Yet another intro to MCMC
Focusing on 2 main methods

Konstantinos Pateras

University of Thessaly, Department of Public and One Health

kostas.pateras@gmail.com

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What to expect?

Go to www.menti.com

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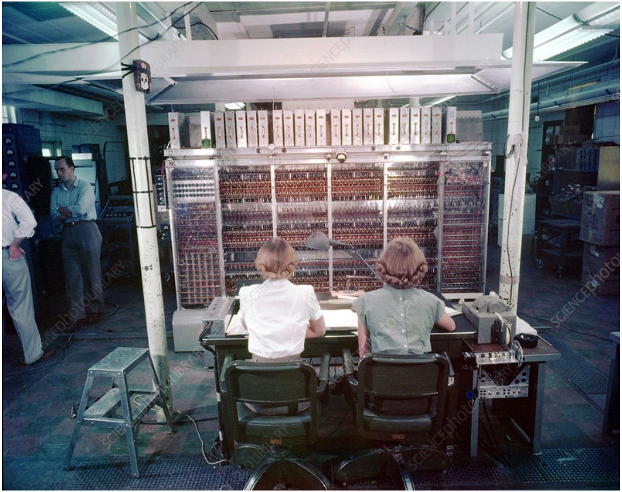
Why bother?

Why bother?

- Monte Carlo: Physical sciences (Astrophysics), Engineering (Thermodynamics), Climate change, Computational biology (Phylogenetics), Applied statistics (Bayesian approach), Artificial intelligence, among many
- MCMC: Computational statistics, computational physics and computational biology among others. Hierarchical modelling in Bayesian statistics

MANIAC I




MANHATTAN PROJECT
A
BOMB

Charles III of Monaco

Historical notes

- Monte carlo methods since 1920 (Enrico Fermi)
- Named after Nicholas Metropolis, Monte Carlo casino.
- Los Alamos labs 1940s (Stanislaw Ulam, John von Neumann, Nicholas Metropolis and others)
- Metropolis-Hastings 1970, Geman Geman Gibbs (1984)
- Mainstream in stats by Gelman and Rubin 1992 among others
- Mainstream software (BUGS 1996 (Gibbs), JAGS (Slice), Stan (Hamiltonian))

Basic notions

1. How to generate completely random numbers (not easy). R uses pseudo-random number generators.
2. Main assumption: Be able to generate from a Uniform(0,1)
3. Inverse transform method, inv-CDF,, (Rizzo pg 49)

Acceptance-Rejection method

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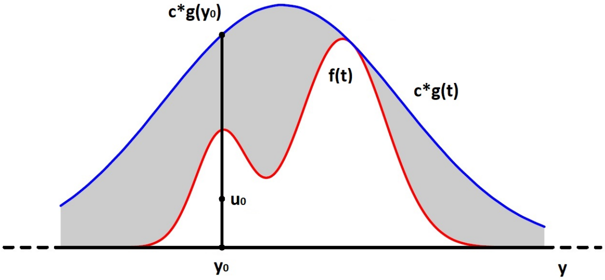
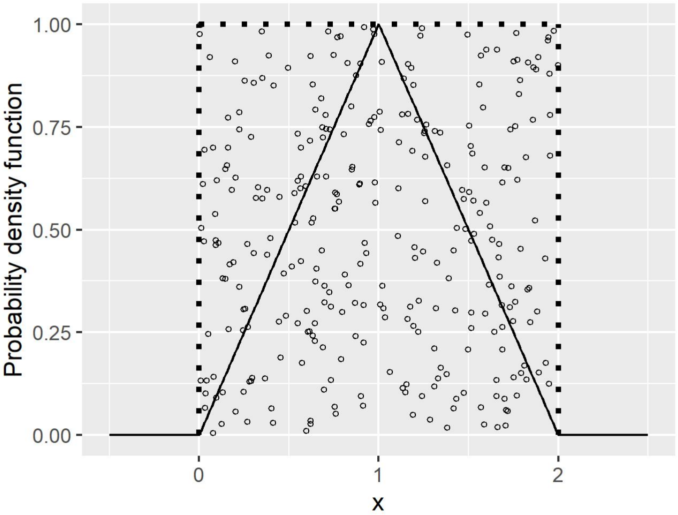
1. Find and generate Y from g for which $f(t) \leq c \cdot g(t), f(t) > 0$
   - i Generate a random $y^* \sim g$
   - ii Generate a random $u \sim Uniform(0, 1)$
   - iii If $u < f(y^*)/(c \cdot g(y^*))$ accept y^* as sample, otherwise reject y^*.
   - iv Repeat from step i.

Acceptance-Rejection figure



Acceptance-Rejection (quiz)



Acceptance-Rejection method

Example (Triangle probability density)

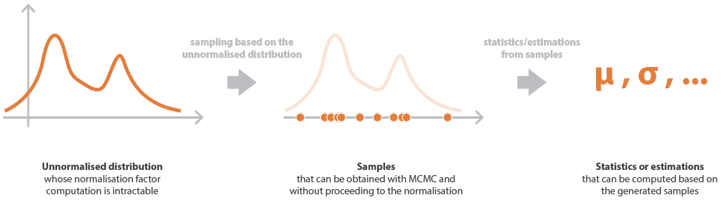
```
triangle.pdf = function(x){ # Definition of triangle pdf.
ifelse((0 < x) & (x < 1), x,
ifelse((1 <= x) & (x < 2), 2 - x, 0))
}

#simulates a sample of size (n) from the pdf f(x) via the acceptance/rejection algorithm
accept_reject = function(fx, n = 100, prop.val=1) {

x = numeric(n);count = 0

while(count < n) {
temp.x <- runif(1, 0, 2)
y <- runif(1, 0, 1)

if (y < fx(temp.x)) {
count = count + 1
x[count] <- temp.x
}

}

return(x)
}
sample = accept_reject(triangle.pdf, 50000)
length(sample)/50000 # Probability of acceptance
plot(density(sample), adjust=0.5)
```

Markov Chains

Some brief notions

- First order Markov Chains (Depend on last value)
- Irreducibility (Any state can reach another state)
- Aperiodicity
- (Positive) recurrent
- Stationary distribution

Markov Chains Concept



Source: Joseph Rocca, Bayesian inference problem, MCMC and variational inference

Markov Chains Concept 2

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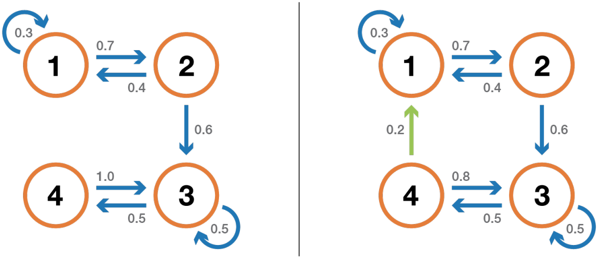
Markov Chains Assumption 1

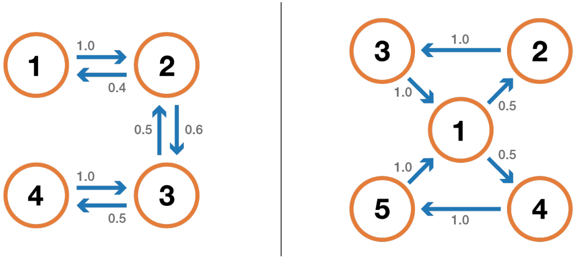
Illustration of the irreducibility property. The chain on the left is not irreducible: from 3 or 4 we can't reach 1 or 2. The chain on the right (one edge has been added) is irreducible: each state can be reached from any other state.



Source: Joseph Rocca, Bayesian inference problem, MCMC and variational inference

Markov Chains Assumption 2

Illustration of the aperiodicity property. The chain on the left is 2-periodic: when leaving any state, it always takes a multiple of 2 steps to come back to it. The chain on the right is 3-periodic.



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  2b Generate U from Uniform(0,1)

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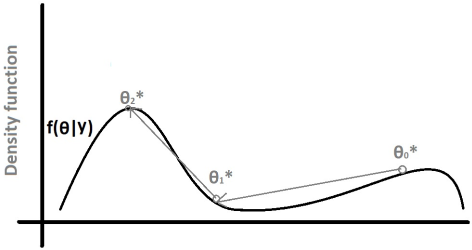
- 2a Generate θ^* from $N(\theta, s_\theta)$, what about s_θ?
- 2b Generate U from Uniform(0,1)
- 2c If $U \leq \dfrac{f(\theta^*|y)}{f(\theta|y)} = \dfrac{f(y|\theta^*)p(\theta^*)}{f(y|\theta)p(\theta)}$, accept θ^* and set $\theta = \theta^*$, otherwise set $\theta = \theta$
- 2d Increment t and repeat

Metropolis figure



Metropolis algorithm

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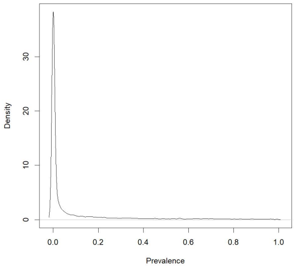

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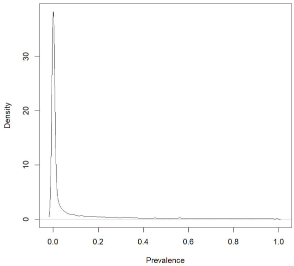


- Toy example: Prevalence of moderate adverse events of Covid-19 vaccine. Observed 50 events in a sample of 10,000, $y \sim B(50, 10^4)$.

Metropolis algorithm

Example (Theorem Slide Code)

```
metropolis <- function(burnin = 0, sample = 10000,
sigma = 0.05, initial_value = 0.05, plot=TRUE)

stopifnot(initial_value > 0, initial_value < 1)
stopifnot(sigma > 0)
burnin <- as.integer(burnin)
sample <- as.integer(sample)
stopifnot(burnin >= 0)
stopifnot(sample > 0)

# Redefine these to work on the log scale:
llikelihood_fun <- function(prevalence) dbinom(50, 10^4, prevalence, log=TRUE)
lprior_fun <- function(prevalence) dbeta(prevalence, 0.1, 1, log=TRUE)

parameters <- numeric(burnin+sample)
parameters[1] <- initial_value
current <- initial_value

post <- llikelihood_fun(current) + lprior_fun(current)
```

Metropolis algorithm

Example (Theorem Slide Code)

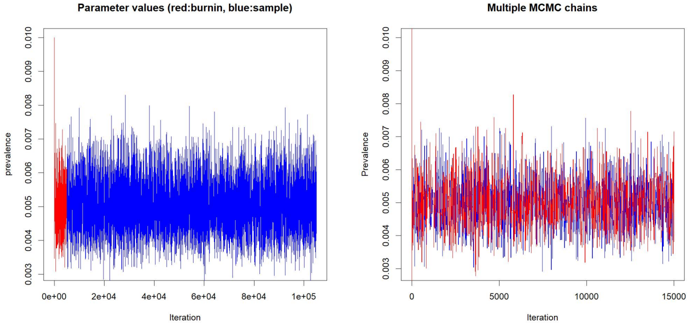
```
for(i in 2:(burnin+sample)){

proposal <- rnorm(1, current, sigma)

if(proposal > 0 \& proposal < 1){
U=log(runif(1,0,1))
newpost <- llikelihood_fun(proposal) + lprior_fun(proposal)
accept <- U <= newpost-post

if(accept){
current <- proposal
post <- newpost
}
}
parameters[i] <- current
}
```

Metropolis results



- ESS: 10000/647.67 = 15.43 iterations for an independent sample
- Geweke diagnostic: p-value=0.67
- Autocorrelation? How to fix this?

Gibbs sampler background

Named after JW Gibbs, invented 80 years after his death.
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2 For each iteration $t = 1, 2, ...T$ repeat

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   - 2a Set $\theta = \theta^{(t-1)}$
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- 2b For each parameter $j = 1, 2..., d$
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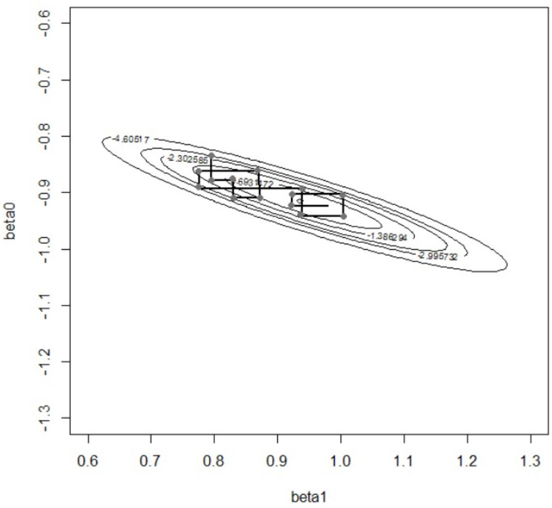
- 2c Increase t and repeat

One component is updated at a time. Conditionally conjugate models and others.

Gibbs sampler figure



Gibbs sampler

1 Example with a normal variable indicating average temperature for July in a time-span of 12 years. (Ntzoufras 2009)

- $\mu \sim N(\mu_0, \sigma_0^2)$ and $\sigma^2 \sim IG(a_0, b_0)$
- Compute conditional distributions $f(\mu|\sigma^2, y)$ and $f(\sigma^2|\mu, y)$
- $\mu|\sigma^2, y \sim N(w\tilde{y} + (1-w)\mu_0, w\frac{\sigma^2}{n})$, $w = \frac{\sigma_0^2}{\sigma^2/n + \sigma_0^2}$
  $\sigma|\mu, y \sim IG[(a_0) + n/2, b_0 + 1/2 \sum_1^n (y_i - \mu)^2]$

Gibbs sampler

Example (Gibbs with non-conjugate priors)

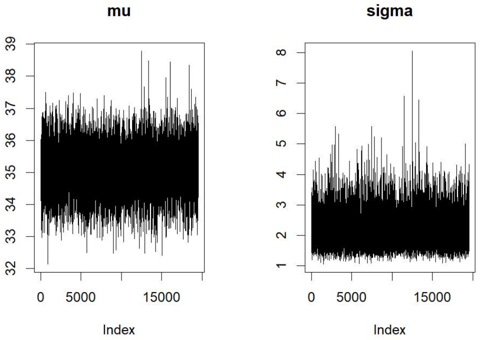
```
y<-c(32,36,37,34,38,36,33,36,37,35,32,35)
bary<-mean(y); n<-length(y)  # Set up data

# Set number of iterations
Iterations<-5000

# Set prior parameters.
mu0<-0; s0<-100; a0<-0.001; b0<-0.001

# Initialize vectors of sample values mu and sigma
theta <- matrix(nrow=Iterations, ncol=2)

# Set initial current mu(0) and sigma(0)
cur.mu<-0; cur.tau<-1; cur.s<-sqrt(1/cur.tau)
```

Gibbs sampler

Example (Gibbs with non-conjugate priors)

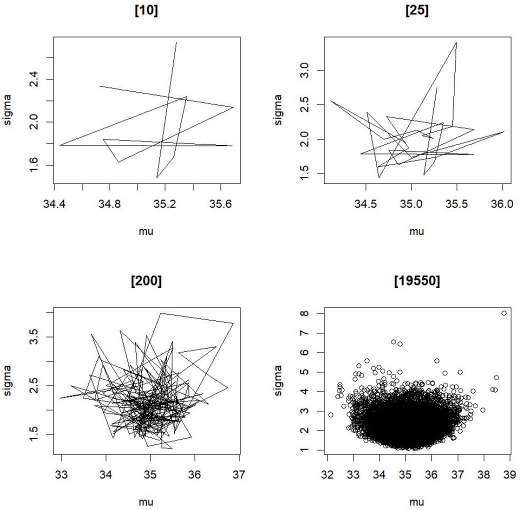
```
for (t in 1:Iterations){  # Repeat for t=1,...,T iterations

w<- s0^2/( cur.s^2/n+ s0^2) # Calculate w

m <- w*bary + (1-w)*mu0  # Calculate m
s <- sqrt( w * cur.s^2/n) # Calculate s

cur.mu <- rnorm(1, m, s) # Calculate mu

a <- a0 + 0.5*n # Calculate alpha
b <- b0 + 0.5 * sum( (y-cur.mu)^2) # Calculate beta

cur.tau <- rgamma( 1, a, b) # Calculate tau from gamma
cur.s <- sqrt(1/cur.tau) # Calculate sigma (inversed tau)

theta[t,]<-c( cur.mu, cur.s) # Set mu(t)=mu, sigma(t)=sigma
} # End of for loop
```

Gibbs results [univariate]

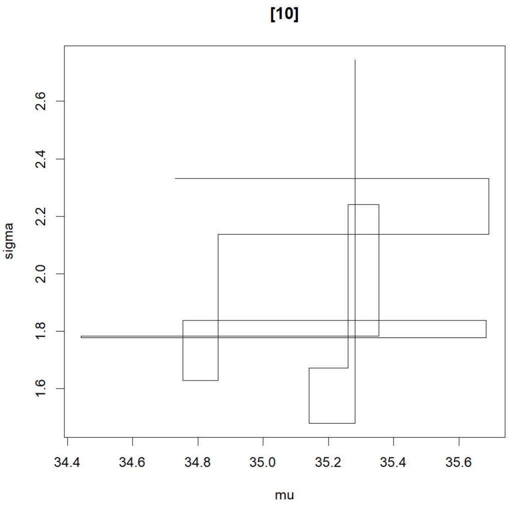


- ESS: $20000/18757.47 = 1.07$ iterations for an independent sample of μ
- Geweke diagnostic: p-value $= 0.49$

Gibbs results [both simultaneously]



Gibbs results [both step by step]



JAGS/WinBUGS code - Examples

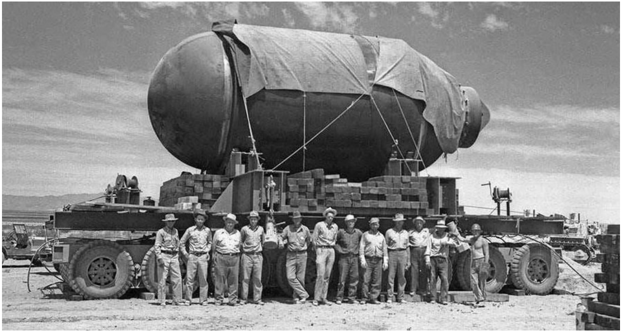
Metropolis example with $y = 50$ and $n = 10^4$

```
"model{
y ~ dbinom(main.ap, n)
main.ap  ~ dbeta(0.1,1)
}"
```

Gibbs example with y temperatures

```
"model{
for (i in 1:12){
y[i] ~ dnorm (mu, prec)
}
mu ~ dnorm (0, 0.01)
prec ~ dgamma (0.001, 0.001)
s2 <- 1/prec
}
}"
```

Epilogue



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Bibliography

- Maria L Rizzo, Statistical computing with R, 2008
- Ioannis Ntzoufras, Bayesian modelling using WinBUGS, 2009
- Martin Haugh, Monte-Carlo Simulation, MCMC and Bayesian Modelling
- Joseph Rocca, Bayesian inference problem, MCMC and variational inference
- Pre-course material - HARMONY Training School - Larissa Greece 2020