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

There are generally **two approaches** to defining probability:

Frequentist The probability that event A is true is the proportion of an infinitely repeated series of A that are true.
Parameters are fixed; data are random.

Bayesian Probabilities represent subjective beliefs that range between zero ("cannot occur") and one ("must occur").
Belief about parameters can be expressed by a random variable; the data we see are fixed.

Bayes's Rule

Deriving Bayes rule (for events A and B):

$$P(B \mid A) = \frac{P(A \text{ and } B)}{P(A)} \qquad \text{(definition of cond. prob.)}$$
$$= \frac{P(A \mid B)P(B)}{P(A)} \quad \text{(again, using def. cond. prob.)}$$

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

Putting the "Bayes" in "Bayesian"

If Bayes' Rule is uncontroversial, so why "Bayesian statistics?"

If θ were a **random variable**, then Bayes' Rule states:

$$\pi(\theta \mid x) = \frac{f(x \mid \theta)\, p(\theta)}{\int f(x \mid \theta)\, p(\theta)\, d\theta}$$

- $p(\theta)$: The **prior distribution** of θ
- $\pi(\theta \mid x)$: The **posterior distribution** of θ
- $f(x \mid \theta)$: 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, $f(x)$)

Using Bayesian Statistics

Suppose we are willing to pick a model for the data ($f(x \mid \theta)$) and a prior for θ ($p(\theta)$).

After observing x, **posterior distribution of θ** answers:

- What is the most likely value of θ? ($\sup \pi(\theta \mid x)$, "maximum a posteriori (MAP) estimator")
- What value of $\hat{\theta}$ would minimize MSE? ($\hat{\theta} = E(\theta \mid x)$, "Bayes estimator")
- What is the probability that θ is positive? ($P(\theta > 0 \mid x)$)
- What is the smallest interval for θ with probability $1 - \alpha$? ("credible interval")

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

Integrals of posterior

With the exception of MAP estimator from the previous slide, all of those ideas require **integrating the posterior** π:

$$E(g(\theta) \mid x) = a$$

Naturally, we can estimate a using Monte Carlo techniques if we can **draw from the posterior**.

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

Inference for binomial θ

You are tutoring a student. If the student can learn 75% of the material, you will be happy with the results.

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 $\theta > 0.75$.

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

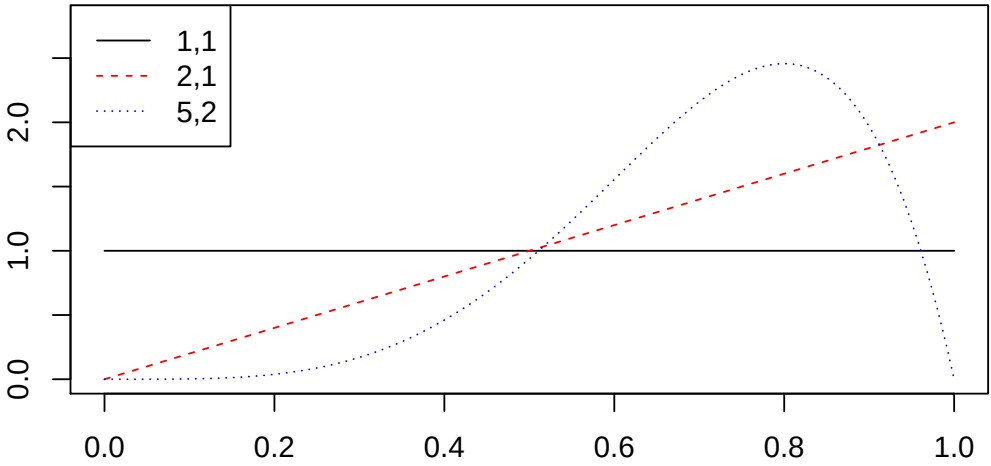
For the parameter θ, we need a **prior distribution** that captures our beliefs about how well we did at teaching (i.e., **a distribution for θ**).

A common model for random variables in (0, 1) is the **beta distribution**:

$$p(\theta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$

It has parameters α and β, which we will pick to capture our beliefs.

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

Recall **Bayes Rule** states

$$\pi(\theta \mid x) = \frac{f(x \mid \theta)\, p(\theta)}{\int f(x \mid \theta)\, p(\theta)\, d\theta}$$

The **marginal likelihood** ($\int f(x \mid \theta)\, p(\theta)\, d\theta$) is often **difficult to compute**

It is often helpful to consider the portion of the RHS that **only depends on** θ:

$$\pi(\theta \mid x) \propto f(x \mid \theta)\, p(\theta) \quad \text{(proportional to)}$$

We would still like to know the full posterior π.

Proportionality

We can often infer π from the **kernel** of $f(x \mid \theta)p(\theta)$.

Let $f^*(x)$ be a **kernel (unnormalized PDF)** such that

$$f^*(x) \geq 0, \int_{-\infty}^{\infty} f^*(x)\, dx = \frac{1}{c}$$

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

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

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

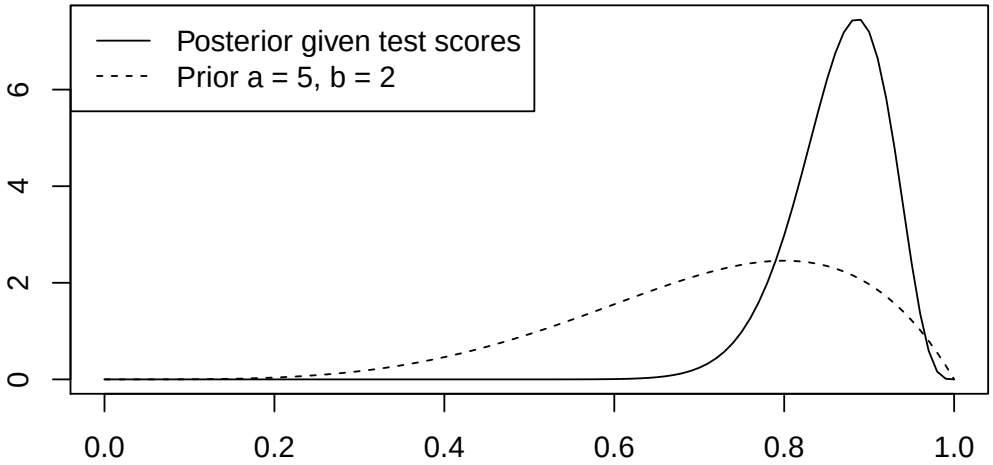
Posterior for beta prior and binomial likelihood

In our case, we have:

$$\begin{aligned}\pi(\theta \mid x) &\propto \binom{30}{x}\theta^x(1-\theta)^{30-x}\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1} \\ &\propto \theta^x(1-\theta)^{30-x}\theta^{\alpha-1}(1-\theta)^{\beta-1} \\ &= \theta^{(\alpha+x)-1}(1-\theta)^{(\beta+30-x)-1}\end{aligned}$$

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



Using the posterior

What is the probability that you were successful at teaching?

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

```
[1] 0.9658
```

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
```

More complex problems

We were able to get a **closed form solution** because we picked our likelihood and prior carefully, but **not every problem can be expressed as conjugates**.

General issues:

- Normalizing constant needed for **inversion method**, often difficult.
- Even if we can figure out the posterior, might **unable to draw from it directly**.
- **Multiple parameters** make life even harder.

Markov Chain Monte Carlo

Markov Chain Monte Carlo

We already know what **Monte Carlo** means.

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

$$\theta(t) \,|\, \theta(t-1), \theta(t-2), \ldots, \theta(0) \sim \theta(t) \,|\, \theta(t-1)$$

(i.e., observation t only depends on observation $t-1$. We suppress dependence on x for simplicity).

Such a stochastic process is called a **(discrete) Markov Chain**.

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

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

Achieving a SLLN

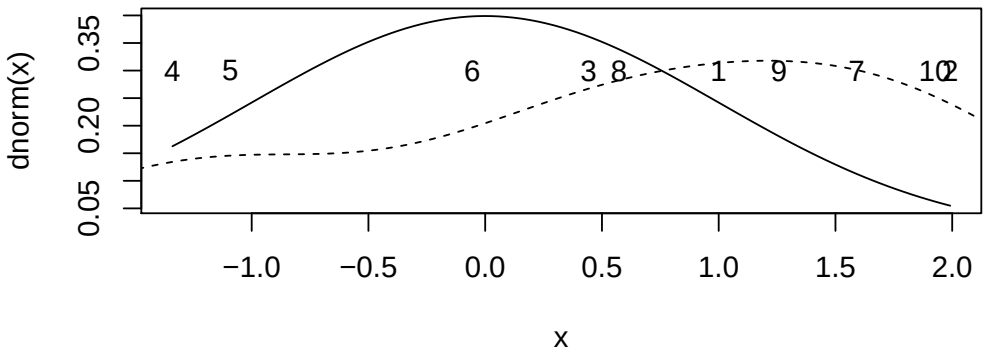
To achieve the desired result, we require Markov Chains that the following properties:

- **Stationary distribution:** A chain is stationary if, when $\theta(t-1) \sim \pi$, $\theta(t) \sim \pi$.
- **Irreproducible**: No matter the start of the chain $\theta(0)$, there positive probability of visiting any region in the support of θ.
- **Aperiodic**: There is no region such that if $\theta(t) \in \mathcal{R}_1$ we cannot reach $\mathcal{R}_2$.

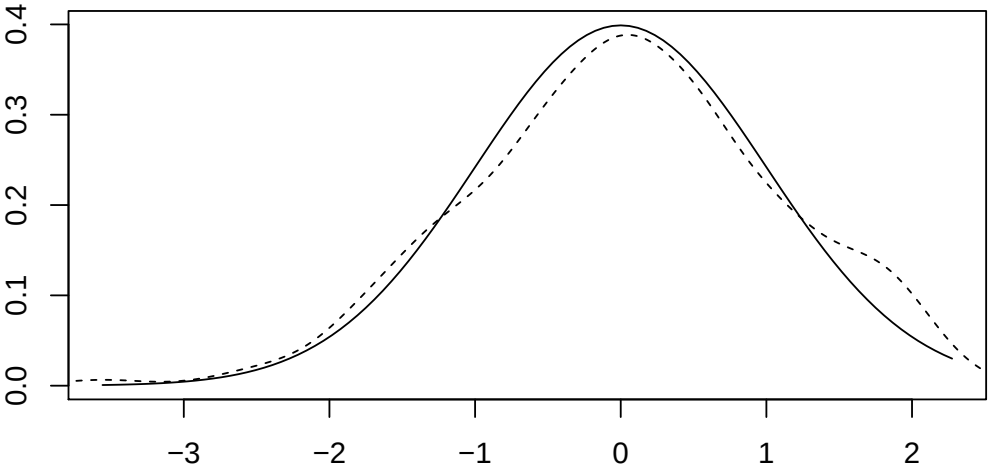
(The last two imply a condition called **ergodicity**, which you may see elsewhere.)

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

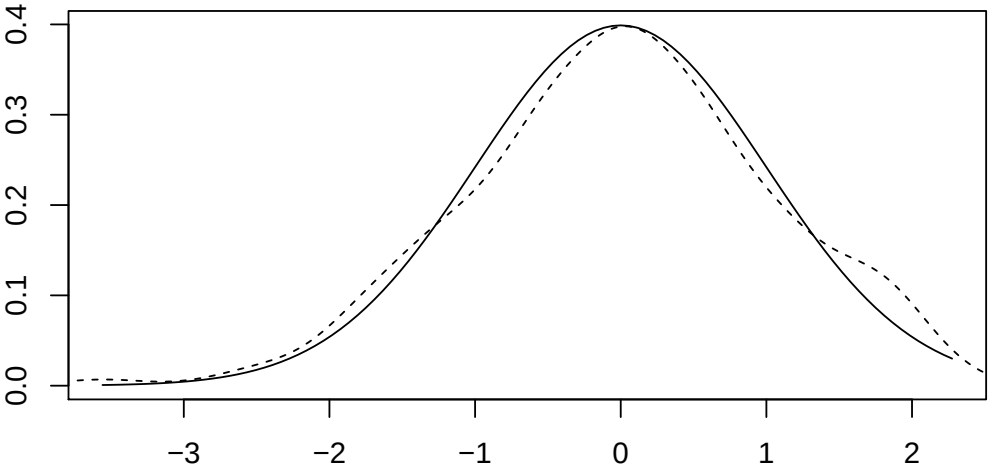
Visual Interpretation: Starting the chain at 1



Visual Interpretation: After many samples



Drop Burn In



Metropolis-Hastings

Accept-reject Review

Recall the **accept-reject algorithm** for IID random variables:

- We wish to draw X from **target density** f but doing so is difficult.
- We pick **candidate density** g that we can draw from.
- We find a c such that $f(x)/cg(x) < 1$, for any x in the support of X
- Draw Y from g and U from $U(0,1)$
- Accept $X = Y$ if $U < f(Y)/cg(Y)$, reject and repeat otherwise.

Metropolis-Hastings: AR for MCMC

The **Metropolis-Hastings algorithm** applies the accept reject concept to **Markov Chains**.

MH draws from $\theta^* | \theta(t-1)$ and either

1. Sets $\theta(t) = \theta^*$ if
$$U \leq \frac{\pi(\theta^*)}{\pi(\theta(t-1))} \frac{g(\theta(t-1) \,|\, \theta^*)}{g(\theta^* \,|\, \theta(t-1))}$$
2. Sets $\theta(t) = \theta(t-1)$, otherwise.

Example: Rayleigh Density

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

$$f(x) = \frac{x}{\sigma^2} \exp\left\{\frac{-x^2}{2\sigma^2}\right\}, \quad x \geq 0, \sigma^2 > 0$$

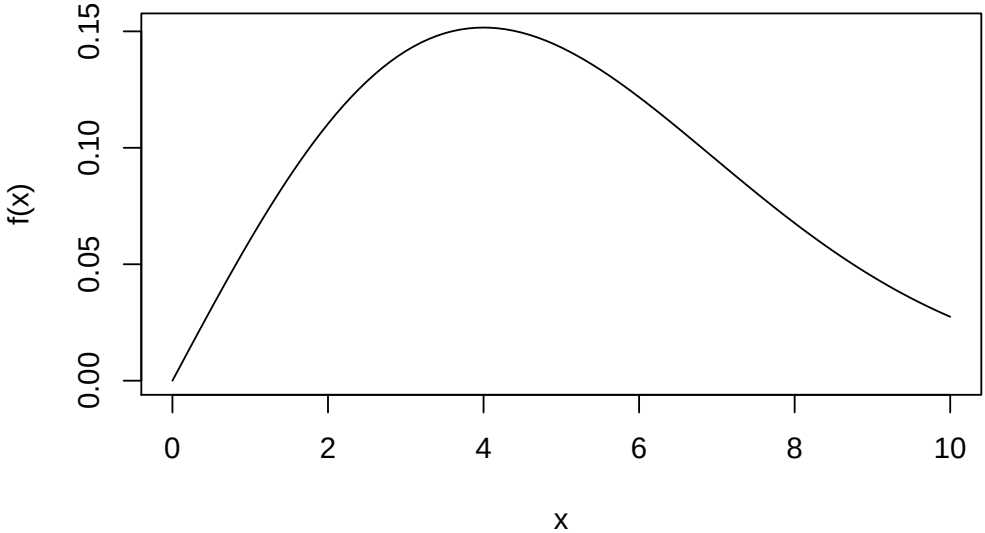
To be clear: we want a sequence $X(0), X(1), \ldots$ that converges to f (we'll fix σ^2 to a constant).

The main requirement we have for the **candidate distribution** is that it have the **same support** as the target.

It should also be **conditional on** $X(t-1)$.

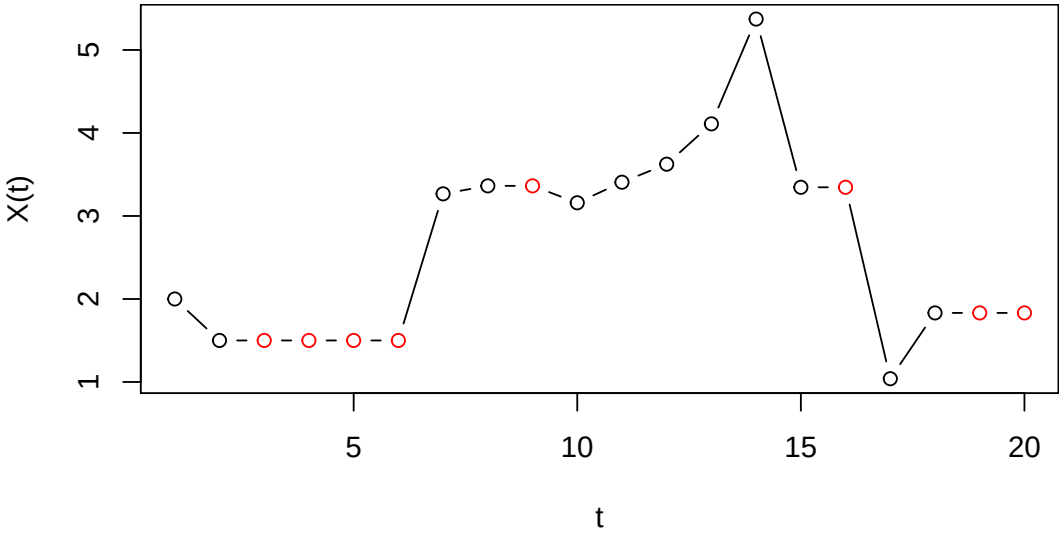
We'll use a χ^2 distribution with $X(t-1)$ degrees of freedom.

```
> # 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
```

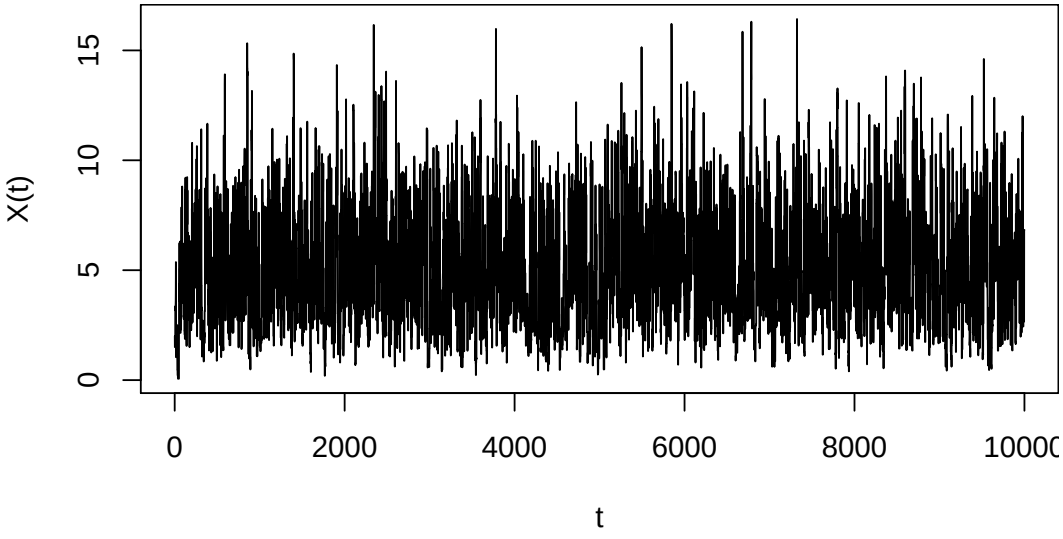

f(x)
0.00
0.05
0.10
0.15
0
2
4
6
8
10
x

```
> # 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



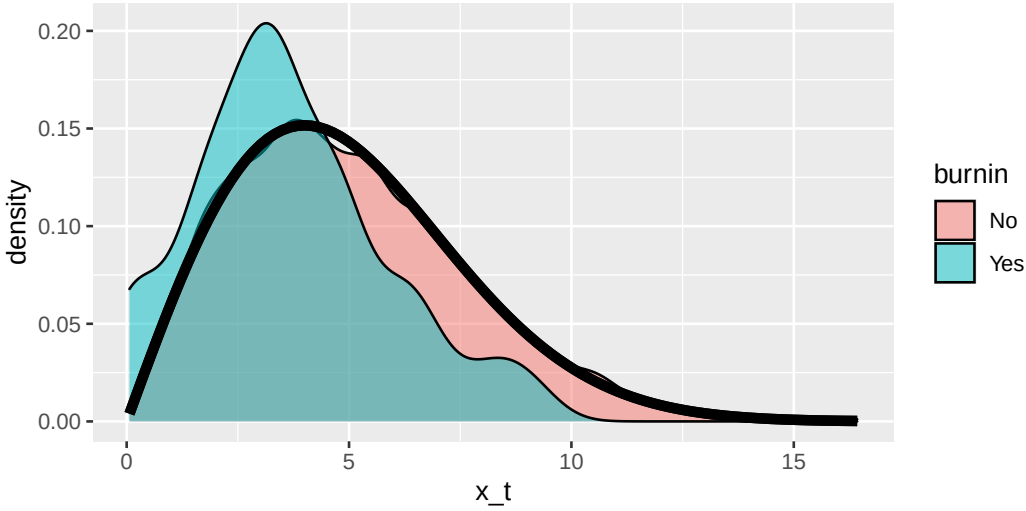
Full Chain



Burn In

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

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**.

This holds true in MH as well since

$$\frac{\pi(\theta^*)}{\pi(\theta(t-1))} = \frac{c\pi^*(\theta^*)}{c\pi^*(\theta(t-1))} = \frac{\pi^*(\theta^*)}{\pi^*(\theta(t-1))}$$

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?

Binomial likelihood:

$$f(x \mid \theta) = \binom{n}{x} \theta^x (1-\theta)^{n-x} \quad \propto \theta^x (1-\theta)^{n-x}$$

Beta prior:

$$p(\theta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1}(1-\theta)^{\beta-1} \quad \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$$

Posterior is proportional to the product of prior and likelihood:

$$\pi^*(\theta \mid x) = \theta^x (1-\theta)^{n-x} \theta^{\alpha-1}(1-\theta)^{\beta-1} = \theta^{\alpha+x-1}(1-\theta)^{\beta+(n-x)-1}$$

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

MCMC for π^*

We need to **pick a candidate distribution** for θ^*.

Since $\theta^* \in (0, 1)$, a candidate **uniform distribution** can be selected.

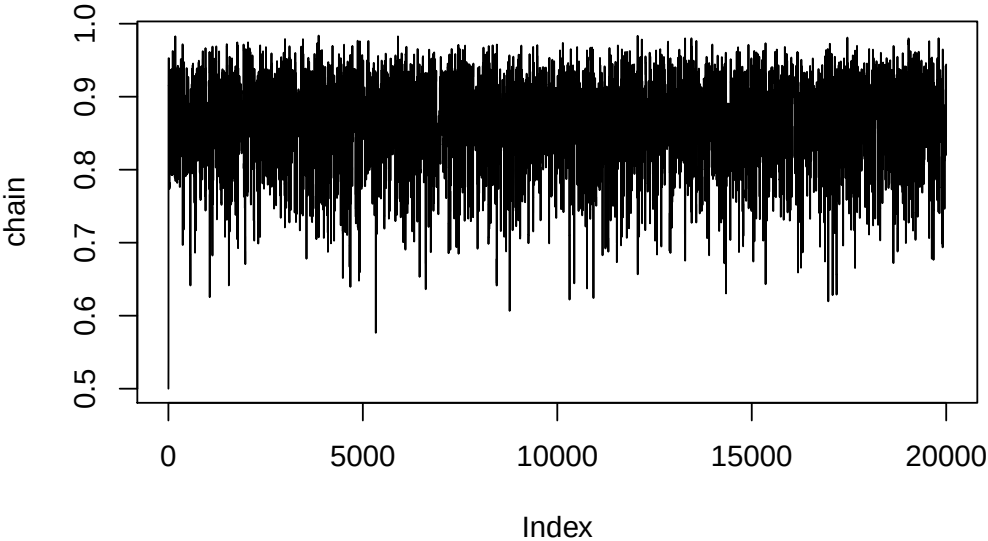
The candidate should be based on $\theta(t-1)$ in some way. We'll do something simple:

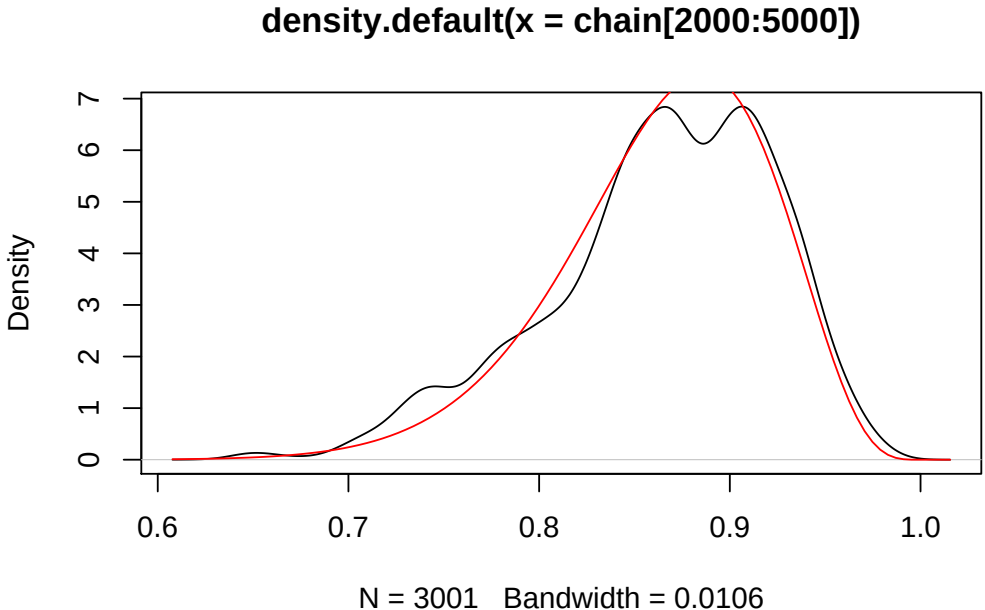
- If $\theta(t-1) < 0.5$, we'll draw from $U(0, 0.6)$
- If $\theta(t-1) \geq 0.5$, we'll draw from $U(0.4, 1)$

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
1.0
0.9
0.8
0.7
0.6
0.5
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.

$$g(\theta^* \mid \theta(t-1)) = g(\theta^*)$$

Then we have the ratio:

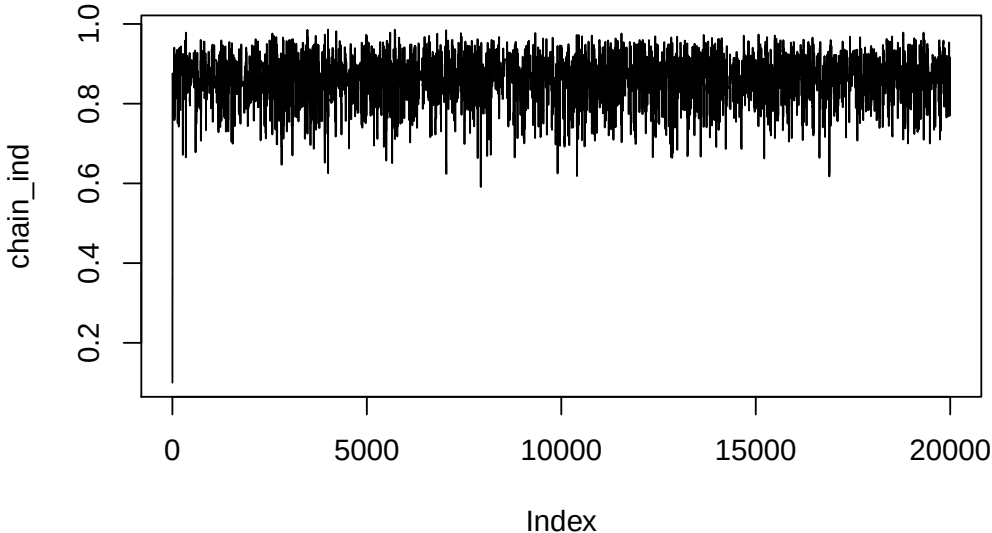
$$\frac{1}{\pi(\theta(t-1))/g(\theta(t-1))} \frac{\pi(\theta^*)}{g(\theta^*)}$$

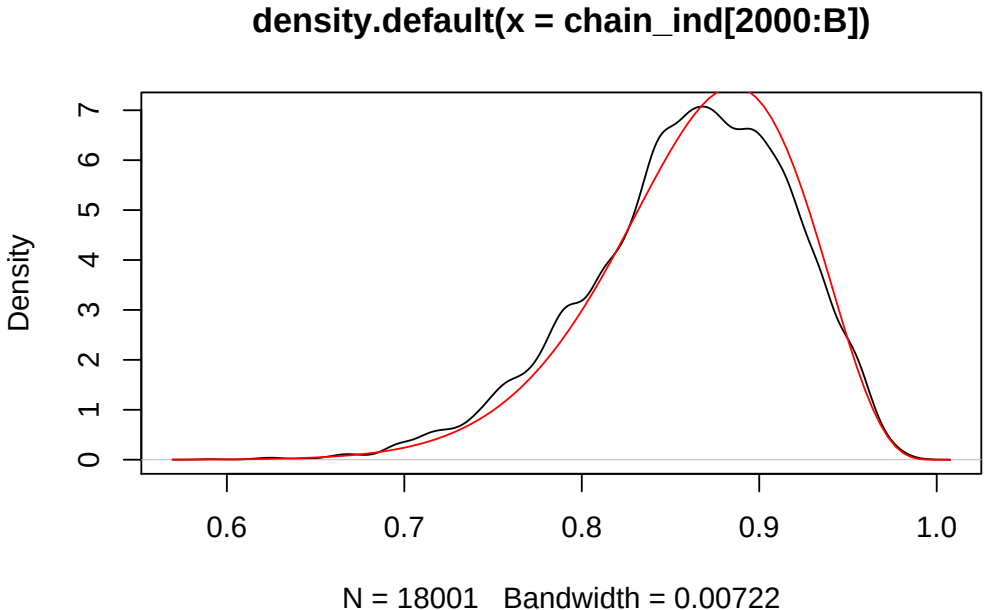
This notation is to highlight the connection to **accept-reject** where we had

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

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
```


chain_ind
0.2
0.4
0.6
0.8
1.0
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?

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

$$g(\theta * \,|\, \theta(t-1)) = g(\theta(t-1) \,|\, \theta*)$$

so that the ratio reduced to:

$$\frac{\pi(\theta^*)}{\pi(\theta(t-1))}$$

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.

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

Example: $N(0, 1)$

Suppose we are trying to generate $N(0, 1)$ using a Markov Chain.

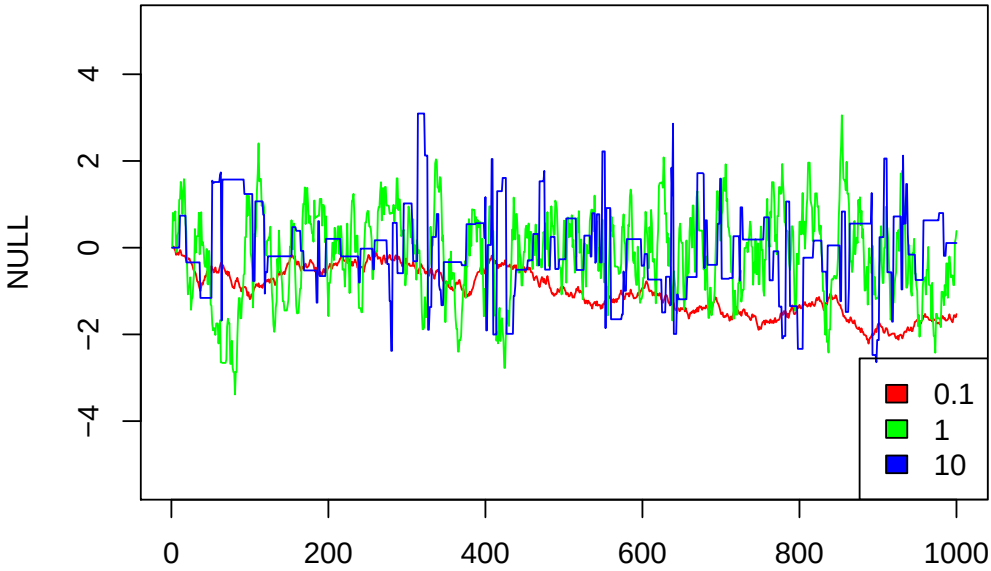
As a proposal, we will use

$$\theta^* = \theta(t - 1) + U(-\delta, \delta)$$

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).
- **Inference** frequently requires **integrals on posteriors**.
- In some cases, we can deduce posteriors (or something **proportional to the posterior**)
- 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**