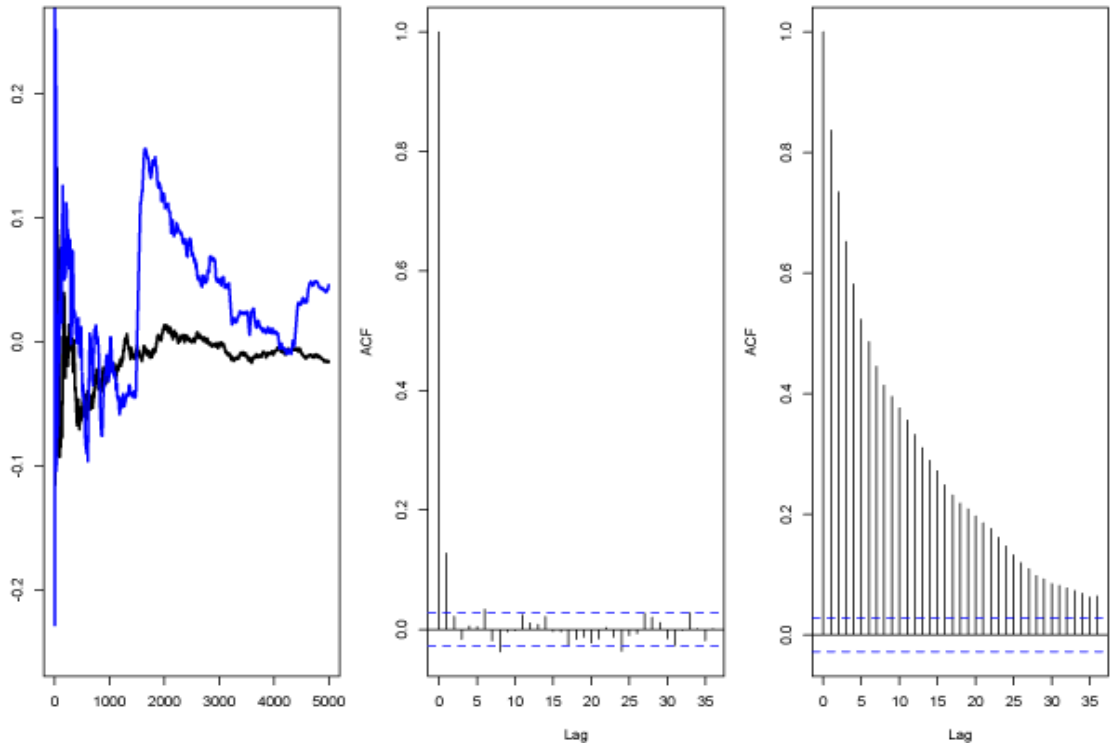
Acceptance Rates
Normals from Double Exponentials

- In the Accept–Reject algorithm
  - To generate a $\mathcal{N}(0,1)$ from a double-exponential $\mathcal{L}(\alpha)$
  - The choice $\alpha = 1$ optimizes the acceptance rate

- In an independent Metropolis–Hastings algorithm
  - We can use the double-exponential as an independent candidate q

- Compare the behavior of Metropolis–Hastings algorithm
  - When using the $\mathcal{L}(1)$ candidate or the $\mathcal{L}(3)$ candidate

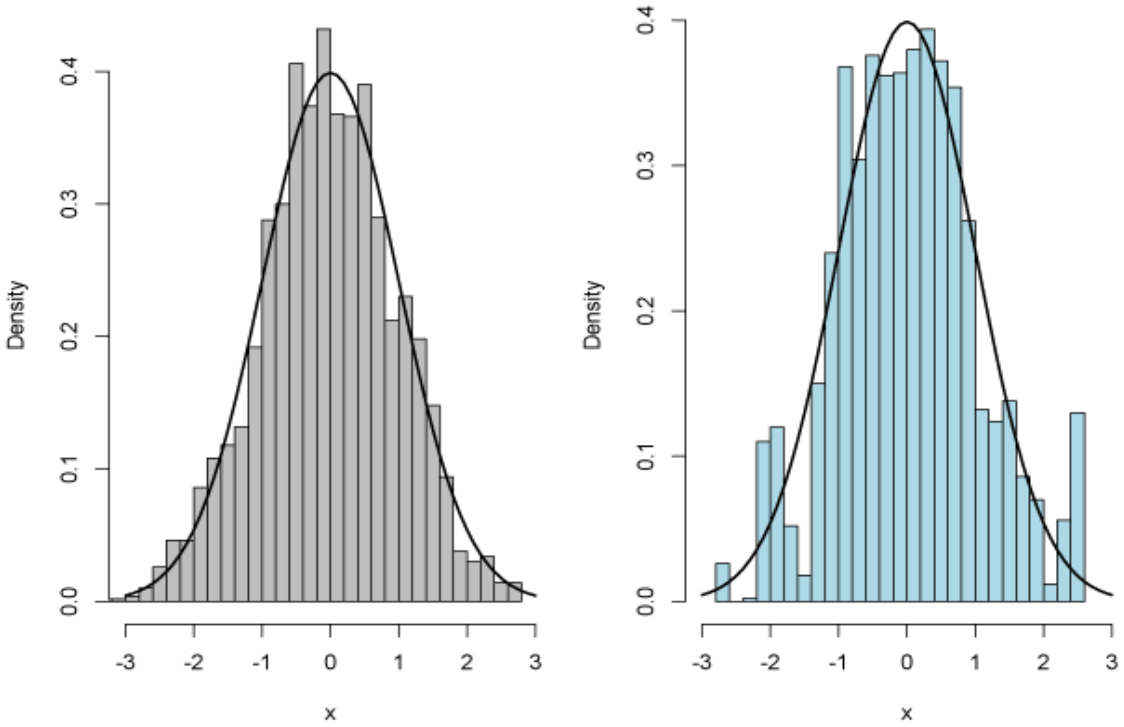
Acceptance Rates
Normals from Double Exponentials Comparison



- $\mathcal{L}(1)$ (black)
  - ▷ Acceptance Rate = 0.83
- $\mathcal{L}(3)$ (blue)
  - ▷ Acceptance Rate = 0.47
- $\mathcal{L}(3)$ has terrible acf (right)
- $\mathcal{L}(3)$ has not converged

Acceptance Rates

Normals from Double Exponentials Histograms

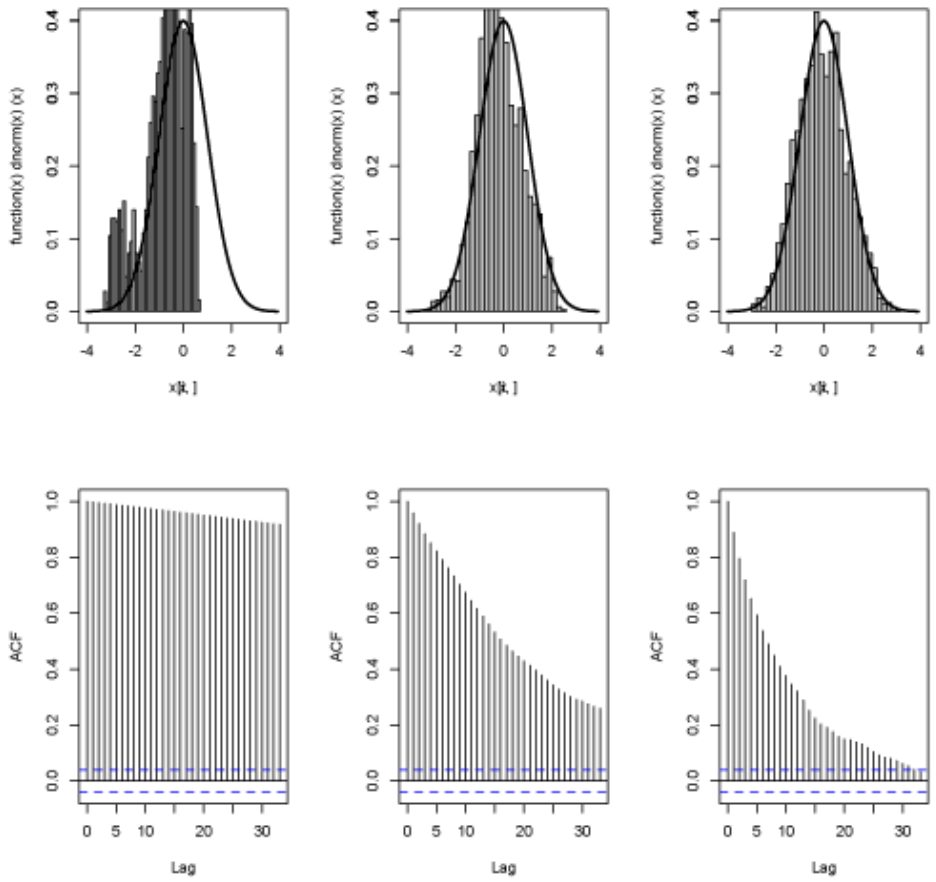


- $\mathcal{L}(1)$ has converged (gray)
- $\mathcal{L}(3)$ not yet there (blue)
- R code

Acceptance Rates
Random Walk Metropolis–Hastings

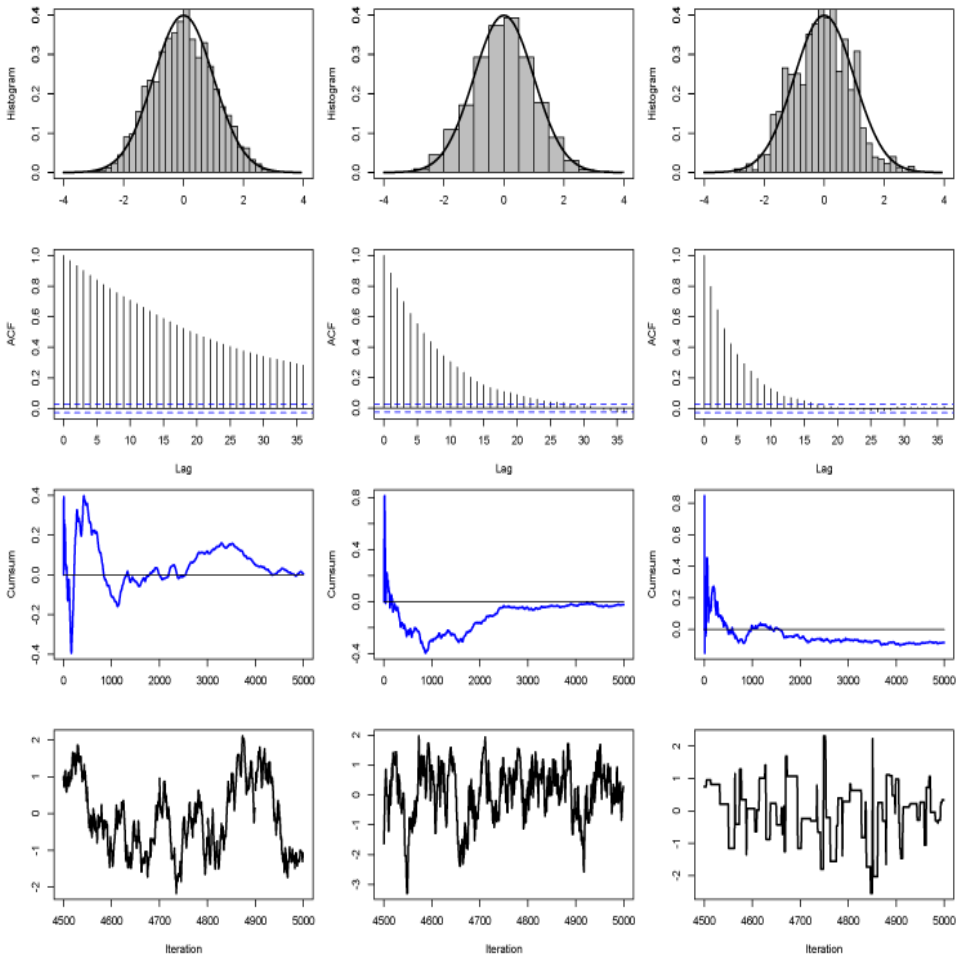
- Independent Metropolis–Hastings algorithms
  - Can be optimized or compared through their acceptance rate
  - This reduces the number of replicas in the chain
  - And reduces the correlation level in the chain
- Not true for other types of Metropolis–Hastings algorithms
  - In a random walk, higher acceptance is not always better.
- The historical example of Hastings generates a $\mathcal{N}(0,1)$ from
  - $Y_t = X_{t-1} + \varepsilon_t$
  - $\rho(x^{(t)}, y_t) = \min\{\exp\{(x^{(t)2} - y_t^2)/2\}, 1\}, \quad \varepsilon_t \sim \mathcal{U}[-\delta, \delta]$
  - δ controls the acceptance rate

Acceptance Rates
Random Walk Metropolis–Hastings Example



- $\delta = 0.1, 1,$ and 10
- $\delta = 0.1$
  - $\triangleright \uparrow$ autocovariance, $\downarrow$ convergence
- $\delta = 10$
  - $\triangleright \downarrow$ autocovariance, ? convergence

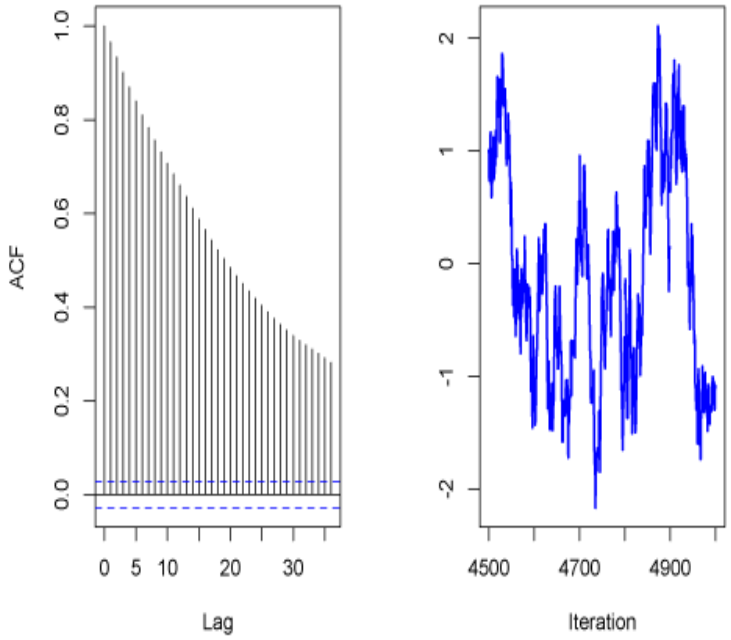
Acceptance Rates
Random Walk Metropolis–Hastings – All of the Details



- Acceptance Rates
  - $\delta = 0.1$: 0.9832
  - $\delta = 1$: 0.7952
  - $\delta = 10$: 0.1512
- Medium rate does better
  - lowest better than the highest

Random Walk Acceptance Rates
Comments

- Random walk Metropolis–Hastings needs careful calibration of acceptance rates



- High acceptance rate
  - ▷ May not have satisfactory behavior
  - ▷ The chain may be moving too slowly on the surface of f
- This is not always the case.
  - ▷ f nearly flat $\Rightarrow$ high acceptance OK

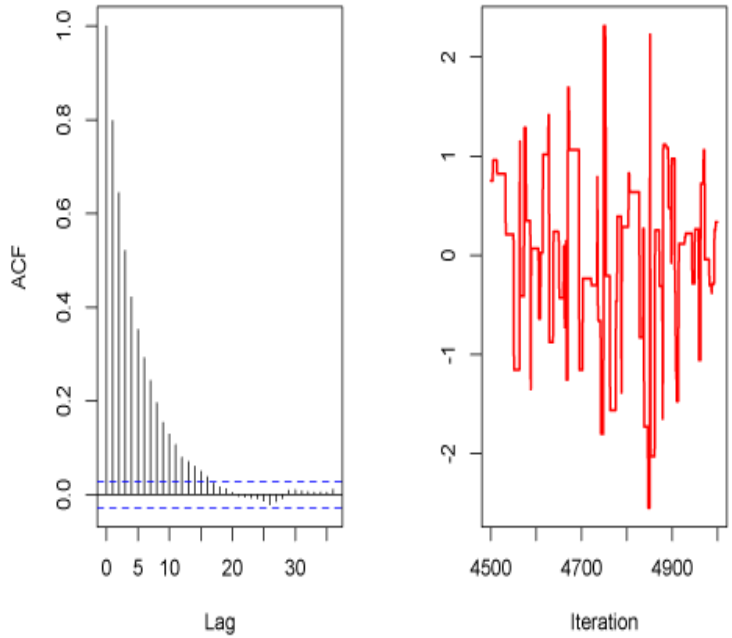
- But, unless f is completely flat, parts of the domain may be missed

Random Walk Acceptance Rates
More Comments

- In contrast, if the average acceptance rate is low
  - ▷ Successive values of $f(y_t)$ are often are small compared to $f(x^{(t)})$

- Low acceptance ⇒
  - ▷ The chain may not see all of f
  - ▷ May miss an important but isolated mode of f

- Nonetheless, low acceptance is less of an issue



- Golden acceptance rate:
  - ▷ 1/2 for the models of dimension 1 or 2
  - ▷ 1/4 in higher dimensions

Chapter 7: Gibbs Samplers

"Come, Watson , come!" he cried. "The game is afoot."

Arthur Conan Doyle

The Adventure of the Abbey Grange

This Chapter

- We cover both the two-stage and the multistage Gibbs samplers
- The two-stage sampler has superior convergence properties
- The multistage Gibbs sampler is the workhorse of the MCMC world
- We deal with missing data and models with latent variables
- And, of course, hierarchical models

Gibbs Samplers
Introduction

- Gibbs samplers gather most of their calibration from the target density
- They break complex problems (high dimensional) into a series of easier problems
  - ▷ May be impossible to build random walk Metropolis–Hastings algorithm
- The sequence of simple problems may take a long time to converge
- But Gibbs sampling is an interesting and useful algorithm.

- *Gibbs sampling* is from the landmark paper by Geman and Geman (1984)
  - ▷ The Gibbs sampler is a special case of Metropolis–Hastings
- Gelfand and Smith (1990) sparked new interest
  - ▷ In Bayesian methods and statistical computing
  - ▷ They solved problems that were previously unsolvable

The Two-Stage Gibbs Sampler
Introduction

- Creates a Markov chain from a joint distribution
- If two random variables X and Y have joint density $f(x, y)$
- With corresponding conditional densities $f_{Y|X}$ and $f_{X|Y}$
- Generates a Markov chain (X_t, Y_t) according to the following steps

Two-stage Gibbs sampler

Take $X_0 = x_0$

For $t = 1, 2, \ldots,$ generate

1. $Y_t \sim f_{Y|X}(\cdot|x_{t-1})$;
2. $X_t \sim f_{X|Y}(\cdot|y_t)$.

The Two-Stage Gibbs Sampler
Convergence

- The algorithm straightforward if simulating from both conditionals is feasible
- The stationary distribution is $f(x, y)$
- Convergence of the Markov chain insured
  - Unless the supports of the conditionals are not connected

Example: Normal bivariate Gibbs

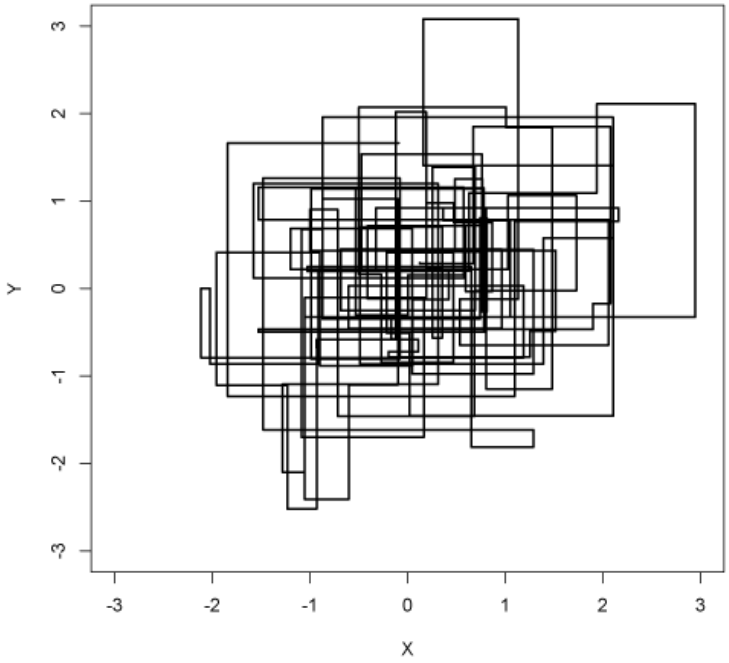
- Start with simple illustration, the bivariate normal model:

$$(X, Y) \sim \mathcal{N}_2 \left(0, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right),$$

- The the Gibbs sampler is `Given` x_t`, generate`

$$\begin{aligned} Y_{t+1} \mid x_t &\sim \mathcal{N}(\rho x_t,\ 1 - \rho^2), \\ X_{t+1} \mid y_{t+1} &\sim \mathcal{N}(\rho y_{t+1},\ 1 - \rho^2). \end{aligned}$$

The Two-Stage Gibbs Sampler
Bivariate Normal Path



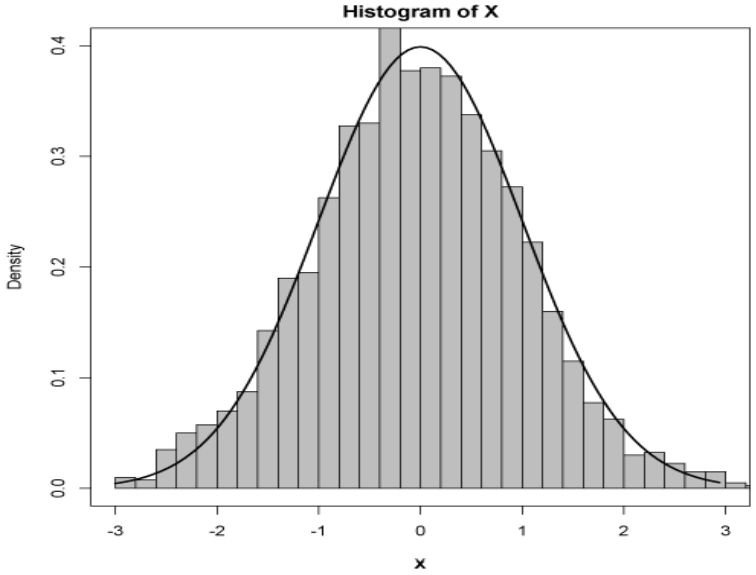
- Iterations $(X_t, Y_t) \to (X_{t+1}, Y_{t+1})$
- Parallel to the axes
- Correlation affects mixing
- R code

The Two-Stage Gibbs Sampler
Bivariate Normal Convergence

- The subchain $(X_t)_t$ satisfies $X_{t+1}|X_t = x_t \sim \mathcal{N}(\rho^2 x_t,\ 1-\rho^4)$,
- A recursion shows that

$$X_t|X_0 = x_0 \sim \mathcal{N}(\rho^{2t}x_0,\ 1-\rho^{4t}) \to \mathcal{N}(0,1)\,,$$

- We have converged to the *joint* distribution and both *marginal distributions*.



- Histogram of Marginal
- 2000 Iterations

The Two-Stage Gibbs Sampler
A First Hierarchical Model

- Gibbs sampling became popular
  - Since it was the perfect computational complement to hierarchical models
- A hierarchical model specifies a joint distribution
  - As successive layers of conditional distributions

Example: Generating beta-binomial random variables

- Consider the hierarchy

$$\begin{aligned} X|\theta &\sim \mathcal{B}\text{in}(n,\theta) \\ \theta &\sim \mathcal{B}e(a,b), \end{aligned}$$

- Which leads to the joint distribution

$$f(x,\theta) = \binom{n}{x} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{x+a-1}(1-\theta)^{n-x+b-1}.$$

The Two-Stage Gibbs Sampler
Beta-Binomial Conditionals

- The joint distribution

$$f(x,\theta) = \binom{n}{x} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{x+a-1}(1-\theta)^{n-x+b-1}.$$

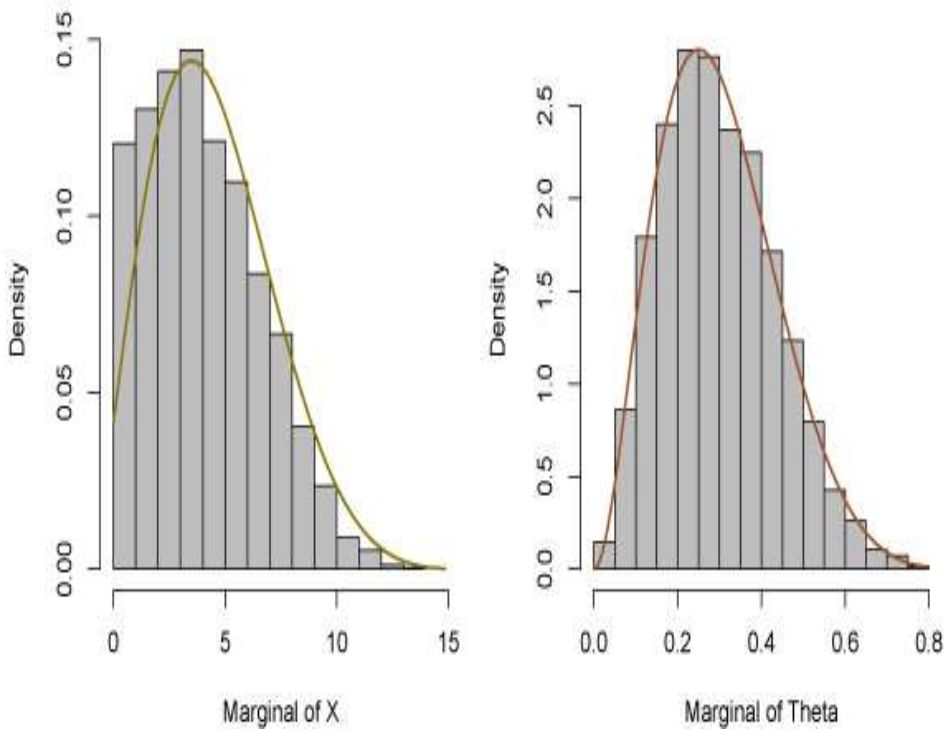
- Has full conditionals
  - $X|\theta \sim \mathcal{B}\text{in}(n,\theta)$
  - $\theta|X \sim \mathcal{B}e(X+a, n-X+b)$
- This can be seen from

$$f(x,\theta) = \binom{n}{x} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{x+a-1}(1-\theta)^{n-x+b-1}.$$

The Two-Stage Gibbs Sampler
Beta-Binomial Marginals

- The marginal distribution of X is the Beta-Binomial

$$m(x) = \int_0^1 \binom{n}{x} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{x+a-1}(1-\theta)^{n-x+b-1} d\theta$$



- Output from the Gibbs sampler
- X and θ marginals

The Two-Stage Gibbs Sampler
A First Normal Hierarchy

- A study on metabolism in 15-year-old females yielded the following data

```
> x=c(91,504,557,609,693,727,764,803,857,929,970,1043,
+     1089,1195,1384,1713)
```

  - ▷ Their energy intake, measured in megajoules, over a 24 hour period.

- We model

$$\log(X) \sim \mathcal{N}(\theta, \sigma^2), \quad i = 1, \ldots, n$$

  - ▷ And complete the hierarchy with

$$\begin{aligned} \theta &\sim \mathcal{N}(\theta_0, \tau^2), \\ \sigma^2 &\sim \mathcal{IG}(a, b), \end{aligned}$$

  where $\mathcal{IG}(a, b)$ is the inverted gamma distribution.

The Two-Stage Gibbs Sampler
θ Conditional

- The posterior distribution $\propto$ joint distribution is

$$f(\theta, \sigma^2|\mathbf{x}) \propto \left[\frac{1}{(\sigma^2)^{n/2}} e^{-\sum_i (x_i-\theta)^2/(2\sigma^2)}\right] \times \left[\frac{1}{\tau} e^{-(\theta-\theta_0)^2/(2\tau^2)}\right] \times \left[\frac{1}{(\sigma^2)^{a+1}} e^{1/b\sigma^2}\right]$$

  (Here $x = \log(x)$)

  - And now we can get the full conditionals

- θ conditional

$$f(\theta, \sigma^2|\mathbf{x}) \propto \left[\frac{1}{(\sigma^2)^{n/2}} e^{-\sum_i (x_i-\theta)^2/(2\sigma^2)}\right] \times \left[\frac{1}{\tau} e^{-(\theta-\theta_0)^2/(2\tau^2)}\right] \times \left[\frac{1}{(\sigma^2)^{a+1}} e^{1/b\sigma^2}\right]$$

  $\Rightarrow$

$$\theta|\mathbf{x}, \sigma^2 \sim \mathcal{N}\left(\frac{\sigma^2}{\sigma^2 + n\tau^2}\, \theta_0 + \frac{n\tau^2}{\sigma^2 + n\tau^2}\, \bar{x},\ \frac{\sigma^2\tau^2}{\sigma^2 + n\tau^2}\right)$$

The Two-Stage Gibbs Sampler
σ^2 Conditional

- Again from the joint distribution

$$f(\theta,\sigma^2|\mathbf{x}) \propto \left[\frac{1}{(\sigma^2)^{n/2}} e^{-\sum_i (x_i-\theta)^2/(2\sigma^2)}\right] \times \left[\frac{1}{\tau} e^{-(\theta-\theta_0)^2/(2\tau^2)}\right] \times \left[\frac{1}{(\sigma^2)^{a+1}} e^{1/b\sigma^2}\right]$$

$$\Rightarrow$$

$$\sigma^2|\mathbf{x},\theta \sim \mathcal{IG}\left(\frac{n}{2}+a, \frac{1}{2}\sum_i (x_i-\theta)^2 + b\right),$$

- We now have a Gibbs sampler using

$$\theta|\sigma^2 \sim \texttt{rnorm} \text{ and } (1/\sigma^2)|\theta \sim \texttt{rgamma}$$

- R code

The Multistage Gibbs Sampler
Introduction

- There is a natural extension from the two-stage to the multistage Gibbs sampler
- For $p > 1$, write $\mathcal{X} = \mathbf{X} = (X_1, \ldots, X_p)$
  - ▷ suppose that we can simulate from the full conditional densities

$$X_i|x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p \sim f_i(x_i|x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p)$$

- The multistage Gibbs sampler has the following transition from $X^{(t)}$ to $X^{(t+1)}$:

The Multi-stage Gibbs Sampler

At iteration $t = 1, 2, \ldots,$ given $\mathbf{x}^{(t)} = (x_1^{(t)}, \ldots, x_p^{(t)})$, generate

1. $X_1^{(t+1)} \sim f_1(x_1|x_2^{(t)}, \ldots, x_p^{(t)})$;
2. $X_2^{(t+1)} \sim f_2(x_2|x_1^{(t+1)}, x_3^{(t)}, \ldots, x_p^{(t)})$;

$\vdots$

p. $X_p^{(t+1)} \sim f_p(x_p|x_1^{(t+1)}, \ldots, x_{p-1}^{(t+1)})$.

The Multistage Gibbs Sampler
A Multivariate Normal Example

Example: Normal multivariate Gibbs

- We previously saw a simple bivariate normal example
- Consider the multivariate normal density

$$(X_1, X_2, \ldots, X_p) \sim \mathcal{N}_p\left(0, (1-\rho)I + \rho J\right),$$

  - I is the $p \times p$ identity matrix
  - J is a $p \times p$ matrix of ones
  - $\text{corr}(X_i, X_j) = \rho$ for every i and j

- The full conditionals are

$$X_i | x_{(-i)} \sim \mathcal{N}\left(\frac{(p-1)\rho}{1+(p-2)\rho}\bar{x}_{(-i)}, \frac{1+(p-2)\rho-(p-1)\rho^2}{1+(p-2)\rho}\right),$$

The Multistage Gibbs Sampler
Use of the Multivariate Normal Gibbs sampler

- The Gibbs sampler that generates from these univariate normals
  - ▷ Can then be easily derived
  - ▷ But it is not needed for this problem

- It is, however, a short step to consider
  - ▷ The setup where the components are restricted to a subset of $\mathbb{R}^p$.
  - ▷ If this subset is a hypercube,

$$\mathfrak{H} = \prod_{i=1}(a_i, b_i)\,, \quad i = 1, \ldots, p$$

  the corresponding conditionals are the normals above restricted to (a_i, b_i)

- These are easily simulated

The Multistage Gibbs Sampler
A Hierarchical Model for the Energy Data

- The oneway model can be a hierarchical model.
- Let X_{ij} be the energy intake, $i = 1, 2$ (girl or boy), $j = 1, n$.

$$\log(X_{ij}) = \theta_i + \varepsilon_{ij}, \quad , N(0, \sigma^2)$$

- We can complete this model with a hierarchical specification.
- There are different ways to parameterize this model. Here is one:

$$\log(X_{ij}) \sim \mathcal{N}(\theta_i, \sigma^2), \quad i = 1, \ldots, k, \quad j = 1, \ldots, n_i,$$

$$\theta_i \sim \mathcal{N}(\mu, \tau^2), \quad i = 1, \ldots, k,$$

$$\mu \sim \mathcal{N}(\mu_0, \sigma_\mu^2),$$

$$\sigma^2 \sim \mathcal{IG}(a_1, b_1), \quad \tau^2 \sim \mathcal{IG}(a_2, b_2), \quad \sigma_\mu^2 \sim \mathcal{IG}(a_3, b_3).$$

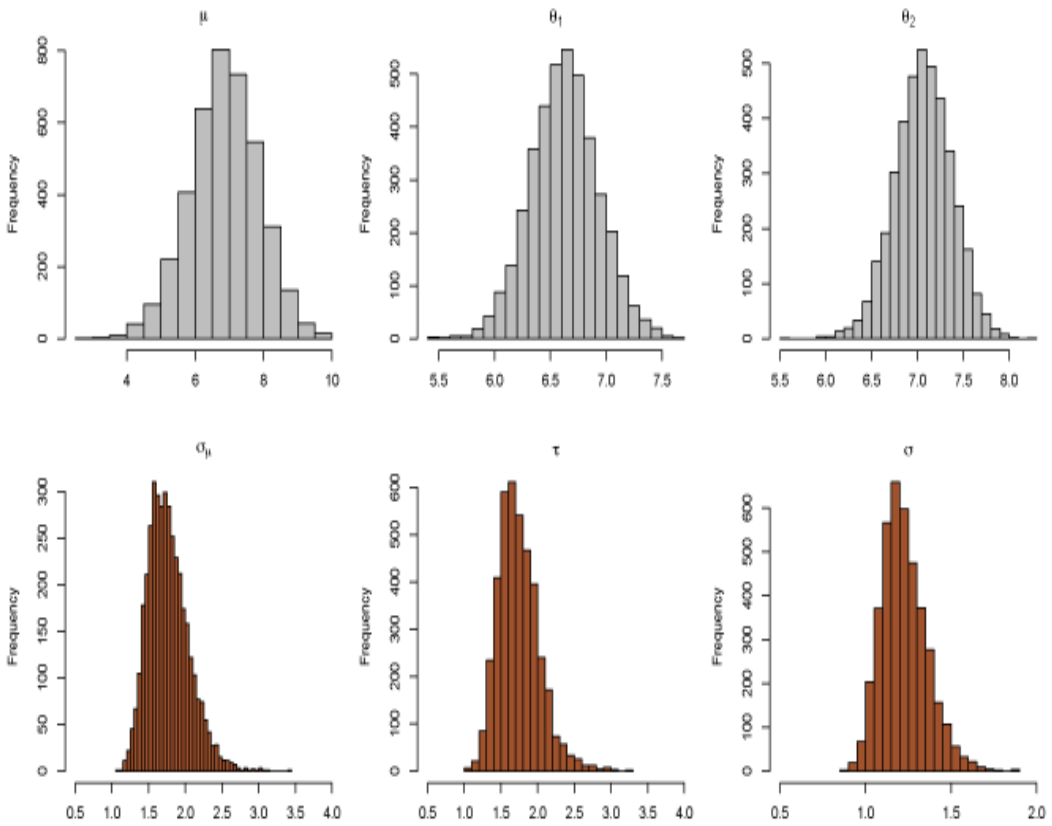
The Multistage Gibbs Sampler
Full Conditionals for a Oneway Model

▶ Now, if we proceed as before we can derive the set of full conditionals

$$
\begin{aligned}
\theta_i &\sim \mathcal{N}\left(\frac{\sigma^2}{\sigma^2+n_i\tau^2}\mu + \frac{n_i\tau^2}{\sigma^2+n_i\tau^2}\bar{X}_i,\ \frac{\sigma^2\tau^2}{\sigma^2+n_i\tau^2}\right), \quad i=1,\ldots,k,\\
\mu &\sim \mathcal{N}\left(\frac{\tau^2}{\tau^2+k\sigma_\mu^2}\mu_0 + \frac{k\sigma_\mu^2}{\tau^2+k\sigma_\mu^2}\bar{\theta},\ \frac{\sigma_\mu^2\tau^2}{\tau^2+k\sigma_\mu^2}\right),\\
\sigma^2 &\sim \mathcal{IG}\left(n/2+a_1,\ (1/2)\sum_{ij}(X_{ij}-\theta_i)^2+b_1\right),\\
\tau^2 &\sim \mathcal{IG}\left(k/2+a_2,\ (1/2)\sum_{i}(\theta_i-\mu)^2+b_2\right),\\
\sigma_\mu^2 &\sim \mathcal{IG}\left(1/2+a_3,\ (1/2)(\mu-\mu_0)^2+b_3\right),
\end{aligned}
$$

where $n=\sum_i n_i$ and $\bar{\theta}=\sum_i n_i\theta_i/n$.

The Multistage Gibbs Sampler
Output From the Energy Data Analysis



- The top row:
  - ▷ Mean μ and θ_1 and θ_2,
  - ▷ For the girl's and boy's energy
- Bottom row:
  - ▷ Standard deviations.

- A variation is to give μ a flat prior, which is equivalent to setting $\sigma_\mu^2 = \infty$
- R code

Missing Data and Latent Variables
Introduction

- Missing Data Models start with the relation

$$g(x|\theta) = \int_z f(x, z|\theta)\, \mathrm{d}z$$

  - $g(x|\theta)$ is typically the sample density or likelihood
  - f is arbitrary and can be chosen for convenience

- We implement a Gibbs sampler on f
- Set $y = (x, z) = (y_1, \ldots, y_p)$ and run the Gibbs sampler

$$\begin{aligned}
Y_1|y_2, \ldots, y_p &\sim f(y_1|y_2, \ldots, y_p),\\
Y_2|y_1, y_3, \ldots, y_p &\sim f(y_2|y_1, y_3, \ldots, y_p),\\
&\vdots\\
Y_p|y_1, \ldots, y_{p-1} &\sim f(y_p|y_1, \ldots, y_{p-1}).
\end{aligned}$$

Missing Data and Latent Variables
Completion Gibbs Sampler

- For $g(x|\theta) = \int_{\mathcal{Z}} f(x, z|\theta)\, \mathrm{d}z$
- And $y = (x, z) = (y_1, \ldots, y_p)$ with

$$
\begin{aligned}
Y_1|y_2, \ldots, y_p &\sim f(y_1|y_2, \ldots, y_p),\\
Y_2|y_1, y_3, \ldots, y_p &\sim f(y_2|y_1, y_3, \ldots, y_p),\\
&\vdots\\
Y_p|y_1, \ldots, y_{p-1} &\sim f(y_p|y_1, \ldots, y_{p-1}).
\end{aligned}
$$

  - $Y^{(t)} = (X^{(t)}, Z^{(t)}) \to Y \sim f(x, z)$
  - $X^{(t)} \to Y \sim f(x)$
  - $Z^{(t)} \to Y \sim f(z)$

- $X^{(t)}$ and $Z^{(t)}$ are not Markov chains
  - But the subchains converge to the correct distributions

Missing Data and Latent Variables
Censored Data Models

Example: Censored Data Gibbs

- Recall the censored data likelihood function

$$g(x|\theta) = L(\theta|x) \propto \prod_{i=1}^{m} e^{-(x_i-\theta)^2/2},$$

- And the complete-data likelihood

$$f(x, z|\theta) = L(\theta|x, z) \propto \prod_{i=1}^{m} e^{-(x_i-\theta)^2/2} \prod_{i=m+1}^{n} e^{-(z_i-\theta)^2/2}$$

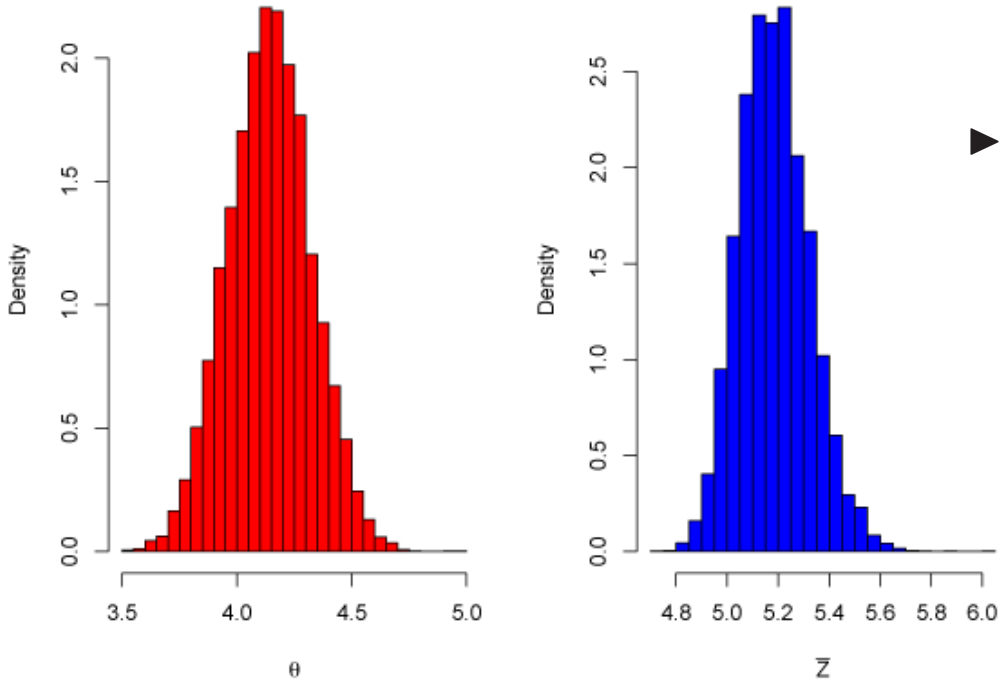
  - With $\theta \sim \pi(\theta)$ we have the Gibbs sampler

$$\pi(\theta|x, z) \quad \text{and} \quad f(z|x, \theta)$$

  - With stationary distribution $\pi(\theta, z|x)$, the posterior of θ and z.

Missing Data and Latent Variables

Censored Normal



- Flat prior $\pi(\theta) = 1$,

$$\theta|x, z \sim \mathcal{N}\left(\frac{m\bar{x} + (n-m)\bar{z}}{n}, \frac{1}{n}\right),$$

$$Z_i|x, \theta \sim \frac{\varphi(z-\theta)}{\{1 - \Phi(a-\theta)\}}$$

- Each Z_i must be greater than the truncation point a
- Many ways to generate Z (AR, `rtrun` from the package `bayesm`, PIT)
- `R` code

Missing Data and Latent Variables
Genetic Linkage

- We previously saw the classic genetic linkage data
- Such models abound
- Here is another, more complex, model

Observed genotype frequencies on blood type data

Genotype	Probability	Observed	Probability	Frequency
AA	p_A^2	A	$p_A^2 + 2p_Ap_O$	$n_A = 186$
AO	$2p_Ap_O$			
BB	p_B^2	B	$p_B^2 + 2p_Bp_O$	$n_B = 38$
BO	$2p_Bp_O$			
AB	$2p_Ap_B$	AB	$2p_Ap_B$	$n_{AB} = 13$
OO	p_O^2	O	p_O^2	$n_O = 284$

- Dominant allele $\rightarrow$ missing data
- Cannot observe AO or BO

- Observe $X \sim \mathcal{M}_4\left(n; p_A^2 + 2p_Ap_O,\ p_B^2 + 2p_Bp_O,\ p_Ap_B,\ p_O^2\right)$
  - $p_A + p_B + p_O = 1$

Missing Data and Latent Variables
Latent Variable Multinomial

- The observed data likelihood is

$$L(p_A, p_B, p_O|X) \propto (p_A^2 + 2p_Ap_O)^{n_A}(p_B^2 + 2p_Bp_O)^{n_B}(p_Ap_B)^{n_{AB}}(p_O^2)^{n_O}$$

- With missing data (latent variables) Z_A and Z_B, the complete-data likelihood is

$$L(p_A, p_B, p_O|X, Z_A, Z_B) \propto (p_A^2)^{Z_A}(2p_Ap_O)^{n_A-Z_A}(p_B^2)^{Z_B}(2p_Bp_O)^{n_B-Z_B}(p_Ap_B)^{n_{AB}}(p_O^2)^{n_O}.$$

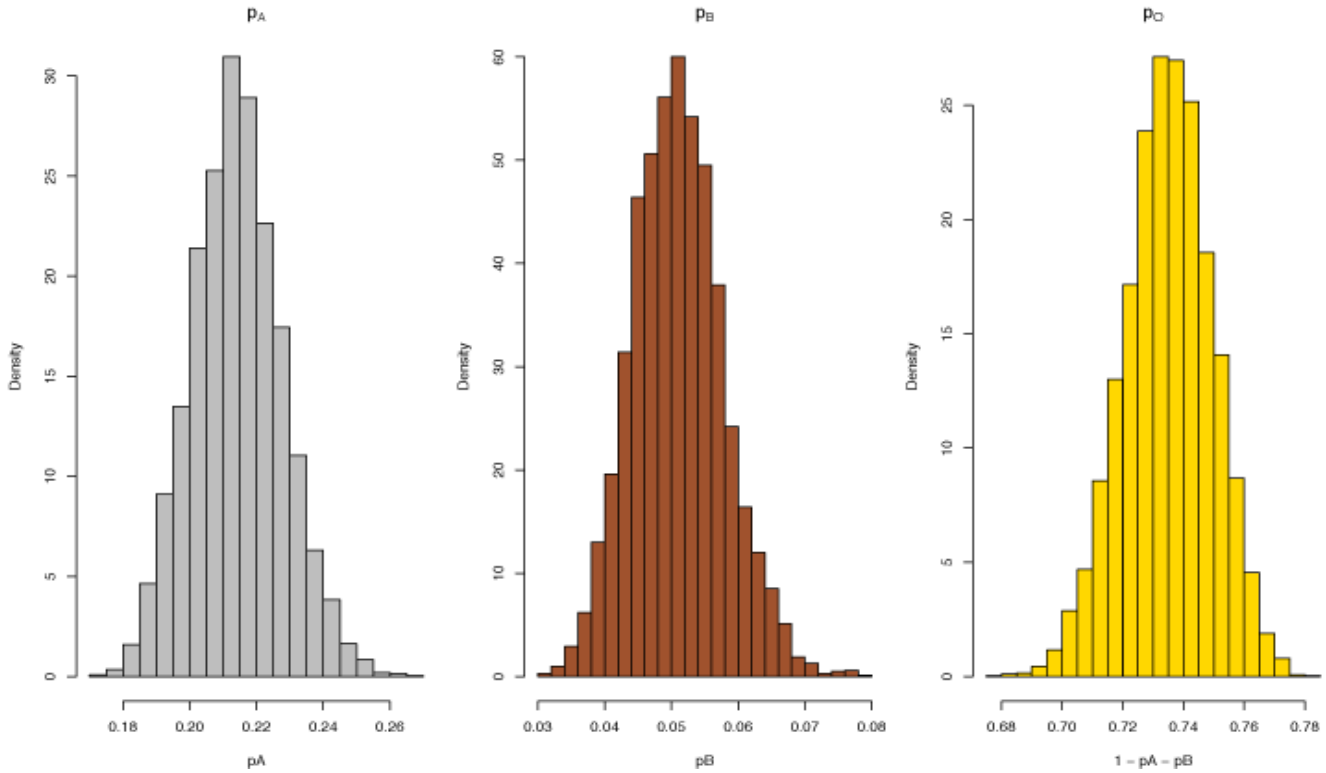
- Giving the missing data density

$$\left(\frac{p_A^2}{p_A^2 + 2p_Ap_O}\right)^{Z_A}\left(\frac{2p_Ap_O}{p_A^2 + 2p_Ap_O}\right)^{n_A-Z_A}\left(\frac{p_B^2}{p_B^2 + 2p_Bp_O}\right)^{Z_B}\left(\frac{2p_Bp_O}{p_B^2 + 2p_Bp_O}\right)^{n_B-Z_B}$$

- And the Gibbs sampler

$$p_A, p_B, p_O|X, Z_A, Z_B \sim \text{Dirichlet}, \quad Z_A, Z_B|p_A, p_B, p_O \sim \text{Independent Binomial}$$

Missing Data and Latent Variables
Analysis of Blood Types



- Estimated genotype frequencies
- Fisher had first developed these models
  - But he could not do the estimation: No EM, No Gibbs in 1930

Multi-Stage Gibbs Samplers
Hierarchical Structures

- We have seen the multistage Gibbs sampler applied to a number of examples
  - Many arising from missing-data structures.
- But the Gibbs sampler can sample from any hierarchical model
- A hierarchical model is defined by a sequence of conditional distributions
  - For instance, in the two-level generic hierarchy

$$\begin{aligned} X_i &\sim f_i(x|\theta), \quad i = 1, \ldots, n\,, \quad \theta = (\theta_1, \ldots, \theta_p)\,, \\ \theta_j &\sim \pi_j(\theta|\gamma), \quad j = 1, \ldots, p\,, \quad \gamma = (\gamma_1, \ldots, \gamma_s)\,, \\ \gamma_k &\sim g(\gamma), \quad k = 1, \ldots, s. \end{aligned}$$

- The joint distribution from this hierarchy is

$$\prod_{i=1}^{n} f_i(x_i|\theta) \prod_{j=1}^{p} \pi_j(\theta_j|\gamma) \prod_{k=1}^{s} g(\gamma_k)\,.$$

Multi-Stage Gibbs Samplers
Simulating from the Hierarchy

▶ With observations x_i the full posterior conditionals are

$$\theta_j \propto \pi_j(\theta_j|\gamma) \prod_{i=1}^{n} f_i(x_i|\theta), \quad j = 1, \ldots, p\,,$$

$$\gamma_k \propto g(\gamma_k) \prod_{j=1}^{p} \pi_j(\theta_j|\gamma), \quad k = 1, \ldots, s\,.$$

▷ In standard hierarchies, these densities are straightforward to simulate from

▷ In complex hierarchies, we might need to use a Metropolis–Hastings step

▷ Main message: full conditionals are easy to write down given the hierarchy

ϟ Note:

▶ When a full conditional in a Gibbs sampler cannot be simulated directly

▷ One Metropolis–Hastings step is enough

Multi-Stage Gibbs Samplers
The Pump Failure Data

Example: Nuclear Pump Failures

- A benchmark hierarchical example in the Gibbs sampling literature
- Describes multiple failures of pumps in a nuclear plant
- Data:

Pump	1	2	3	4	5	6	7	8	9	10
Failures	5	1	5	14	3	19	1	1	4	22
Time	94.32	15.72	62.88	125.76	5.24	31.44	1.05	1.05	2.10	10.48

- Model: Failure of i^{th} pump follows a Poisson process
- For time t_i, the number of failures $X_i \sim \mathcal{P}(\lambda_i t_i)$

Multi-Stage Gibbs Samplers
The Pump Failure Hierarchy

- The standard priors are gammas, leading to the hierarchical model

$$\begin{aligned} X_i &\sim \mathcal{P}(\lambda_i t_i), \quad i = 1, \ldots 10, \\ \lambda_i &\sim \mathcal{G}(\alpha, \beta), \quad i = 1, \ldots 10, \\ \beta &\sim \mathcal{G}(\gamma, \delta). \end{aligned}$$

- With joint distribution

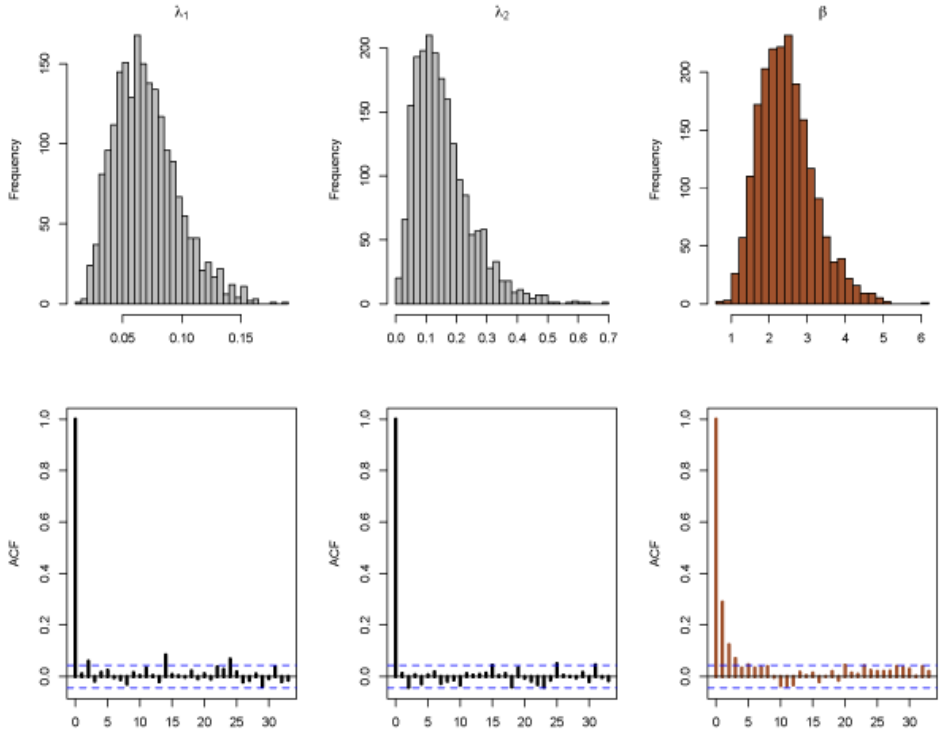
$$\prod_{i=1}^{10} \left\{ (\lambda_i t_i)^{x_i} \, e^{-\lambda_i t_i} \, \lambda_i^{\alpha-1} e^{-\beta\lambda_i} \right\} \beta^{10\alpha} \beta^{\gamma-1} e^{-\delta\beta}$$

- And full conditionals

$$\lambda_i | \beta, t_i, x_i \sim \mathcal{G}(x_i + \alpha, t_i + \beta), \quad i = 1, \ldots 10,$$

$$\beta | \lambda_1, \ldots, \lambda_{10} \sim \mathcal{G}\left(\gamma + 10\alpha, \delta + \sum_{i=1}^{10} \lambda_i \right).$$

Multi-Stage Gibbs Samplers
The Pump Failure Gibbs Sampler



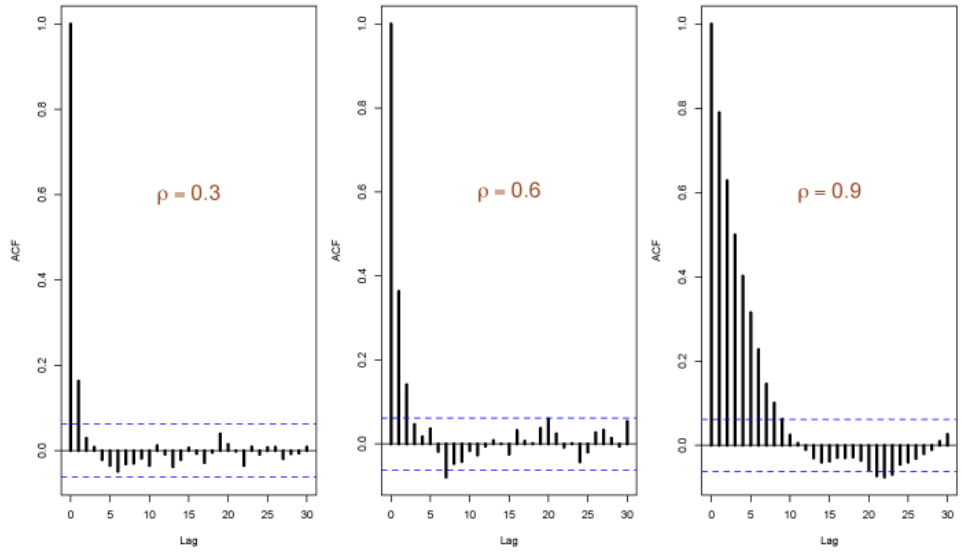
- The Gibbs sampler is easy
- Some selected output here
- Nice autocorrelations
- R code

- Goal of the pump failure data is to identify which pumps are more reliable.
  - Get 95% posterior credible intervals for each λ_i to assess this

Other Considerations
Reparameterization

- Many factors contribute to the convergence properties of a Gibbs sampler
- Convergence performance may be greatly affected by the parameterization
- High covariance may result in slow exploration.

Simple Example



- $(X, Y) \sim \mathcal{N}_2\left(0, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$
- $X + Y$ and $X - Y$ are independent
- Autocorrelation for $\rho = .3, .6, .9$

Reparameterization
Oneway Models

- Poor parameterization can affect both Gibbs sampling and Metropolis–Hastings
- No general consensus on a solution
  - ▷ Overall advice ⇒ make the components as independent as possible
- Example: Oneway model for the energy data
  - Then

$$\begin{aligned} Y_{ij} &\sim \mathcal{N}(\theta_i, \sigma^2), \\ \theta_i &\sim \mathcal{N}(\mu, \tau^2), \\ \mu &\sim \mathcal{N}(\mu_0, \sigma_\mu^2), \end{aligned}$$

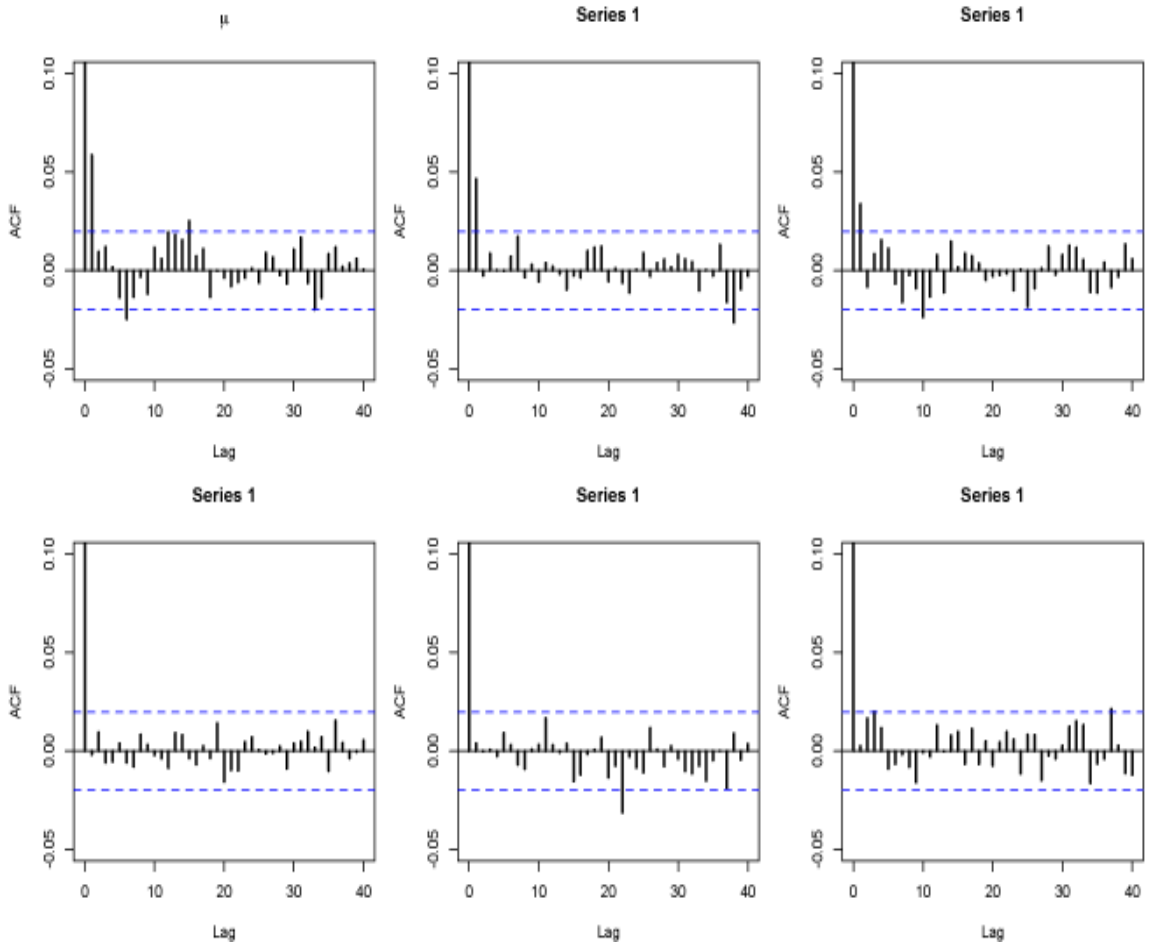
  - μ at second level
  - Now

$$\begin{aligned} Y_{ij} &\sim \mathcal{N}(\mu + \theta_i, \sigma^2), \\ \theta_i &\sim \mathcal{N}(0, \tau^2), \\ \mu &\sim \mathcal{N}(\mu_0, \sigma_\mu^2). \end{aligned}$$

  - μ at first level

Reparameterization

Oneway Models for the Energy Data



- Top = Then
- Bottom = Now
- Very similar
- Then slightly better?

Reparameterization
Covariances of the Oneway Models

- But look at the covariance matrix of the subchain $(\mu^{(t)}, \theta_1^{(t)}, \theta_2^{(t)})$

Then: $Y_{ij} \sim \mathcal{N}(\theta_i, \sigma^2)$

$$\begin{pmatrix} 1.056 & -0.175 & -0.166 \\ -0.175 & 1.029 & 0.018 \\ -0.166 & 0.018 & 1.026 \end{pmatrix}$$

Now: $Y_{ij} \sim \mathcal{N}(\mu + \theta_i, \sigma^2)$

$$\begin{pmatrix} 1.604 & 0.681 & 0.698 \\ 0.681 & 1.289 & 0.278 \\ 0.698 & 0.278 & 1.304 \end{pmatrix},$$

- So the new model is not as good as the old
- The covariances are all bigger
  - ▷ It will not mix as fast
- A pity: I like the new model better

Rao–Blackwellization
Introduction

- We have already seen Rao–Blackwellization in Chapter 4
  - Produced improved variance over standard empirical average
- For $(X, Y) \sim f(x, y)$, parametric Rao–Blackwellization is based on
  - $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X|Y]] = \mathbb{E}[\delta(Y)]$
  - $\text{var}[\delta(Y)] \leq \text{var}(X)$

Example: Poisson Count Data

- For 360 consecutive time units
- Record the number of passages of individuals per unit time past some sensor.

Number of passages	0	1	2	3	4 or more
Number of observations	139	128	55	25	13

Rao–Blackwellization
Poisson Count Data

- The data involves a grouping of the observations with four passages or more.
- This can be addressed as a missing-data model
  - Assume that the ungrouped observations are $X_i \sim \mathcal{P}(\lambda)$
  - The likelihood of the model is

$$\ell(\lambda|x_1,\ldots,x_5) \propto e^{-347\lambda}\lambda^{128+55\times 2+25\times 3}\left(1-e^{-\lambda}\sum_{i=0}^{3}\lambda^i/i!\right)^{13}$$

    for $x_1 = 139, \ldots, x_5 = 13$.

- For $\pi(\lambda) = 1/\lambda$ and missing data $\mathbf{z} = (z_1, \ldots, z_{13})$
  - We have a completion Gibbs sampler from the full conditionals

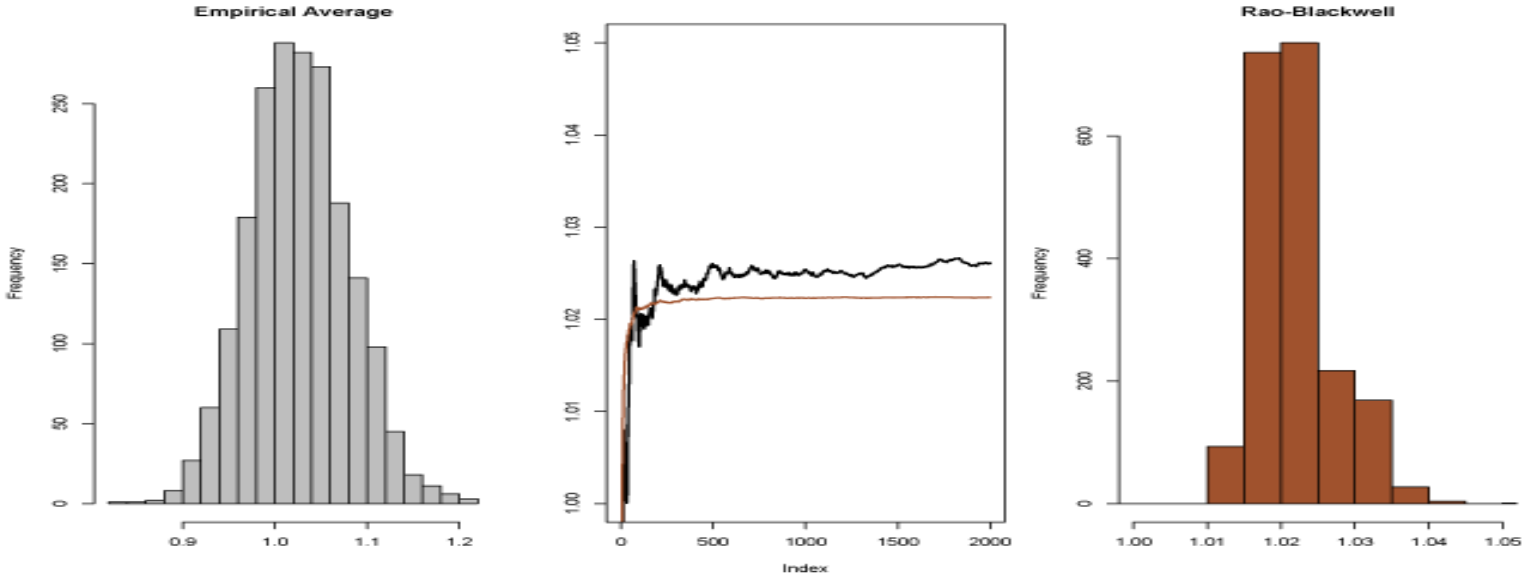
$$\begin{aligned} Z_i^{(t)} &\sim \mathcal{P}(\lambda^{(t-1)})\, \mathbb{I}_{y\geq 4}, \quad i = 1,\ldots,13, \\ \lambda^{(t)} &\sim \mathcal{G}\left(313 + \sum_{i=1}^{13} Z_i^{(t)},\ 360\right). \end{aligned}$$

Rao–Blackwellization
Comparing Estimators

- The empirical average is $\frac{1}{T}\sum_{t=1}^{T}\lambda^{(t)}$
- The Rao–Blackwellized estimate of λ is then given by

$$\mathbb{E}\left[\frac{1}{T}\sum_{t=1}^{T}\lambda^{(t)}\Big|, z_1^{(t)},\ldots,z_{13}^{(t)}\right] = \frac{1}{360T}\sum_{t=1}^{T}\left(313+\sum_{i=1}^{13} z_i^{(t)}\right),$$

- Note the massive variance reduction.



Generating Truncated Poisson Variables
Using While

- The truncated Poisson variable can be generated using the `while` statement

```
> for (i in 1:13){while(y[i]<4) y[i]=rpois(1,lam[j-1])}
```

or directly with

```
> prob=dpois(c(4:top),lam[j-1])
> for (i in 1:13) z[i]=4+sum(prob<runif(1)*sum(prob))
```

- Lets look at a comparison
- R code

Gibbs Sampling with Improper Priors
Introduction

- There is a particular danger resulting from careless use of the Gibbs sampler.
- The Gibbs sampler is based on conditional distributions
- It is particularly insidious is that

  (1) These conditional distributions may be well-defined

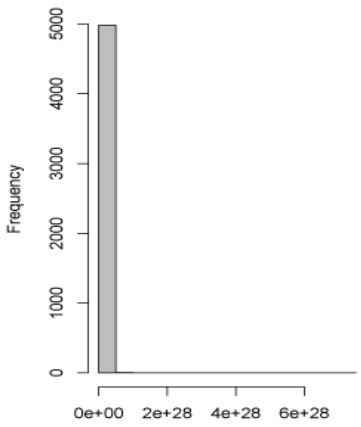
  (2) They may be simulated from

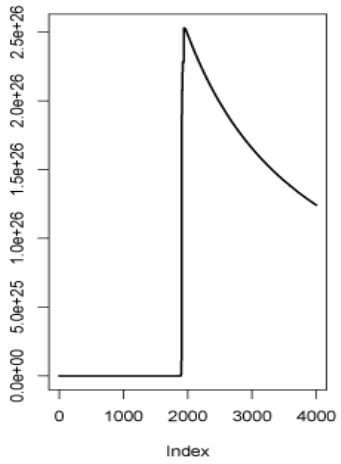
  (3) But may not correspond to any joint distribution!

- This problem is not a defect of the Gibbs sampler
- It reflects use of the Gibbs sampler when assumptions are violated.
- Corresponds to using Bayesian models with improper priors

Gibbs Sampling with Improper Priors
A Very Simple Example

- The Gibbs sampler can be constructed directly from conditional distributions
  - ▷ Leads to carelessness about checking the propriety of the posterior
- The pair of conditional densities $X|y \sim \mathcal{E}xp(y)\,, \quad Y|x \sim \mathcal{E}xp(x)\,,$
  - ▷ Well-defined conditionals with no joint probability distribution.





- The pictures are absolute rubbish!
- Not a recurrent Markov chain
- Stationary measure $= \exp(-xy)$
- No finite integral

- Histogram and cumulative average

Gibbs Sampling with Improper Priors
A Very Scary Example

- Oneway model $Y_{ij} = \mu + \alpha_i + \varepsilon_{ij}$,
  - $\alpha_i \sim \mathcal{N}(0, \sigma^2)$ and $\varepsilon_{ij} \sim \mathcal{N}(0, \tau^2)$
  - The Jeffreys (improper) prior for μ, σ, and τ is $\pi(\beta, \sigma^2, \tau^2) = \frac{1}{\sigma^2\tau^2}$.
- Conditional distributions

$$\begin{aligned}
\alpha_i|y, \mu, \sigma^2, \tau^2 &\sim \mathcal{N}\left(\frac{J(\bar{y}_i - \mu)}{J + \tau^2\sigma^{-2}}, (J\tau^{-2} + \sigma^{-2})^{-1}\right), \\
\mu|\alpha, y, \sigma^2, \tau^2 &\sim \mathcal{N}(\bar{y} - \bar{\alpha}, \tau^2/IJ), \\
\sigma^2|\alpha, \mu, y, \tau^2 &\sim \mathcal{IG}(I/2, (1/2)\sum_i \alpha_i^2), \\
\tau^2|\alpha, \mu, y, \sigma^2 &\sim \mathcal{IG}(IJ/2, (1/2)\sum_{i,j} (y_{ij} - \alpha_i - \mu)^2),
\end{aligned}$$

- Are well-defined
- Can run a Gibbs sampler
- But there is no proper joint distribution
- Often this is impossible to detect by monitoring the output

Gibbs Sampling with Improper Priors
A Final Warning

ϟ

- Graphical monitoring cannot exhibit deviant behavior of the Gibbs sampler.
- There are many examples, some published, of null recurrent Gibbs samplers
  - Undetected by the user
- The Gibbs sampler is valid only if the joint distribution has a finite integral.

- With improper priors in a Gibbs sampler
  - The posterior must always be checked for propriety.
- Improper priors on variances cause more trouble than those on means

Chapter 8: Monitoring Convergence of MCMC Algorithms

"Why does he insist that we must have a diagnosis? Some things are not meant to be known by man."

Susanna Gregory
An Unholy Alliance

This Chapter

- We look at different diagnostics to check the convergence of an MCMC algorithm
- To answer to question: "When do we stop our MCMC algorithm?"
- We distinguish between two separate notions of convergence:
  - Convergence to stationarity
  - Convergence of ergodic averages
- We also discuss some convergence diagnostics contained in the coda package

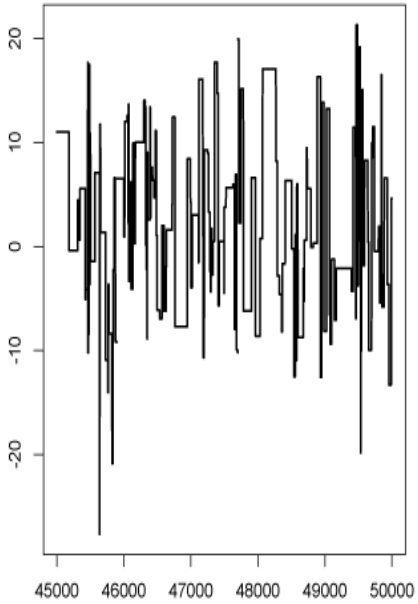
Monitoring Convergence
Introduction

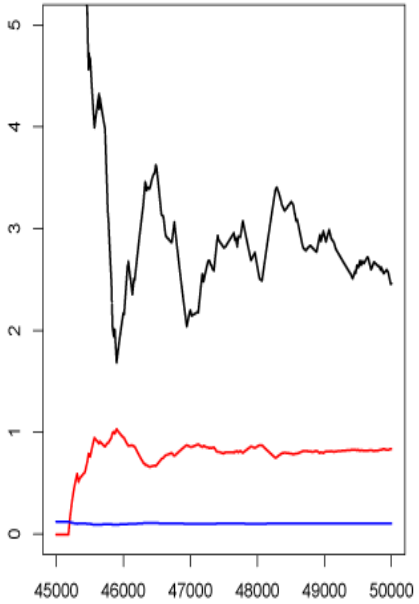
- The MCMC algorithms that we have seen
  - ▷ Are convergent because the chains they produce are ergodic.
- Although this is a necessary theoretical validation of the MCMC algorithms
  - ▷ It is insufficient from the implementation viewpoint
- Theoretical guarantees do not tell us
  - ▷ When to stop these algorithms and produce our estimates with confidence.
- In practice, this is nearly impossible
- Several runs of your program are usually required until
  - ▷ You are satisfied with the outcome
  - ▷ You run out of time and/or patience

Monitoring Convergence

Monitoring What and Why

- There are three types of convergence for which assessment may be necessary.





- Convergence to the stationary distribution
- Convergence of Averages
- Approximating iid Sampling

Monitoring Convergence
Convergence to the Stationary Distribution

- First requirement for convergence of an MCMC algorithm
  - $(x^{(t)}) \sim f$, the stationary distribution
  - This sounds like a minimal requirement
- Assessing that $x^{(t)} \sim f$ is difficult with only a *single realization*
- A slightly less ambitious goal: Assess the independence from the starting point $x^{(0)}$ based on several realizations of the chain using the same transition kernel.

- When running an MCMC algorithm, the important issues are
  - The speed of exploration of the support of f
  - The degree of correlation between the $x^{(t)}$'s

Monitoring Convergence
Tools for AssessingConvergence to the Stationary Distribution

- A major tool for assessing convergence: Compare performance of several chains
- This means that the slower chain in the group governs the convergence diagnostic
- Multiprocessor machines is an incentive for running replicate parallel chains
  - Can check for the convergence by using several chains at once
  - May not be much more costly than using a single chain

- Looking at a single path of the Markov chain produced by an MCMC algorithm makes it difficult to assess convergence
- MCMC algorithms suffer from the major defect that
  - "you've only seen where you've been"
- The support of f that has not yet been visited is almost impossible to detect.

Monitoring Convergence
Convergence of Averages

- A more important convergence issue is convergence of the empirical average

$$\frac{1}{T}\sum_{t=1}^{T} h(x^{(t)}) \to BE_f[h(X)]$$

- Two features that distinguish stationary MCMC outcomes from iid ones
  - ▷ The probabilistic dependence in the sample
  - ▷ The mixing behavior of the transition,
  - ▷ That is, how fast the chain explores the support of f
- "Stuck in a mode" might appear to be stationarity
  - ▷ The missing mass problem again

- Also: The CLT might not be available

Monitoring Convergence
Approximating iid sampling

- Ideally, the approximation to f provided by MCMC algorithms should
  - ▷ Extend to the (approximate) production of iid samples from f.
- A practical solution to this issue is to use *subsampling* (or *batch sampling*)
  - ▷ Reduces correlation between the successive points of the Markov chain.
- Subsampling illustrates this general feature but it loses in efficiency
- Compare two estimators
  - ▷ δ_1: Uses all of the Markov chain
  - ▷ δ_2: Uses subsamples
- It can be shown that

$$\text{var}(\delta_1) \leq \text{var}(\delta_2)$$

Monitoring Convergence
The coda package

- Plummer *et al.* have written an R package called coda
- Contains many of the tools we will be discussing in this chapter
- Download and install with `library(coda)`
- Transform an MCMC output made of a vector or a matrix into an MCMC object that can be processed by coda, as in

```
> summary(mcmc(X))
```

or

```
> plot(mcmc(X))
```

Monitoring Convergence to Stationarity
Graphical Diagnoses

- A first approach to convergence control
  - Draw pictures of the output of simulated chains
- Componentwise as well as jointly
  - In order to detect deviant or nonstationary behaviors

- `coda` provides this crude analysis via the `plot` command
- When applied to an `mcmc` object
  - Produces a trace of the chain across iterations
  - And a non-parametric estimate of its density, parameter by parameter

Monitoring Convergence to Stationarity
Graphical Diagnoses for a Logistic Random Effect Model

Example: Random effect logit model

- Observations y_{ij} are modeled conditionally on one covariate x_{ij} as

$$P(y_{ij} = 1|x_{ij}, u_i, \beta) = \frac{\exp\{\beta x_{ij} + u_i\}}{1 + \exp\{\beta x_{ij} + u_i\}}, i = 1, \ldots, n, \; j = 1, \ldots, m$$

  - $u_i \sim \mathcal{N}(0, \sigma^2)$ is an unobserved random effect
  - This is missing data

- We fit this with a Random Walk Metropolis–Hastings algorithm.

Monitoring Convergence to Stationarity
Fitting a Logistic Random Effect Model

- The complete data likelihood is

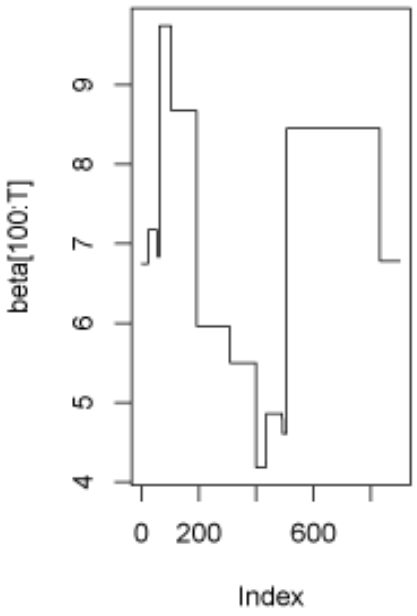
$$\prod_{ij} \left(\frac{\exp\{\beta x_{ij} + u_i\}}{1 + \exp\{\beta x_{ij} + u_i\}} \right)^{y_{ij}} \left(\frac{1}{1 + \exp\{\beta x_{ij} + u_i\}} \right)^{1-y_{ij}}$$

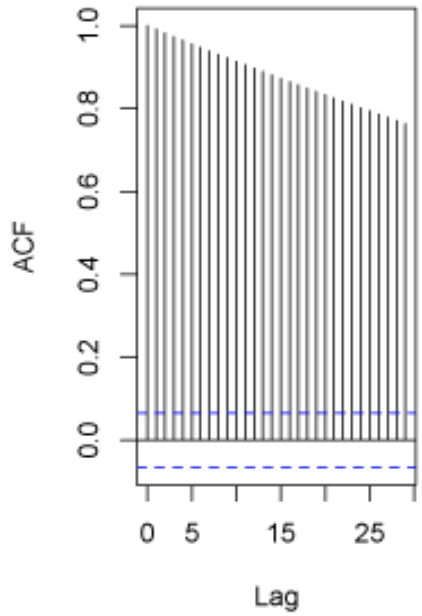
- This is the target in our Metropolis–Hastings algorithm
  - Simulate random effects $u_i^{(t)} \sim N(u_i^{(t-1)}, \sigma^2)$
  - Simulate the logit coefficient $\beta^{(t)} \sim N(\beta^{(t-1)}, \tau^2)$
  - Specify σ^2 and τ^2

- σ^2 and τ^2 affect mixing

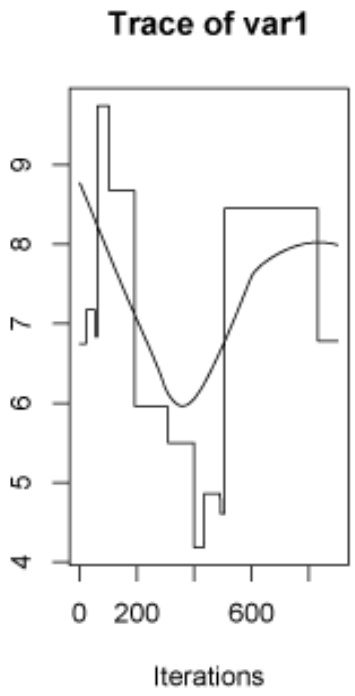
Monitoring Convergence to Stationarity
ACF and Coda

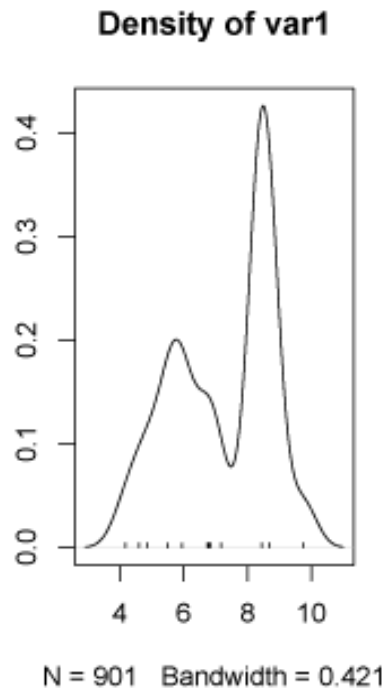
- Trace and acf:





- Coda





- R code

Tests of Stationarity
Nonparametric Tests: Kolmogorov-Smirnov

- Other than a graphical check, we can try to test for independence
- Standard non-parametric tests of fit, such as Kolmogorov–Smirnov
  - Apply to a single chain to compare the distributions of the two halves
  - Also can apply to parallel chains
- There needs to be a correction for the Markov correlation
  - The correction can be achieved by introducing a batch size
- We use

$$K = \frac{1}{M} \sup_{\eta} \left| \sum_{g=1}^{M} \mathbb{I}_{(0,\eta)}(x_1^{(gG)}) - \sum_{g=1}^{M} \mathbb{I}_{(0,\eta)}(x_2^{(gG)}) \right|$$

  - With G = batch size, M = sample size

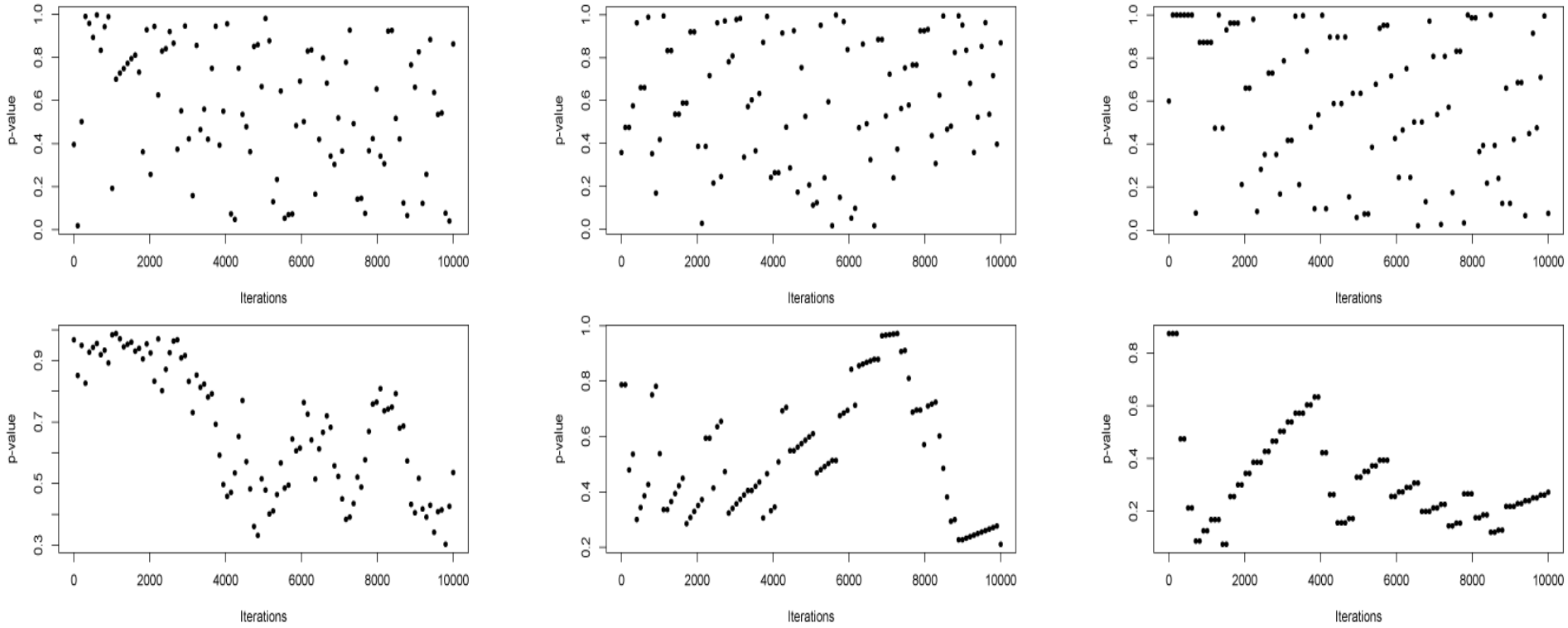
Tests of Stationarity
Kolmogorov-Smirnov for the Pump Failure Data

Example: Poisson Hierarchical Model

- Consider again the nuclear pump failures
- We monitor the subchain $(\beta^{(t)})$ produced by the algorithm
  - ▷ We monitor one chain split into two halves
  - ▷ We also monitor two parallel chains
- Use `R` command `ks.test`
- We will see (next slide) that the results are not clear

Monitoring Convergence

Kolmogorov-Smirnov p-values for the Pump Failure Data



- Upper=split chain; Lower = Parallel chains; L → R: Batch size 10, 100, 200.
- Seems too variable to be of little use
- This is a good chain! (fast mixing, low autocorrelation)

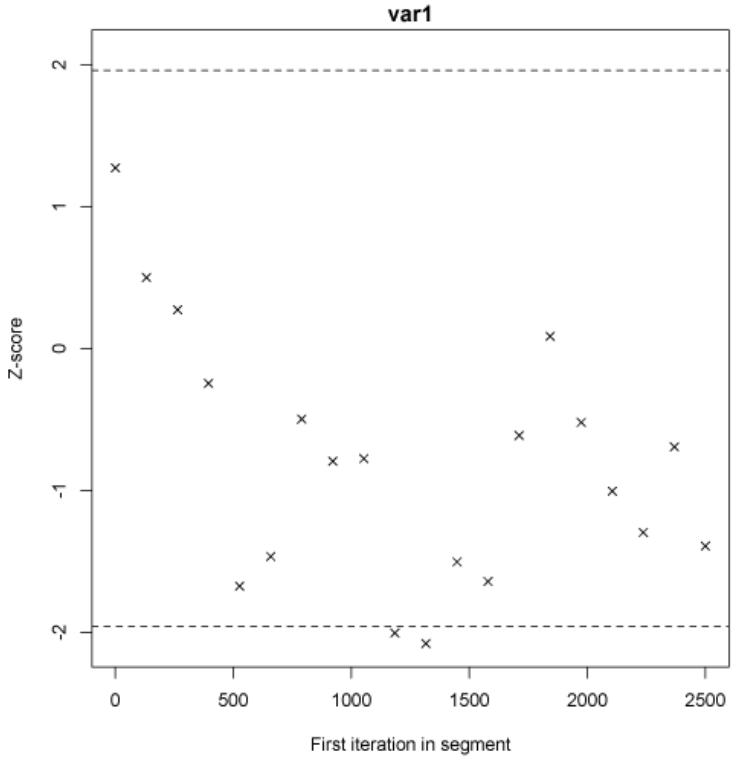
Monitoring Convergence
Tests Based on Spectral Analysis

- There are convergence assessments spectral or Fourier analysis
- One is due to Geweke
  - Constructs the equivalent of a t test
  - Assess equality of means of the first and last parts of the Markov chain.
- The test statistic is

$$\sqrt{T}(\delta_A - \delta_B) \Big/ \sqrt{\frac{\sigma_A^2}{\tau_A} + \frac{\sigma_B^2}{\tau_B}},$$

  - δ_A and δ_B are the means from the first and last parts
  - σ_A^2 and σ_B^2 are the spectral variance estimates
- Implement with `geweke.diag` and `geweke.plot`

Monitoring Convergence
Geweke Diagnostics for Pump Failure Data

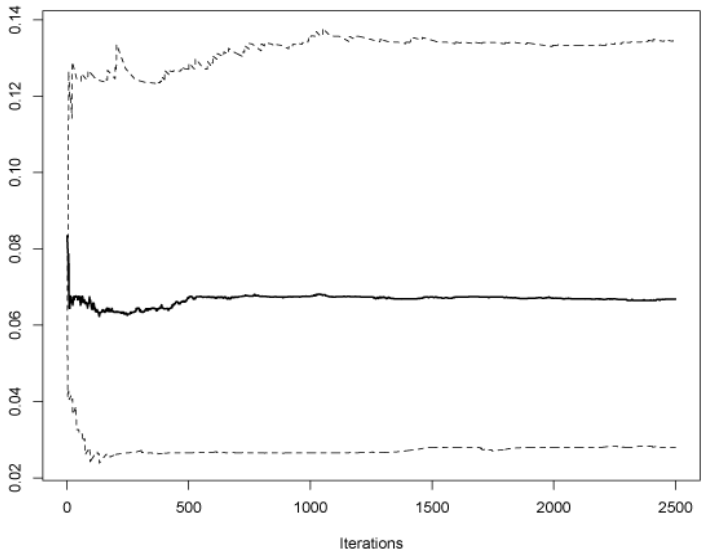


- For λ_1
  - t-statistic $= 1.273$
  - Plot discards successive beginning segments
  - Last z-score only uses last half of chain

- Heidelberger and Welch have a similar test: `heidel.diag`

Monitoring Convergence of Averages
Plotting the Estimator

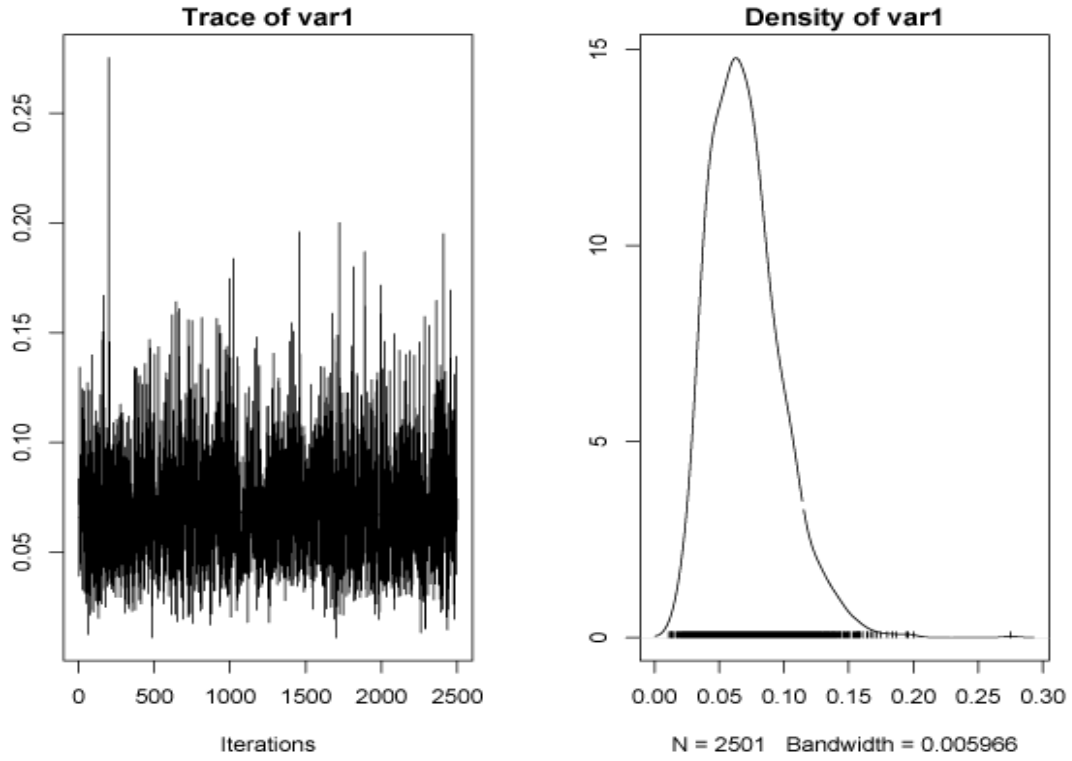
- The initial and most natural diagnostic is to plot the evolution of the estimator
- If the curve of the cumulated averages has not stabilized after T iterations
  - ▷ The length of the Markov chain must be increased.
- The principle can be applied to multiple chains as well.
  - ▷ Can use `cumsum`, `plot(mcmc(coda))`, and `cumuplot(coda)`



- For λ_1 from Pump failures
- `cumuplot` of second half

Monitoring Convergence of Averages
Trace Plots and Density Estimates

- `plot(mcmc(lambda))` produces two graphs

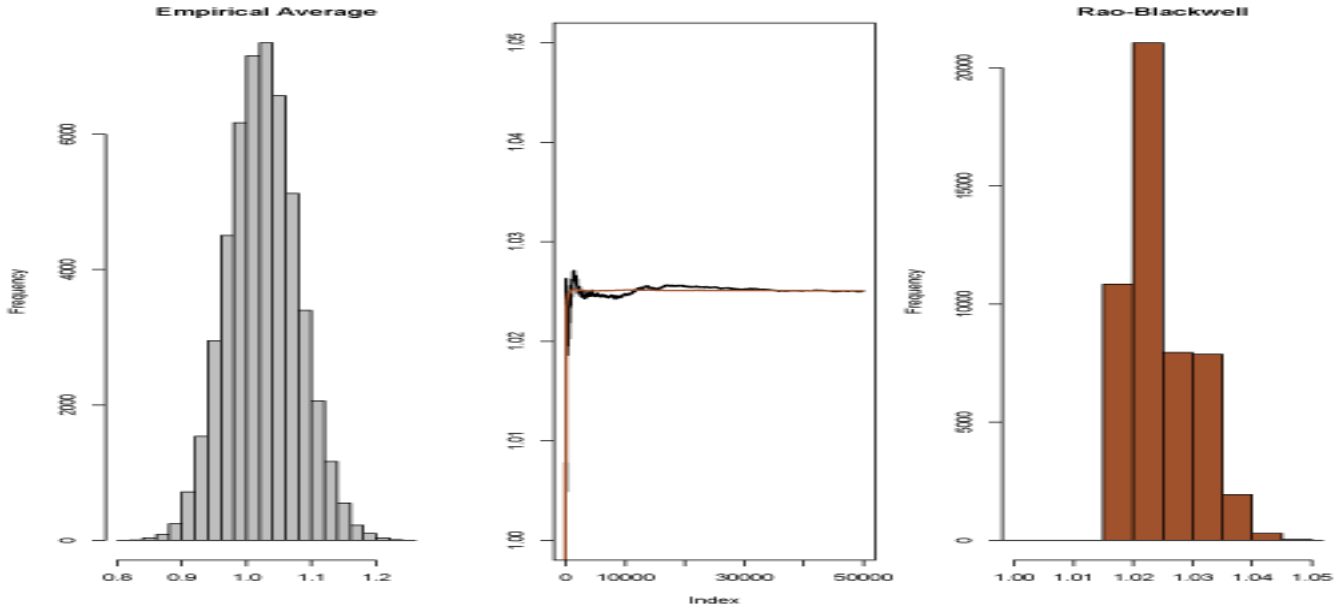


- Trace Plot
- Density Estimate

- Note: To get second half of chain `temp=lambda[2500:5000]`, `plot(mcmc(temp))`

Monitoring Convergence of Averages
Multiple Estimates

- Can use several convergent estimators of $\mathbb{E}_f[h(\theta)]$ based on the same chain
  - Monitor until all estimators coincide
- Recall Poisson Count Data
  - Two Estimators of Lambda: Empirical Average and RB
  - Convergence Diagnostic → Both estimators converge - 50,000 Iterations



Monitoring Convergence of Averages
Computing Multiple Estimates

- Start with a Gibbs sampler $\theta|\eta$ and $\eta|\theta$
- Typical estimates of $h(\theta)$
  - The empirical average $S_T = \frac{1}{T} \sum_{t=1}^{T} h(\theta^{(t)})$
  - The Rao–Blackwellized version $S_T^C = \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[h(\theta)|\eta^{(t)}]$,
  - Importance sampling: $S_T^P = \sum_{t=1}^{T} w_t \, h(\theta^{(t)})$,
    - $w_t \propto f(\theta^{(t)})/g_t(\theta^{(t)})$
    - f = target, g = candidate

Monitoring Convergence of Multiple Estimates
Cauchy Posterior Simulation

- The hierarchical model

$$\begin{aligned} X_i &\sim \text{Cauchy}(\theta), \quad i = 1, \ldots, 3 \\ \theta &\sim N(0, \sigma^2) \end{aligned}$$

- Has posterior distribution

$$\pi(\theta|x_1, x_2, x_3) \propto e^{-\theta^2/2\sigma^2} \prod_{i=1}^{3} \frac{1}{(1 + (\theta - x_i)^2)}$$

- We can use a Completion Gibbs sampler

$$\eta_i|\theta, x_i \sim \mathcal{E}xp\left(\frac{1 + (\theta - x_i)^2}{2}\right),$$

$$\theta|x_1, x_2, x_3, \eta_1, \eta_2, \eta_3 \sim \mathcal{N}\left(\frac{\eta_1 x_1 + \eta_2 x_2 + \eta_3 x_3}{\eta_1 + \eta_2 + \eta_3 + \sigma^{-2}}, \frac{1}{\eta_1 + \eta_2 + \eta_3 + \sigma^{-2}}\right),$$

Monitoring Convergence of Multiple Estimates
Completion Gibbs Sampler

- The Gibbs sampler is based on the latent variables η_i, where

$$\int e^{-\frac{1}{2}\eta_i(1+(x_i-\theta)^2)} d\eta_i = \frac{2}{1+(x_i-\theta)^2}$$

- With

$$\eta_i \sim \text{Exponential}\left(\frac{1}{2}(1+(x_i-\theta)^2)\right)$$

- Monitor with three estimates of θ
  - Empirical Average
  - Rao-Blackwellized
  - Importance sample

Monitoring Convergence of Multiple Estimates
Calculating the Estimates

- Empirical Average

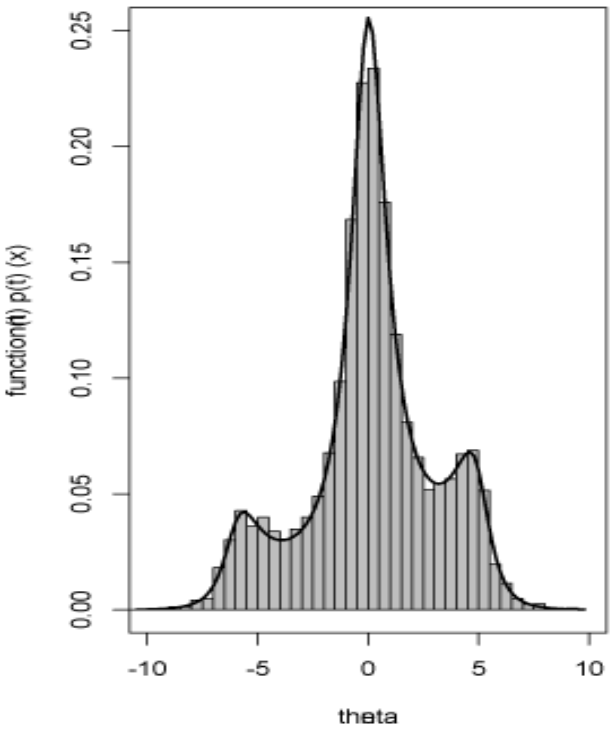
$$\frac{1}{M}\sum_{j=1}^{M}\hat{\theta}^{(j)}$$

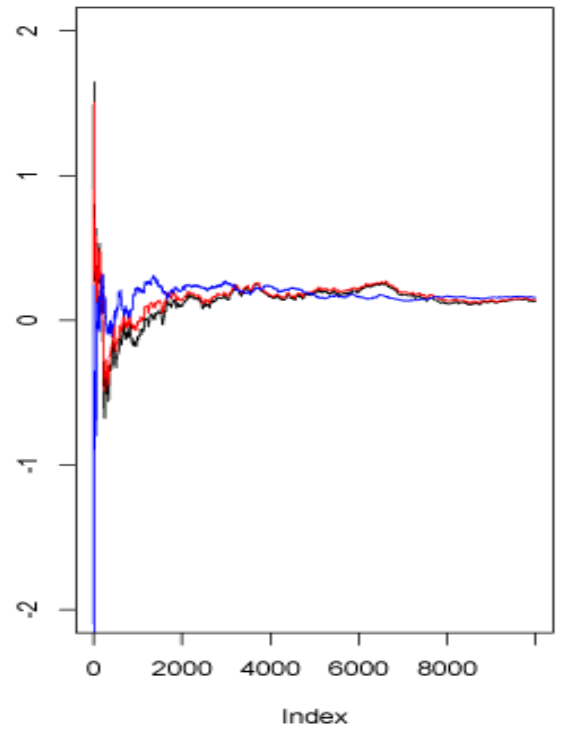
- Rao-Blackwellized

$$\theta|\eta_1,\eta_2,\eta_3 \sim N\left(\frac{\sum_i \eta_i x_i}{\frac{1}{\sigma^2}+\sum_i \eta_i}, \left[\frac{1}{\sigma^2}+\sum_i \eta_i\right]^{-1}\right)$$

- Importance sampling with Cauchy candidate

Monitoring Convergence of Multiple Estimates
Monitoring the Estimates





- Emp. Avg
- RB
- IS
  - ▷ Estimates converged
  - ▷ IS seems most stable

- When applicable, superior diagnostic to single chain
- Intrinsically conservative
  - ▷ Speed of convergence determined by slowest estimate

Monitoring Convergence of Averages
Between and Within Variances

- The Gelman-Rubin diagnostic uses multiple chains
- Based on a between-within variance comparison (anova-like)
  - Implemented in `coda` as `gelman.diag(coda)` and `gelman.plot(coda)`.
- For m chains $\{\theta_1^{(t)}\}, \ldots \{\theta_m^{(t)}\}$
  - The between-chain variance is $B_T = \dfrac{1}{M-1} \displaystyle\sum_{m=1}^{M} (\overline{\theta}_m - \overline{\theta})^2$,
  - The within-chain variance is $W_T = \frac{1}{M-1} \sum_{m=1}^{M} \frac{1}{T-1} \sum_{t=1}^{T} (\theta_m^{(t)} - \overline{\theta}_m)^2$
- If the chains have converged, these variances are the same (anova null hypothesis)

Monitoring Convergence of Averages
Gelman-Rubin Statistic

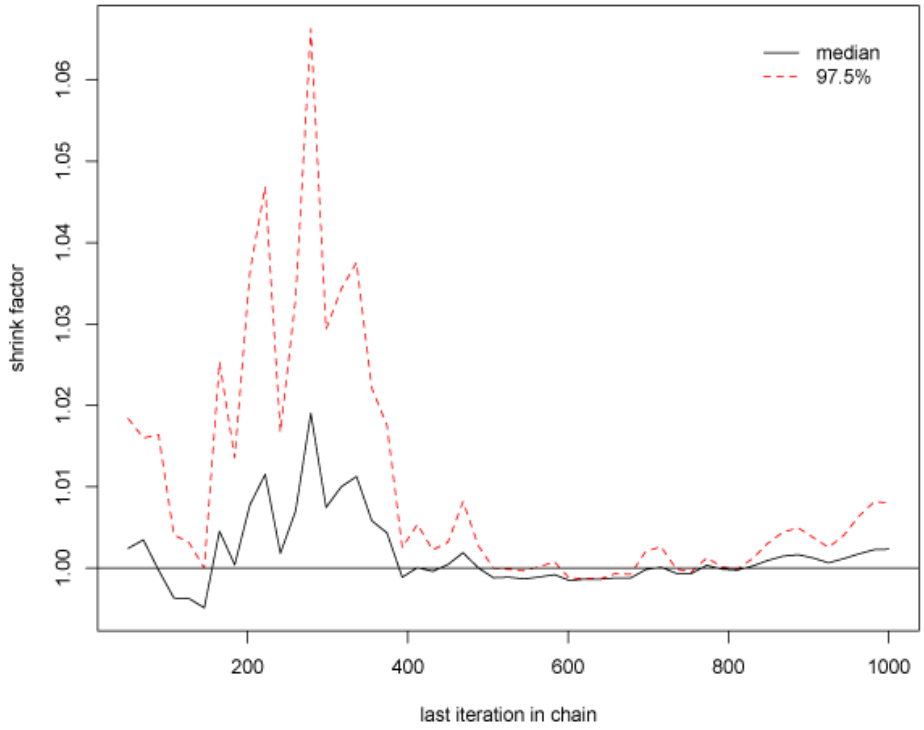
- B_T and W_T are combined into an F-like statistic
- The shrink factor, defined by

$$R_T^2 = \frac{\hat{\sigma}_T^2 + \dfrac{B_T}{M}}{W_T} \, \frac{\nu_T + 1}{\nu_T + 3},$$

  - $\hat{\sigma}_T^2 = \frac{T-1}{T} W_T + B_T$.
  - F-distribution approximation

- Enjoyed wide use because of simplicity and intuitive connections with anova
- R_T does converge to 1 under stationarity,
- However, its distributional approximation relies on normality
- These approximations are at best difficult to satisfy and at worst not valid.

Monitoring Convergence of Averages
Gelman Plot for Pump Failures

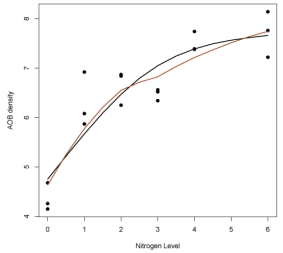


- Three chains for λ_1
- nsim=1000
- Suggests convergence
- `gelman.diag` gives

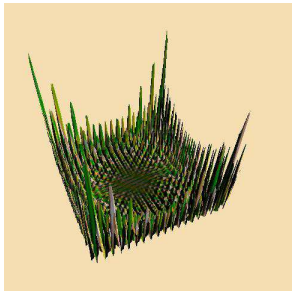
```
Point est.  97.5 % quantile
1.00        1.01
```

- R code

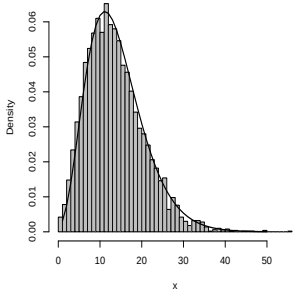
We Did All This!!!



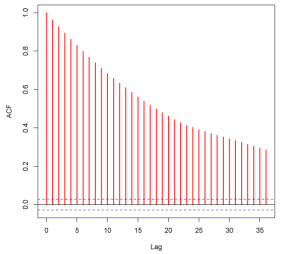
1. Intro



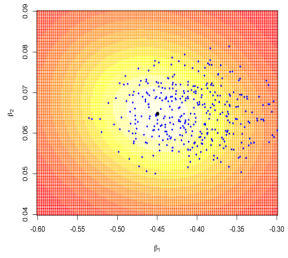
5. Optimization



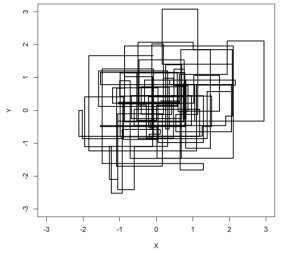
2. Generating



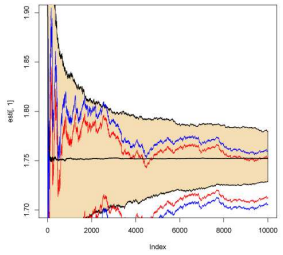
6. Metropolis



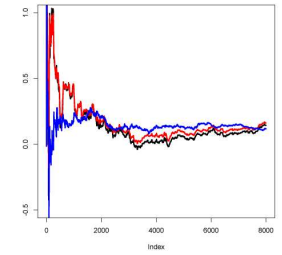
3. MCI



7. Gibbs



4. Acceleration



8. Convergence

Thank You for Your Attention

George Casella

casella@ufl.edu