

Bayesian statistics with R

5. Markov chains Monte Carlo (MCMC)

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**Get posteriors with Markov chains
Monte Carlo (MCMC) methods**

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- $\Pr(\text{data}) = \int L(\text{data} \mid \theta) \Pr(\theta) d\theta$ is a N -dimensional integral if $\theta = \theta_1, \dots, \theta_N$
- Difficult, if not impossible to calculate!

Brute force approach via numerical integration

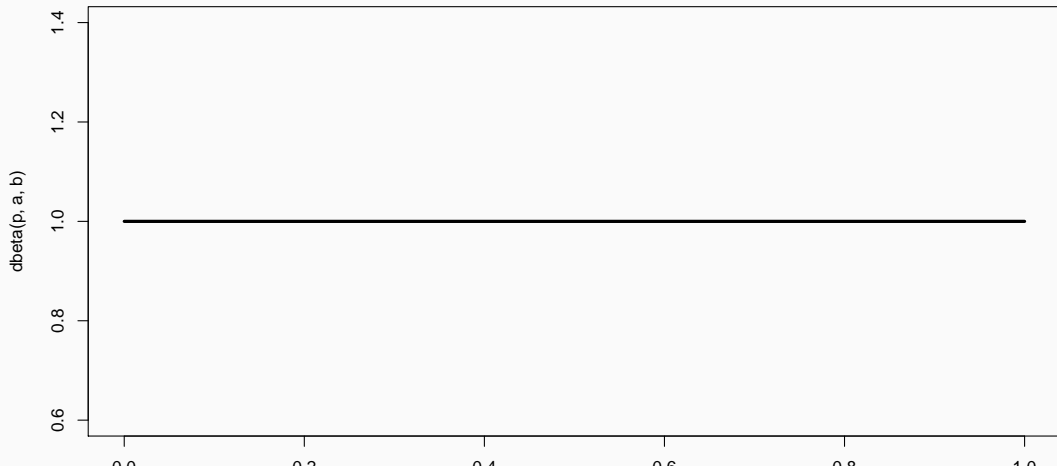
- Deer data

```
y <- 19 # nb of success  
n <- 57 # nb of attempts
```

- Likelihood $\text{Binomial}(57, \theta)$
- Prior $\text{Beta}(a = 1, b = 1)$

Beta prior

```
a <- 1; b <- 1; p <- seq(0,1,.002)
plot(p, dbeta(p,a,b), type='l', lwd=3)
```



Apply Bayes theorem

- Likelihood times the prior: $\Pr(\text{data} \mid \theta) \Pr(\theta)$

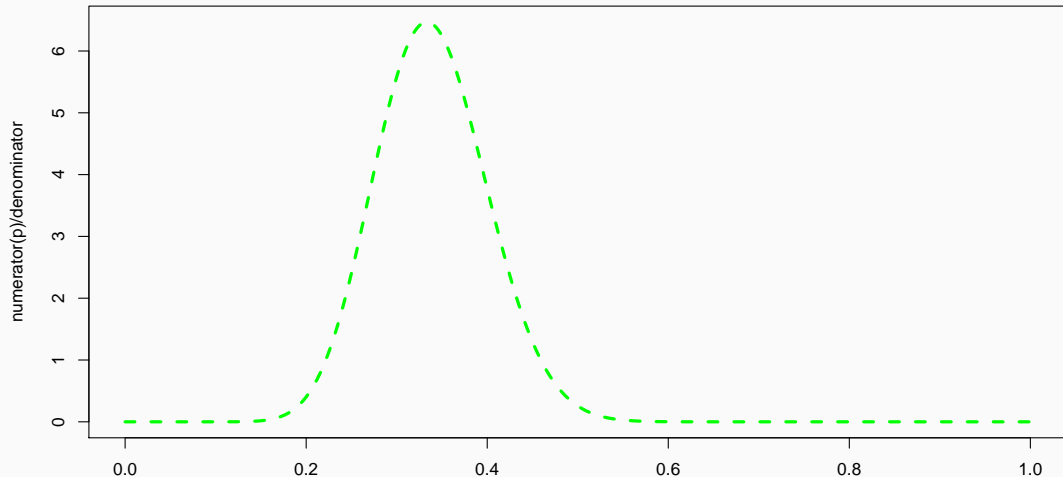
```
numerator <- function(p) dbinom(y,n,p)*dbeta(p,a,b)
```

- Averaged likelihood: $\Pr(\text{data}) = \int L(\theta \mid \text{data}) \Pr(\theta) d\theta$

```
denominator <- integrate(numerator,0,1)$value
```

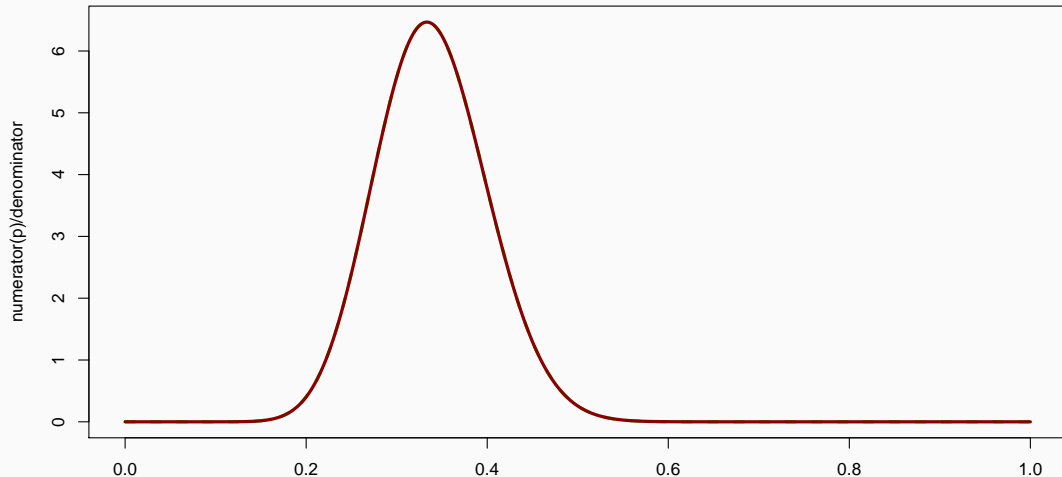
Posterior inference via numerical integration

```
plot(p, numerator(p)/denominator,type="l", lwd=3, col="green", lty=2)
```



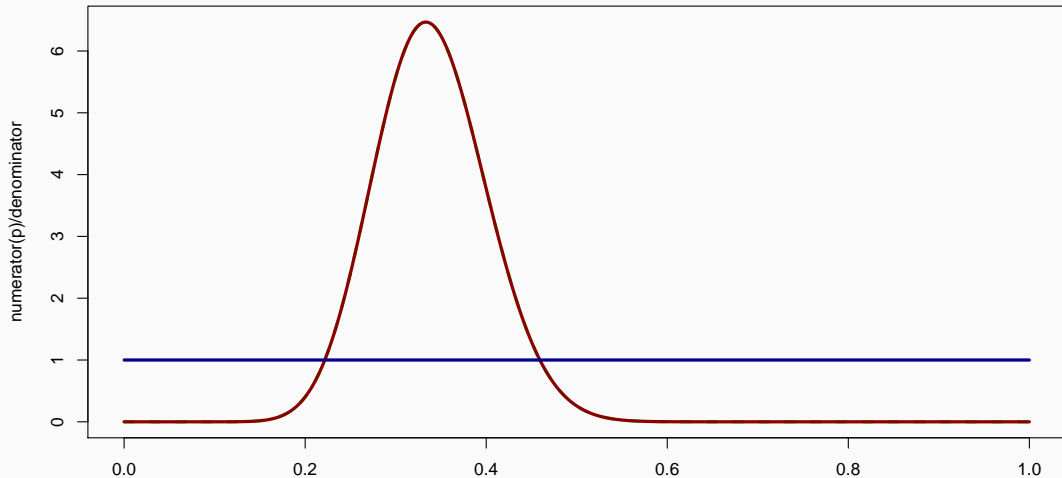
Superimpose explicit posterior distribution (Beta formula)

```
lines(p, dbeta(p,y+a,n-y+b), col='darkred', lwd=3)
```



And the prior

```
lines(p, dbeta(p,a,b), col='darkblue', lwd=3)
```



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- Do we really wish to calculate a 3D integral?

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THE JOURNAL OF CHEMICAL PHYSICS

VOLUME 21, NUMBER 6

JUNE, 1953

Equation of State Calculations by Fast Computing Machines

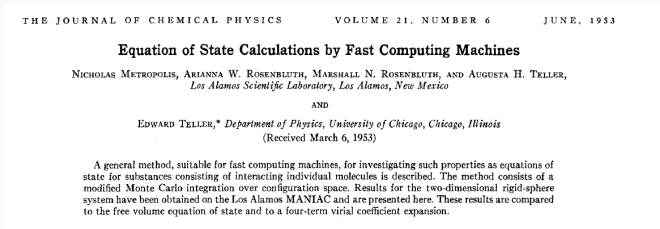
NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

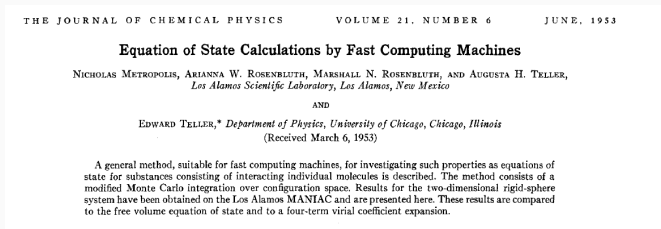
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

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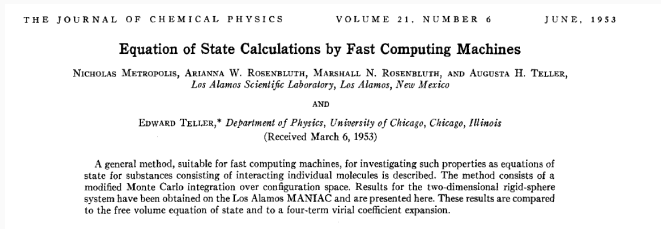
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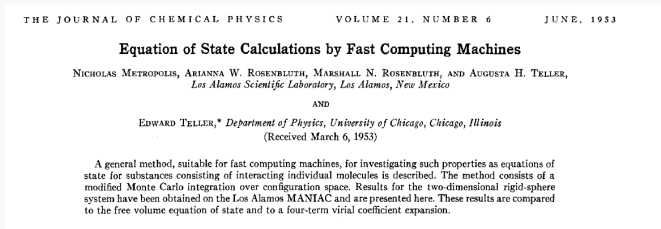
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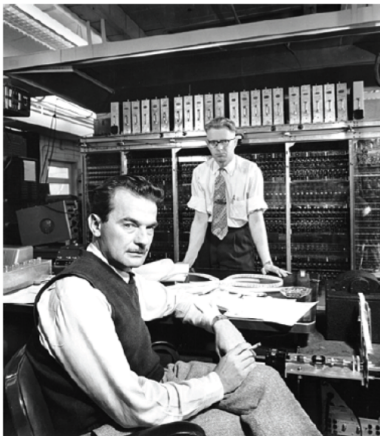
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- Markov chain Monte Carlo = MCMC; boost to Bayesian statistics!

MANIAC: Mathematical Analyzer, Numerical Integrator, and Computer



MANIAC:
1000 pounds
5 kilobytes of memory
70k multiplications/sec

Your laptop:
4-7 pounds
2-8 million kilobytes
Billions of multiplications/sec

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- Converge to equilibrium (aka stationary) distribution.
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- Several ways of constructing these chains: e.g., Metropolis-Hastings, Gibbs sampler, Metropolis-within-Gibbs.
- How to implement them in practice?!

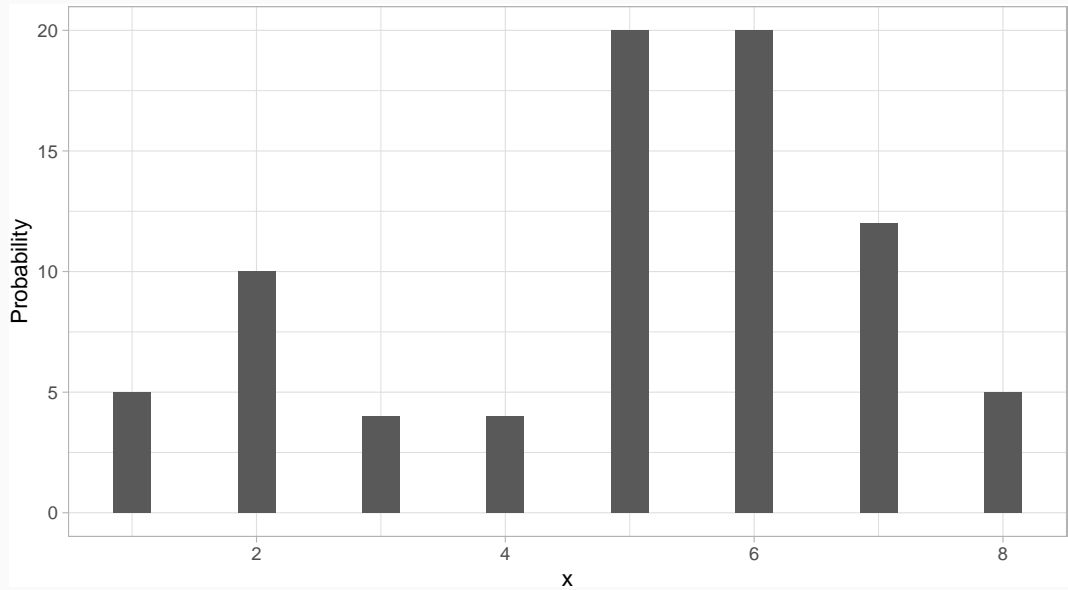
The Metropolis algorithm

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- We illustrate sampling from a discrete distribution. Suppose we define a discrete probability distribution on the integers $1, \dots, K$.
- We write a short function `pd()` in R taking on the values $1, \dots, 8$ with probabilities proportional to the values 5, 10, 4, 4, 20, 20, 12, and 5.

```
pd <- function(x){  
  values <- c(5, 10, 4, 4, 20, 20, 12, 5)  
  ifelse(x %in% 1:length(values), values[x], 0)  
}  
prob_dist <- data.frame(x = 1:8, prob = pd(1:8))  
prob_dist  
#>   x prob  
#> 1 1    5  
#> 2 2   10  
#> 3 3    4  
#> 4 4    4  
#> 5 5   20  
#> 6 6   20  
#> 7 7   12  
#> 8 8    5
```



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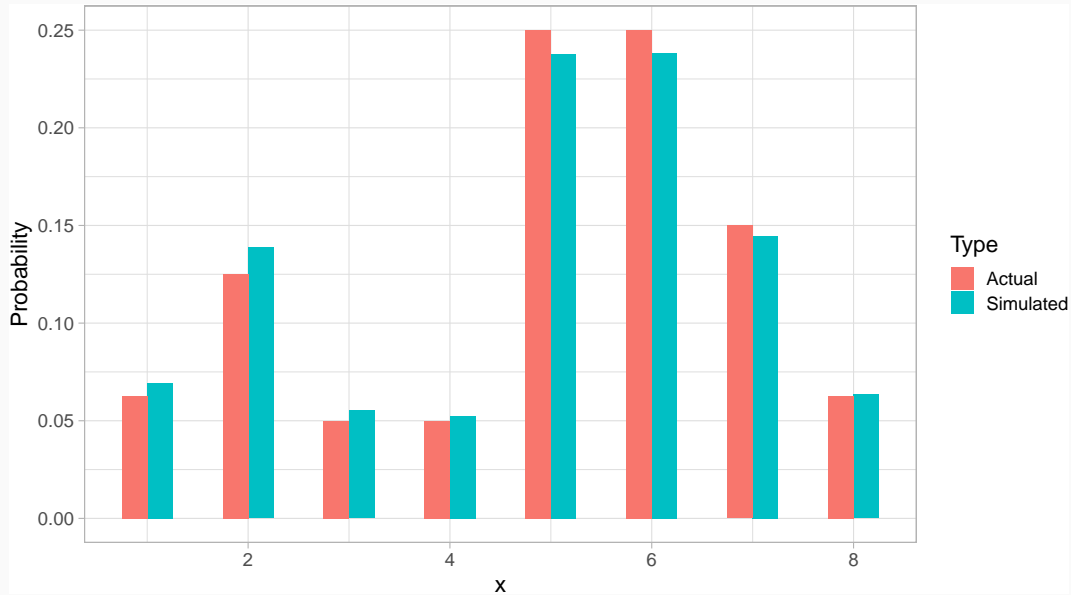
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5. We repeat 2-4 a number of times called **steps** (many steps).

```
random_walk <- function(pd, start, num_steps){  
  y <- rep(0, num_steps)  
  current <- start  
  for (j in 1:num_steps){  
    candidate <- current + sample(c(-1, 1), 1)  
    prob <- pd(candidate) / pd(current)  
    if (runif(1) < prob) current <- candidate  
    y[j] <- current  
  }  
  return(y)  
}
```

Starting at the value $X = 4$ and running the algorithm for $s = 10,000$ iterations.

```
out <- random_walk(pd, 4, 10000)
head(out)
#> [1] 3 2 2 2 1 1
tail(out)
#> [1] 4 5 5 5 6 7
```



Animating the Metropolis algorithm - 2D example

<https://mbjoseph.github.io/posts/2018-12-25-animating-the-metropolis-algorithm/>

The Markov-chain Monte Carlo Interactive Gallery

<https://chi-feng.github.io/mcmc-demo/>