

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

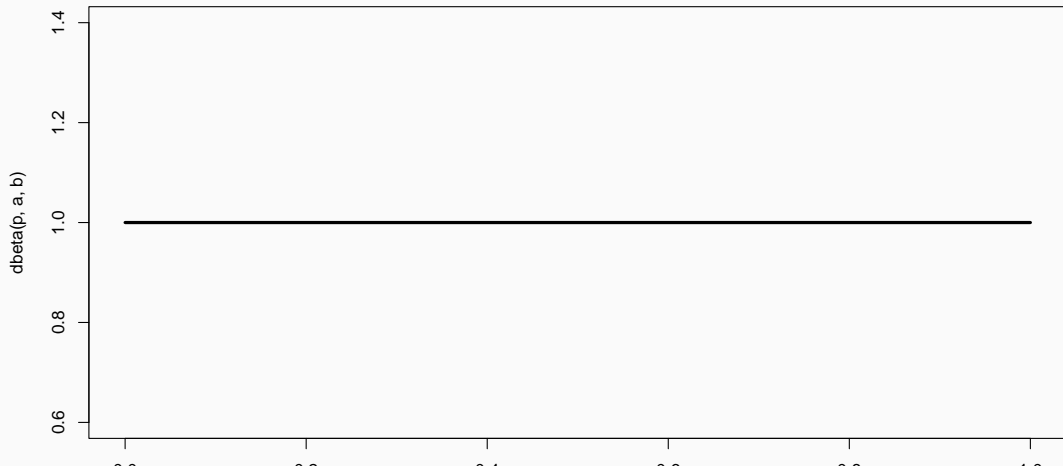
- Deer data

```
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: $\Pr(\text{data} \mid \theta) \Pr(\theta)$

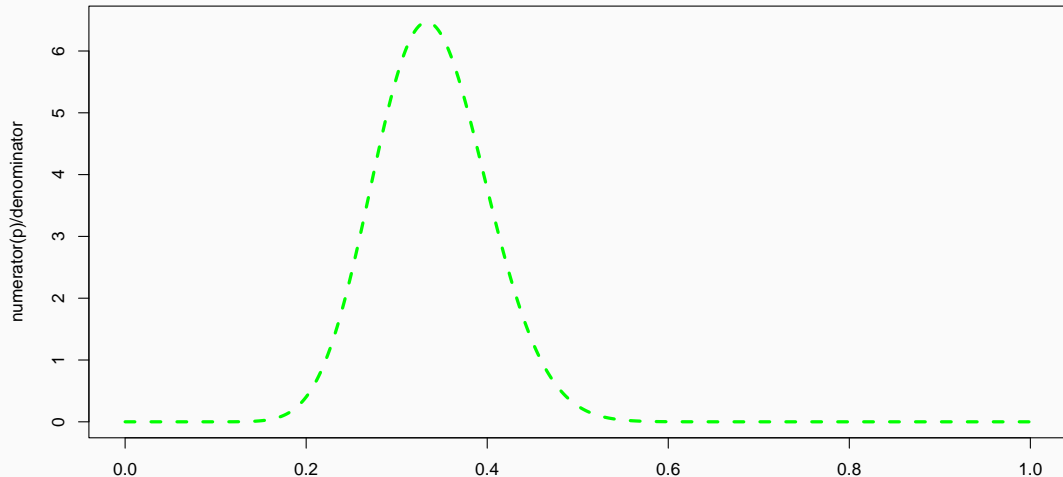
```
numerator <- function(p) dbinom(y,n,p)*dbeta(p,a,b)
```

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

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

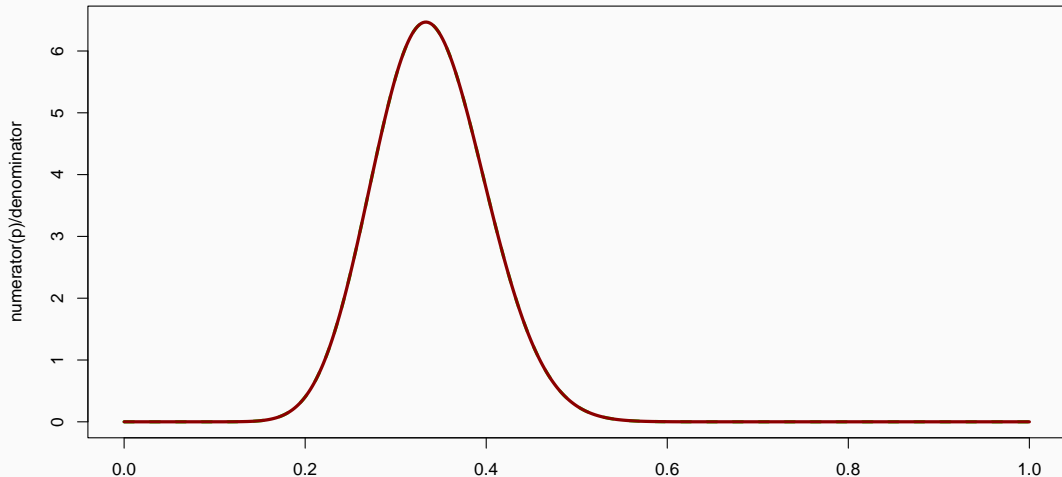
Posterior inference via numerical integration

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



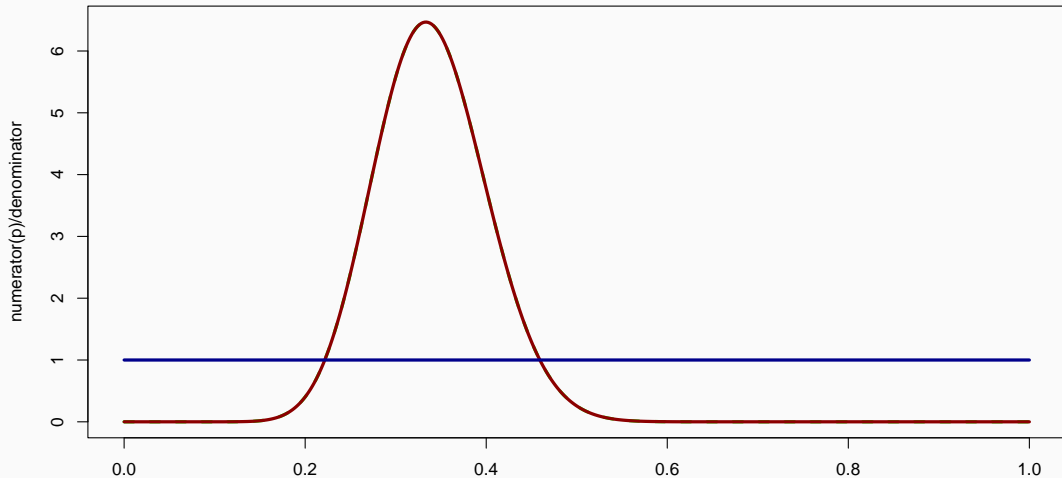
Superimpose explicit posterior distribution (Beta formula)

```
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?

- In the early 1990s, statisticians rediscovered work from the 1950's in physics.

THE JOURNAL OF CHEMICAL PHYSICS

VOLUME 21, NUMBER 6

JUNE, 1953

Equation of State Calculations by Fast Computing Machines

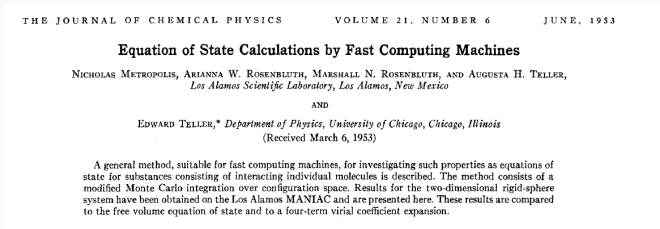
NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

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

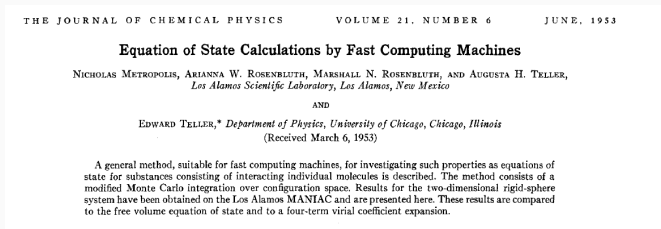
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional 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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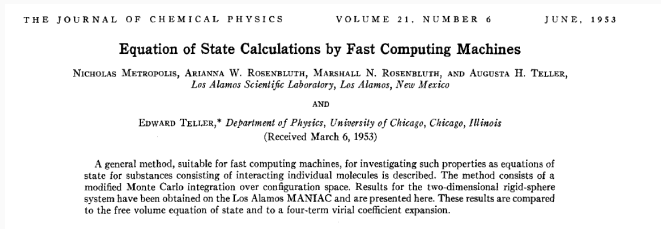
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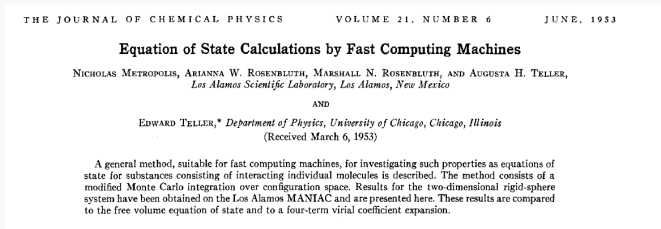
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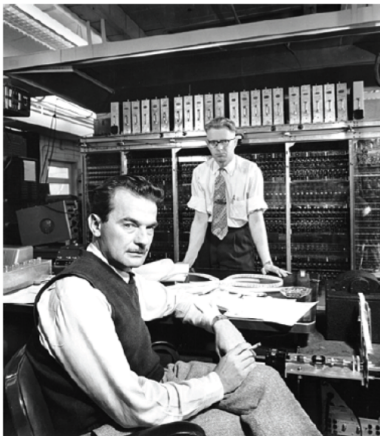
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- Markov chain Monte Carlo = MCMC; boost to Bayesian statistics!

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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- Equilibrium distribution is the desired posterior distribution!
- Several ways of constructing these chains: e.g., Metropolis-Hastings, Gibbs sampler, Metropolis-within-Gibbs.
- How to implement them in practice?!

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- Let's go back to the deer example and survival estimation.
- We illustrate sampling from the posterior distribution of winter survival.
- We write functions in R for the likelihood, the prior and the posterior.

```
# deer data, 19 "success" out of 57 "attempts"
survived <- 19
released <- 57

# log-likelihood function
loglikelihood <- function(x, p){
  dbinom(x = x, size = released, prob = p, log = TRUE)
}

# prior density
logprior <- function(p){
  dunif(x = p, min = 0, max = 1, log = TRUE)
}
```

```
# posterior density function (log scale)
posterior <- function(x, p){
  loglikelihood(x, p) + logprior(p) # - log(Pr(data))
}
```

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3. We compute the ratio of the probabilities at the candidate and current locations $R = \text{posterior}(\text{candidate}) / \text{posterior}(\text{current})$. This is where the magic of MCMC happens, in that $\text{Pr}(\text{data})$ (the denominator of the Bayes theorem) cancels out when we compute R .

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4. We spin a continuous spinner that lands anywhere from 0 to 1 — call the random spin X . If X is smaller than R , we move to the candidate location, otherwise we remain at the current location.

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

```
# propose candidate value
move <- function(x, away = .2){
  logitx <- log(x / (1 - x))
  logit_candidate <- logitx + rnorm(1, 0, away)
  candidate <- plogis(logit_candidate)
  return(candidate)
}

# set up the scene
steps <- 100
theta.post <- rep(NA, steps)
set.seed(1234)
```

```
# pick starting value (step 1)  
inits <- 0.5  
theta.post[1] <- inits
```

```
for (t in 2:steps){ # repeat steps 2-4 (step 5)

  # propose candidate value for prob of success (step 2)
  theta_star <- move(theta.post[t-1])

  # calculate ratio R (step 3)
  pstar <- posterior(survived, p = theta_star)
  pprev <- posterior(survived, p = theta.post[t-1])
  logR <- pstar - pprev
  R <- exp(logR)

  # decide to accept candidate value or to keep current value (step 4)
  accept <- rbinom(1, 1, prob = min(R, 1))
  theta.post[t] <- ifelse(accept == 1, theta_star, theta.post[t-1])
}
```

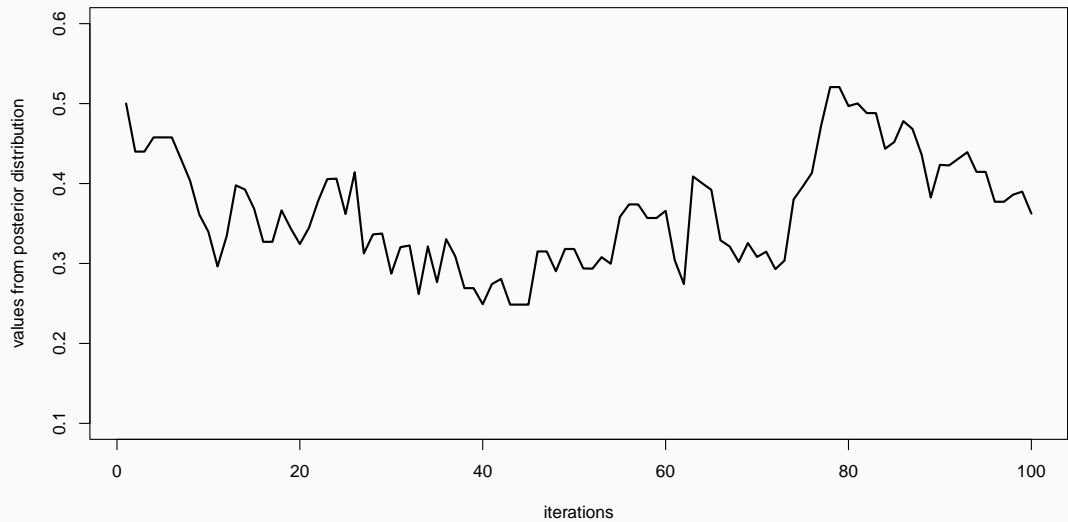

Starting at the value 0.5 and running the algorithm for 100 iterations.

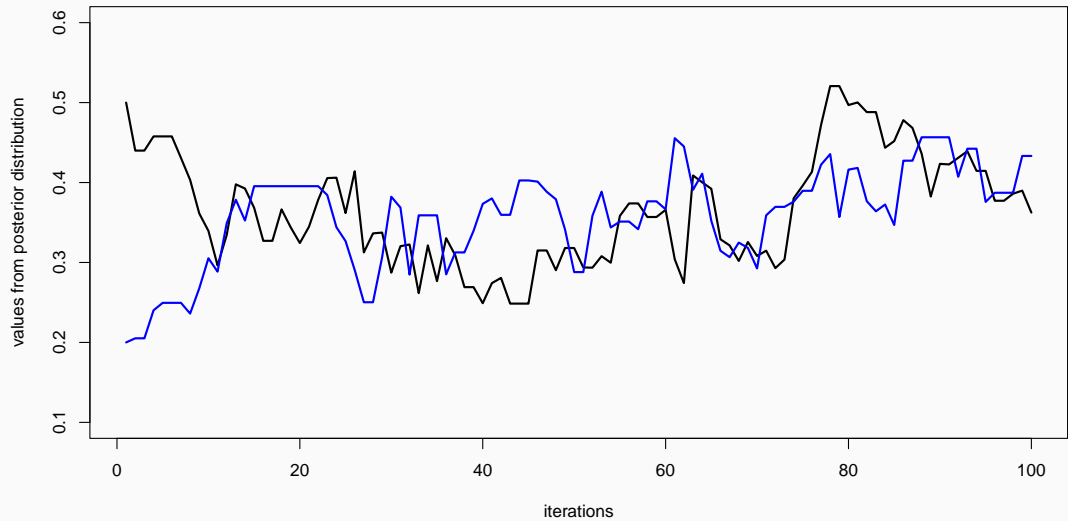
```
head(theta.post)
```

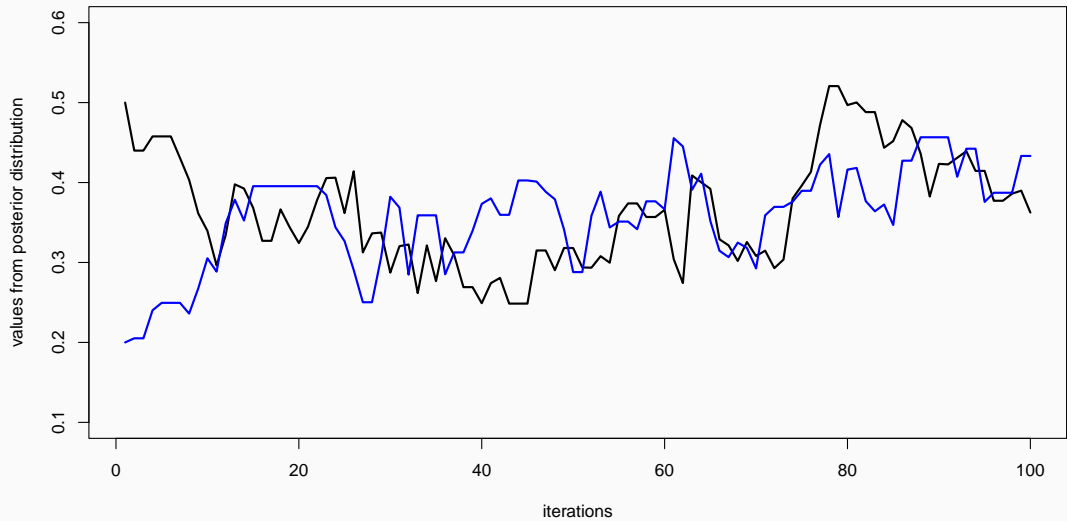
```
#> [1] 0.5000000 0.4399381 0.4399381 0.4577124 0.4577124 0.4577124
```

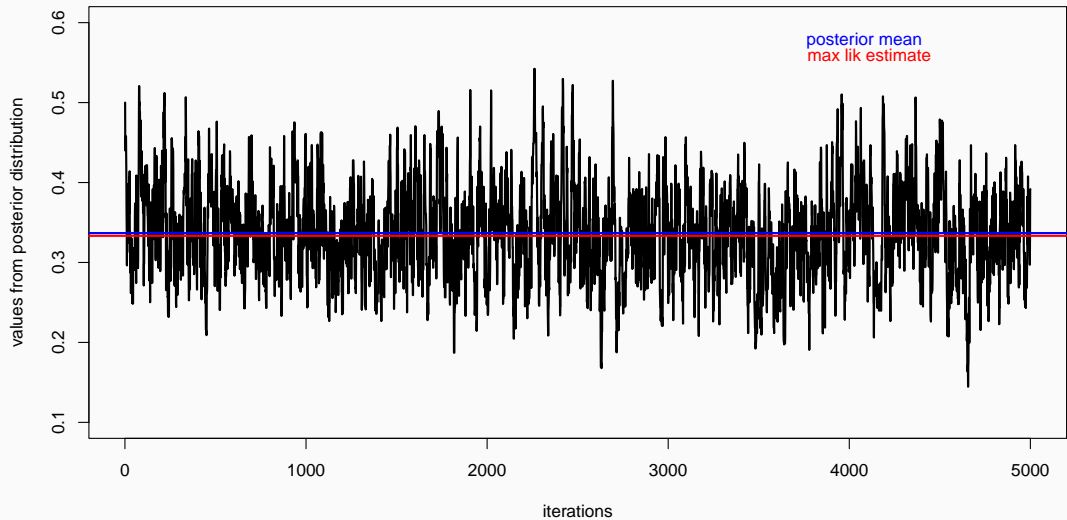
```
tail(theta.post)
```

```
#> [1] 0.4145878 0.3772087 0.3772087 0.3860516 0.3898536 0.3624450
```









Animating the Metropolis algorithm - 1D example

<https://gist.github.com/oliviergimenez/5ee33af9c8d947b72a39ed1764040bf3>

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/>