Bayesian Statistics and Markov-Chain Monte Carlo

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Computational Methods in Statistics and Data Science (Stats 406)

Baysian Statistics

Definitions of Probability

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Belief about parameters can be expressed by a random variable; the data we see are fixed.

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Observe: Frequentist statistical approaches often use Bayes's rule when, e.g., predicting B after observing A.

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- $f(x \mid \theta)$: The **likelihood of** x (given θ)
- $\int f(x \mid \theta)\, p(\theta)\, d\theta$: A **normalizing constant** (also known as the marginal likelihood of X, $f(x)$)

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With two priors, we can compare posterior distributions to get **Bayes Factors** (Bayesian hypothesis tests).

Integrals of posterior

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We'll see an immediate example and then revisit for more complicated examples

Inference for binomial θ

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You adminsiter a test of 30 true/false questions. The student scores

```
[1] 27
```

correctly.

Assumptions and Likelihood

Let us assume that

- All questions are answered with probability $\theta \in (0, 1)$.
- All questions are independent.
- You were successful at teaching if $\theta > 0.75$.

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By these assumptions, we get a **binomial likelihood** for the total X:

$$f(x \mid \theta) = \binom{30}{x} \theta^x (1 - \theta)^{30-x}$$

Prior Distribution

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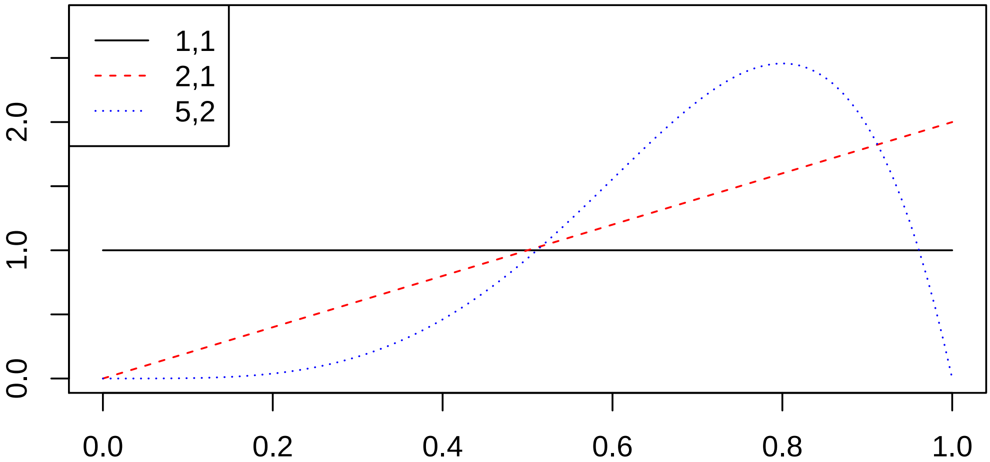
We think that we did a decent job teaching (θ probably close to 0.75), but we want to leave the possibility that we did not do a good job.


1,1
2,1
5,2
0.0
1.0
2.0
0.0
0.2
0.4
0.6
0.8
1.0

Computing posteriors

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We would still like to know the full posterior π.

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Suppose that $g(x)$ is a **proper PDF** and

$$g(x) \propto f^*(x)$$

Then $g(x) = cf^*(x)$.

Posterior for beta prior and binomial likelihood

In our case, we have:

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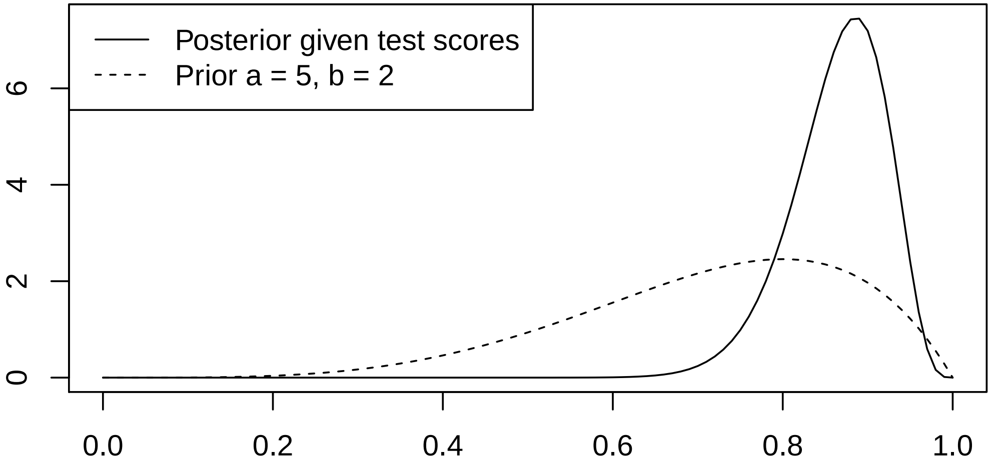
Key insight: since $\pi(\theta \mid x) \propto \text{Beta}(\alpha+x, \beta+30-x)$ it **must also be Beta distributed** (the beta distribution is **conjugate** for the binomial distribution).

Posterior



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What is the probability that you were successful at teaching?

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> 1 - pbeta(0.75, 5 + test_score, 32 - test_score)

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How much did the scores reduce the variance in your uncertainty?

```
> 1 - var(rbeta(1000, 5 + test_score, 32 - test_score)) /
+   var(rbeta(1000, 5, 2)) ## MC estimates of variance

[1] 0.8925
```

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- **Multiple parameters** make life even harder.

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The **Markov Chain** comes from the fact that we will draw samples from a **stochastic process**:

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Goal: Markov chains that lead to a law of large numbers:

$$\frac{1}{B}\sum_{b=1}^{B} g(\theta(b)) \overset{\text{a.s.}}{\to} E(g(\theta) \,|\, x)$$

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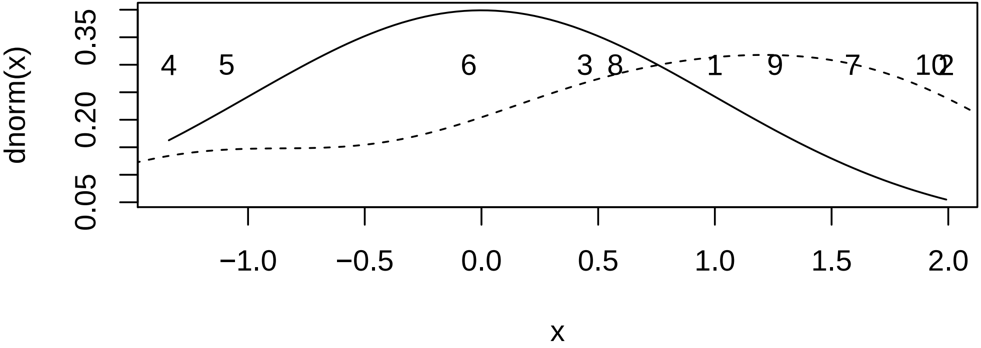
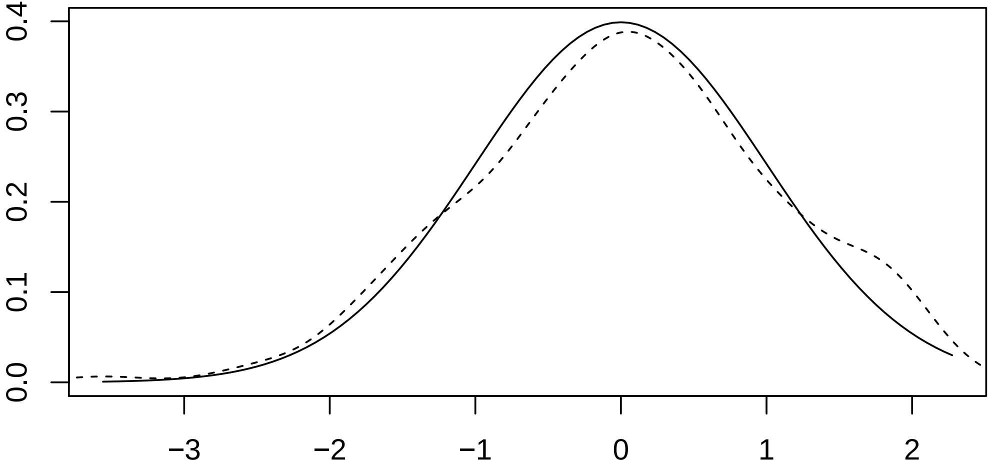
Luckily for us, we can use algorithms that already have these properties established!

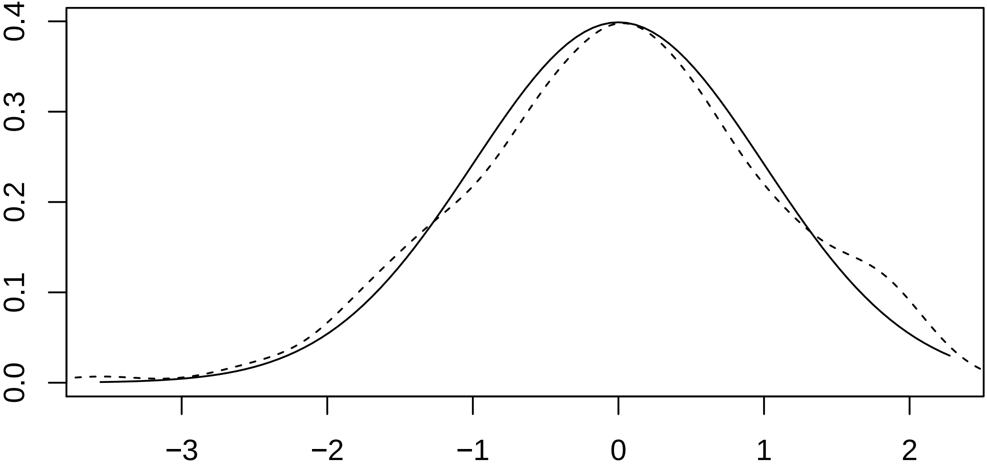
Visual Interpretation: Starting the chain at 1



Visual Interpretation: After many samples



Drop Burn In



Metropolis-Hastings

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- Accept $X = Y$ if $U < f(Y)/cg(Y)$, reject and repeat otherwise.

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Example: Rayleigh Density

We'll start with an example that is not specifically Bayesian: drawing from the Rayleigh density:

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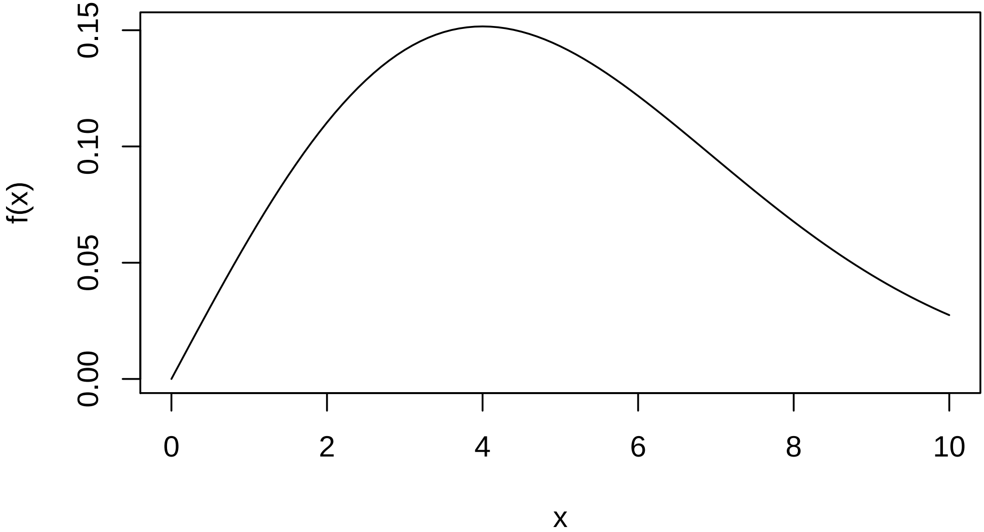
We'll use a χ^2 distribution with $X(t-1)$ degrees of freedom.

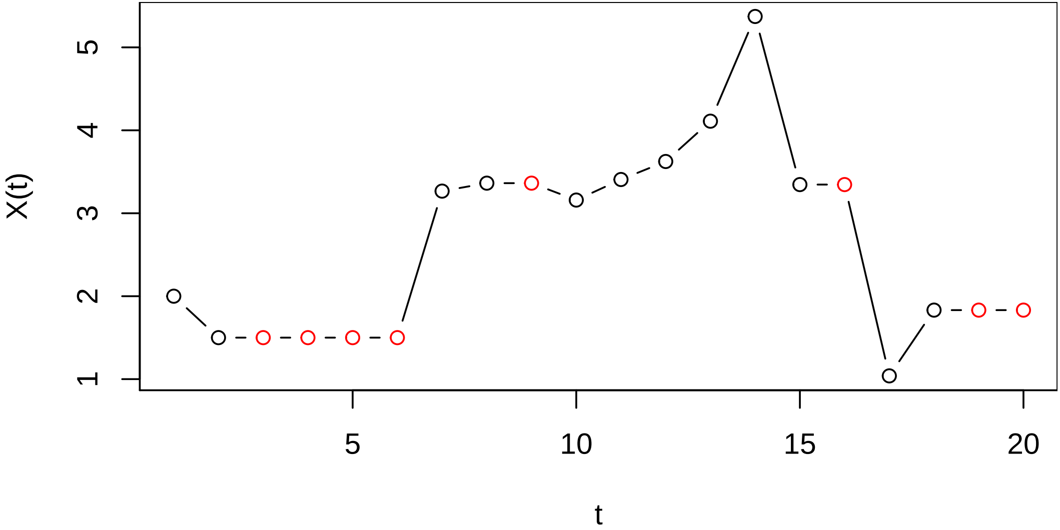
```r
> # we'll fix sigma at 4
> f <- function(x) {
+   (x / 16) * exp(-x^2 / 32)
+ }
> B <- 10000
> xs <- numeric(B)
> xs[1] <- 2 # arbitrary starting point
> # we'll log rejects
> rejected <- logical(B)
> rejected[1] <- FALSE
```



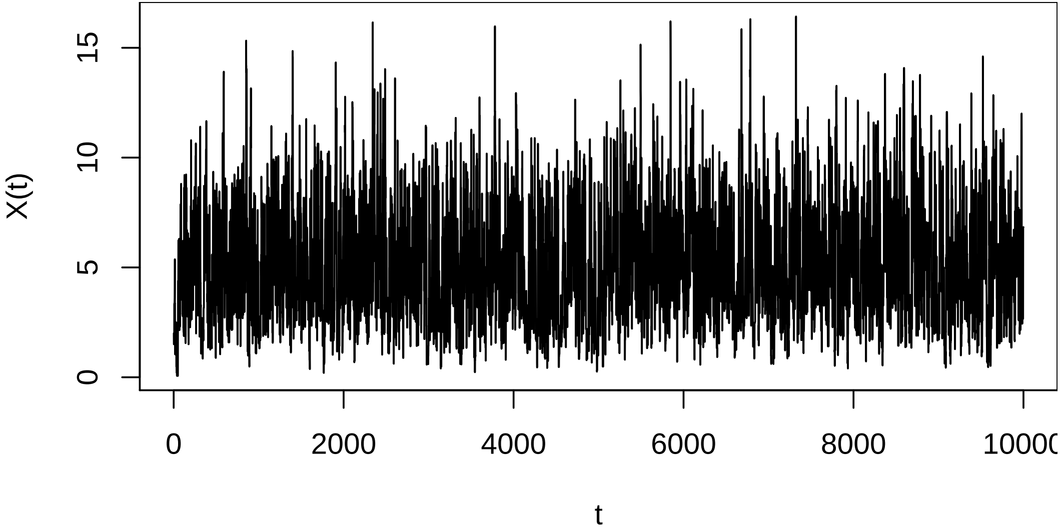
0.00
0.05
0.10
0.15
f(x)
0
2
4
6
8
10
x

```
> # starting i = 2, apply MH
> for (i in 2:B) {
+   x <- xs[i - 1]
+   xstar <- rchisq(1, df = x)
+   ratio <- f(xstar) * dchisq(x, df = xstar) /
+            (f(x) * dchisq(xstar, df = x))
+   u <- runif(1)
+   if (u <= ratio) {
+     xs[i] <- xstar
+     rejected[i] <- FALSE
+   } else {
+     xs[i] <- x
+     rejected[i] <- TRUE
+   }
+ }
```

Start of Chain



Full Chain



Burn In

Recall, guarantees for MCMC only state that **the chain converges to π** (or f).

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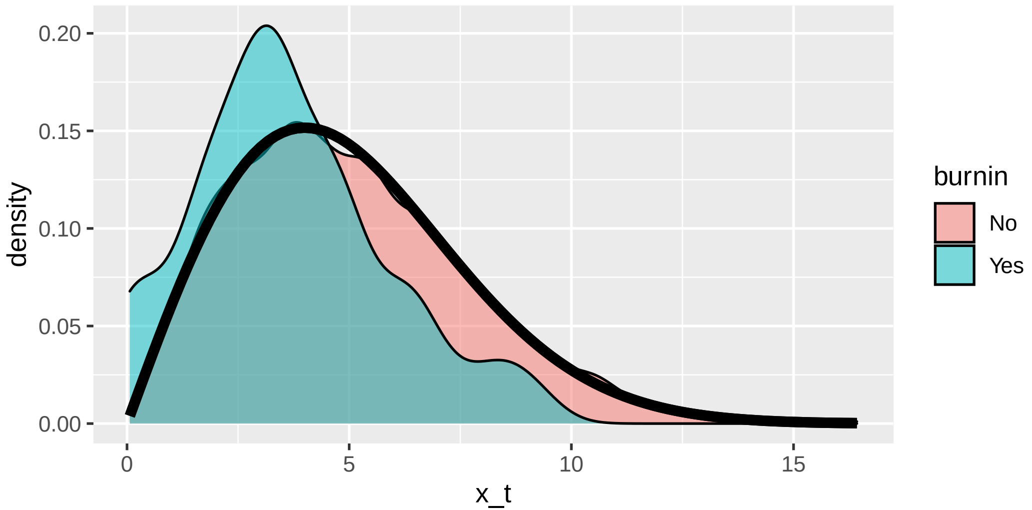
We often ignore the early portion of the chain (**burn in**).


0.20
0.15
0.10
0.05
0.00
density
0
5
10
15
x_t
burnin
No
Yes

Normalizing constants

We saw with **accept-reject** and **importance sampling** we could often ignore **normalizing constants**.

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As we saw, this is useful because it is often much easier to calculate:

$$\pi^*(\theta \mid x) = f(x \mid \theta)\, p(\theta)$$

Binomial θ example, again

We only need **terms that contain θ**. What are they?

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As we saw, **π is be Beta** with $\alpha + x$ and $\beta + n - x$.

MCMC for π^*

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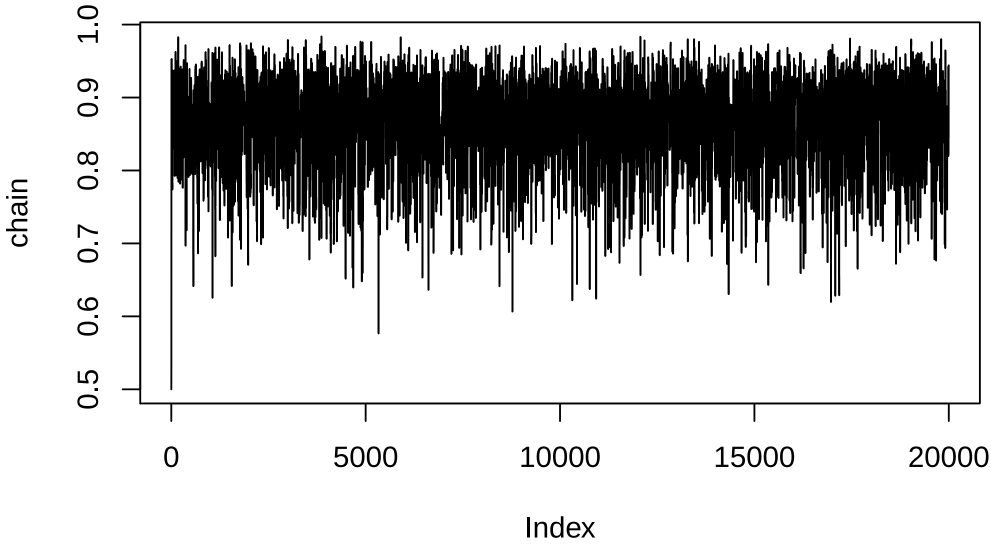
The candidate should be based on $\theta(t-1)$ in some way. We'll do something simple:

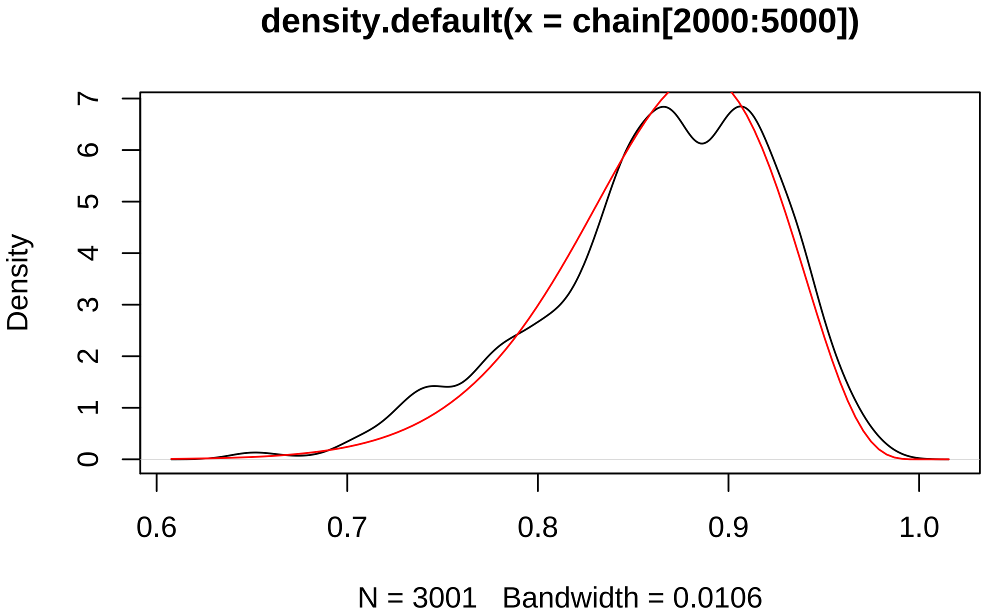
- If $\theta(t-1) < 0.5$, we'll draw from $U(0, 0.6)$
- If $\theta(t-1) \geq 0.5$, we'll draw from $U(0.4, 1)$

Note: the candidate always has density $5/3$.

```
> pi_star <- function(theta) {
+   theta^(5 + test_score - 1) *
+   (1 - theta)^(32 - test_score - 1)
+ }
```

```
> B <- 20000; chain <- numeric(B) ; chain[1] <- 0.5; rejects <- 0
> for (i in 2:B) {
+     candidate <- ifelse(chain[i - 1] < 0.5,
+                         runif(1, 0, 0.6),
+                         runif(1, 0.4, 1))
+     ratio <- pi_star(candidate) * (5/3) /
+         (pi_star(chain[i - 1]) * (5/3))
+     if (runif(1) <= ratio) {
+         chain[i] <- candidate
+     } else {
+         chain[i] <- chain[i - 1]
+         rejects <- rejects + 1
+     }
+ }
> reject_rate <- rejects / B
```


chain
0.5
0.6
0.7
0.8
0.9
1.0
0
5000
10000
15000
20000
Index


density.default(x = chain[2000:5000])
Density
0
1
2
3
4
5
6
7
0.6
0.7
0.8
0.9
1.0
N = 3001 Bandwidth = 0.0106

Independent MH

A special case of the proposal density is to **pick candidate values independently** of the previous value in the chain.

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$$\frac{1}{c} \frac{f(Y)}{g(Y)}$$

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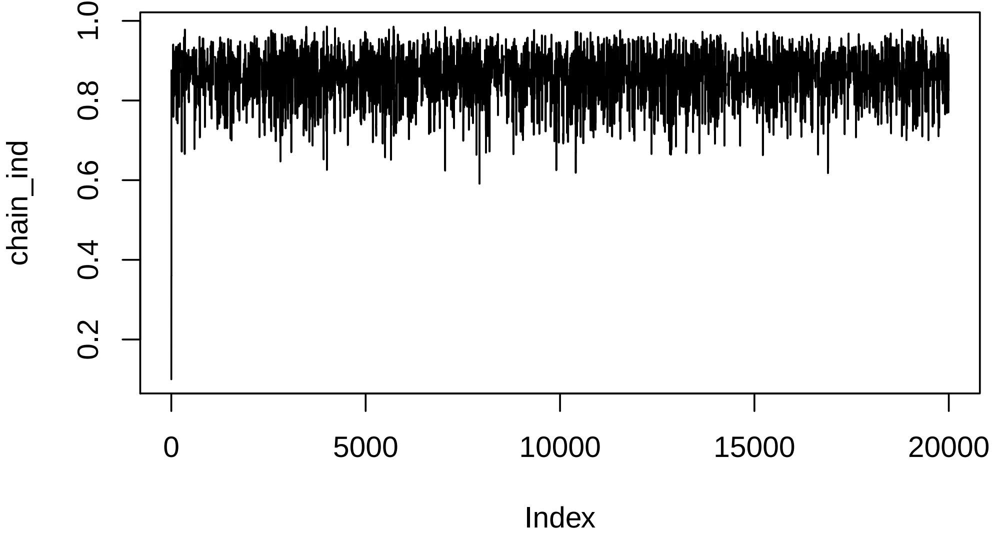
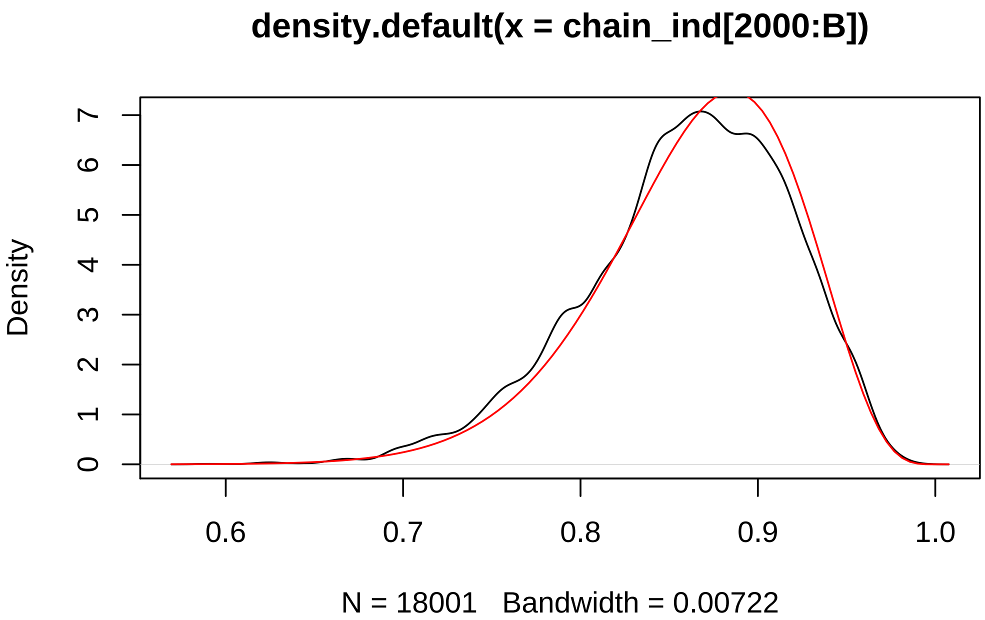
$$\frac{1}{c} \frac{f(Y)}{g(Y)}$$

An advantage of MH is we don't need to find a c.

```
> chain_ind <- numeric(B) ; chain_ind[1] <- 0.1 ; rejects_ind <- 0
> for (i in 2:B) {
+     candidate <- runif(1)
+     ratio <- pi_star(candidate) / pi_star(chain_ind[i - 1])
+     if (runif(1) <= ratio) {
+         chain_ind[i] <- candidate
+     } else {
+         chain_ind[i] <- chain_ind[i - 1]
+         rejects_ind <- rejects_ind + 1
+     }
+ }
> reject_rate_ind <- rejects_ind / B
```


1.0
0.8
0.6
0.4
0.2
chain_ind
0
5000
10000
15000
20000
Index


density.default(x = chain_ind[2000:B])
Density
0
1
2
3
4
5
6
7
0.6
0.7
0.8
0.9
1.0
N = 18001   Bandwidth = 0.00722

Comparing Methods

The independent sampler was easier to implement, does it perform as well?

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Fewer rejects means that we have more **unique samples** in the chain (closer to independent).

```
> reject_rate
[1] 0.7178
> reject_rate_ind
[1] 0.8288
```

Symmetric MH

One nice feature of independent MH is that

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so that the ratio reduced to:

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There are many cases when g is not uniform, but this property (**symmetry**) holds.

Random Walks

An example of symmetry,

$$\theta^* = \theta(t-1) + \epsilon$$

where ϵ is symmetric about 0.

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Here the **proposals are a random walk**, though the chain itself is not (why?).

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As a proposal, we will use

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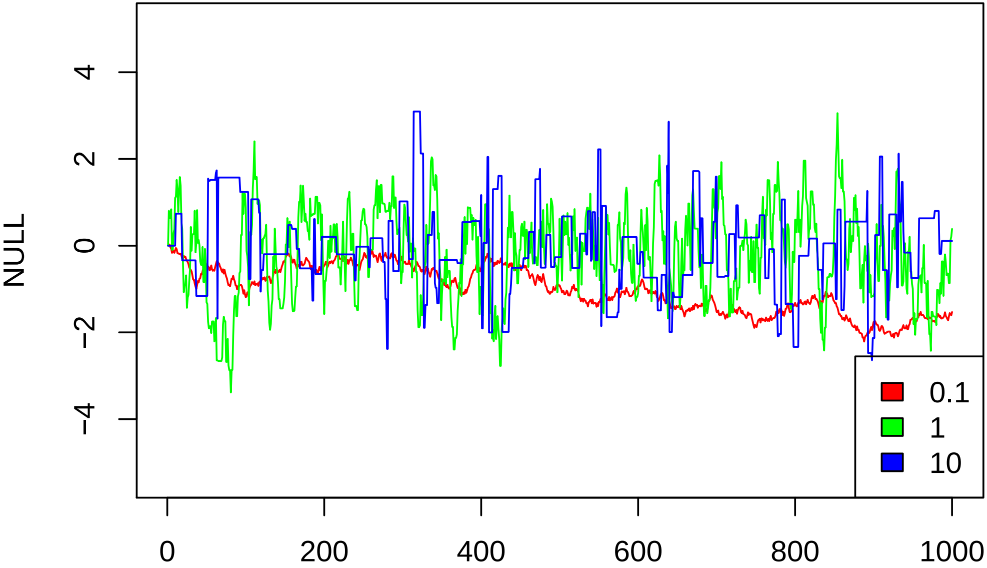
We will try a few different versions of δ to see how it changes the chain behavior.

```
> unif_chain <- function(delta, B = 5000) {
+   chain <- numeric(B); chain[1] <- 0 ; rejects <- 0
+   for (i in 2:B) {
+     candidate <- chain[i - 1] + runif(1, -delta, delta)
+     ratio <- dnorm(candidate) / dnorm(chain[i - 1])
+     if (runif(1) <= ratio) {
+         chain[i] <- candidate
+     } else {
+         chain[i] <- chain[i - 1]
+         rejects <- rejects + 1
+     }
+   }
+   list(reject_rate = rejects / B, chain = chain)
+ }
```

```
> n01_chain_0.1 <- unif_chain(0.1)
> n01_chain_1 <- unif_chain(1)
> n01_chain_10 <- unif_chain(10)
```


NULL
4
2
0
−2
−4
0
200
400
600
800
1000
0.1
1
10

```
> n01_chain_0.1$reject_rate
[1] 0.0254
> n01_chain_1$reject_rate
[1] 0.193
> n01_chain_10$reject_rate
[1] 0.843
```

Summary

- Bayesian statistics **treat parameters as random variables** with distributions (prior, posterior).

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- More complicated cases require **Markov Chain Monte Carlo**: drawing from a **Markov Chain** with a **stationary target distribution**
- Algorithms guarantee (asympotic) convergence: Metropolis-Hastings (regular, independent, random walk), more next time.
- Often a tradeoff between **amount of rejection** and **exploring the posterior**