STA 602 - Intro to Bayesian Statistics

Lecture 10

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Gaussian model with unknown mean and unkown variance

- Sampling model for n readings given the mean θ and variance σ^2 is

$$X_1, X_2, \ldots, X_n \,|\, \theta, \sigma^2 \overset{\text{iid}}{\sim} \mathrm{N}(\theta, \sigma^2)$$

- Prior distribution for the mean θ

$$\theta \,|\, \sigma^2 \sim \mathrm{N}(\mu_0, \tau_0^2)$$

- Now let's assume that the sampling variance σ^2 is also unknown.
- So now we have a two parameter model (θ, σ^2).
- To complete Bayesian inference, we need to specify a joint prior for (θ, σ^2).

Prior independence

- So far we have constrained our conditional prior for θ given σ^2 to be
$$\theta \,|\, \sigma^2 \sim \mathrm{N}(\mu_0, \tau_0^2)$$
where $\tau_0^2 = \sigma^2/\kappa_0$. In particular, *a priori*, θ and σ^2 are *dependent*.
- Suppose instead we want θ and σ^2 to be independent *a priori*. That is,
$$p(\theta, \sigma^2) = p(\theta)p(\sigma^2).$$
- It is convenient to adopt a conjugate prior so that the resulting posterior is analytically tractable.
- Unfortuately, this is not achievable.

A "semi-conjugate" prior

- Note that given the form of the likelihood $p(x|\theta, \sigma^2)$, *a posteriori* θ and σ^2 will be dependent. That is,

$$p(\theta, \sigma^2|\mathbf{x}) \neq p(\theta|\mathbf{x})p(\sigma^2|\mathbf{x})$$

  because

$$p(\theta, \sigma^2|\mathbf{x}) \propto p(\theta)p(\sigma^2)p(\mathbf{x}|\theta, \sigma^2).$$

- For example, after observing some value of x, if θ is much smaller in absolute value than x, then σ^2 must be large. For $p(\sigma^2 \,|\, \theta, \mathbf{x})$ depends on θ.
- Question: What would small values of σ^2 imply about θ?
- In this sense, strict conjugacy is not feasible, as the prior independence will inevitably be lost under the posterior.

- Let's then aim for having a posterior such that $p(\sigma^2|\mathbf{x})$ is in the same family as $p(\sigma^2)$, and $p(\theta \,|\, \sigma^2, \mathbf{x})$ is in the same family as $p(\theta \,|\, \sigma^2)$.
- It turns out that without letting $\tau_0^2 = \sigma^2/\kappa_0$ even this is not achievable.
- Inpsired by the conjugate case, what if we use the following *Normal-inverse-Gamma* prior that is similar to what we had used previously without the constraint that $\tau_0^2 = \sigma^2/\kappa_0$:

$$\begin{aligned} \theta \,|\, \sigma^2 &\sim \mathrm{N}(\mu_0, \tau_0^2) \\ \sigma^2 &\sim \mathrm{IG}(\nu_0/2, \nu_0\sigma_0^2/2) \end{aligned}$$

or

$$\gamma = \frac{1}{\sigma^2} \sim \mathrm{Gamma}(\nu_0/2, \nu_0\sigma_0^2/2).$$

The corresponding conditional posterior

- As before, by Bayes theorem, the conditional posterior distribution for θ given σ^2 is

$$\theta \,|\, \mathbf{x}, \sigma^2 \sim \mathrm{N}(\mu_n, \tau_n^2)$$

where

$$\mu_n = \left(\frac{1/\tau_0^2}{1/\tau_0^2 + n/\sigma^2} \right) \mu_0 + \left(\frac{n/\sigma^2}{1/\tau_0^2 + n/\sigma^2} \right) \bar{x}$$

and

$$\frac{1}{\tau_n^2} = \frac{1}{\tau_0^2} + \frac{n}{\sigma^2}.$$

- This is called the *full conditional* of θ. That is, the conditional posterior of θ given all other *random variables*—that is, all other parameters in the model and the data in this example.
- Again, note that the conditional posterior of θ given σ^2 depends on σ^2. So there is no posterior independence.

The corresponding conditional posterior

- Without the constraint $\tau_0^2 = \sigma^2/\kappa_0$, we can no longer get a simple Gamma marginal posterior for $1/\sigma^2$ as before.
- Fortunately, we can find the *full conditional* (i.e., conditional posterior of $1/\sigma^2$ given the rest of the parameters, here θ, and the data):

$$\sigma^2 \,|\, \mathbf{x}, \theta \sim \text{IG}\left(\frac{\nu_0 + n}{2}, \frac{1}{2}\left(\nu_0\sigma_0^2 + \sum_i (x_i - \theta)^2\right)\right)$$

or

$$\sigma^2 \,|\, \mathbf{x}, \theta \sim \text{IG}\left(\frac{\nu_0 + n}{2}, \frac{1}{2}\left(\nu_0\sigma_0^2 + (n-1)s^2 + n(\bar{x} - \theta)^2\right)\right)$$

where we again use the fact that

$$\sum_i (x_i - \theta)^2 = (n-1)s^2 + n(\bar{x} - \theta)^2.$$

- Compare this to the marginal posterior of $1/\sigma^2$ in the conjugate prior.

Finding the full conditionals

- First write then the full joint density of all parameters and the data

$$\begin{aligned} p(\theta, \gamma, \mathbf{x}) &= p(\theta, \gamma) p(\mathbf{x}|\theta, \gamma) \\ &= p(\theta) p(\gamma) p(\mathbf{x}|\theta, \gamma) \\ &\propto e^{-\frac{(\theta-\mu_0)^2}{2\tau_0^2}} \cdot \gamma^{\frac{\nu_0}{2}-1} e^{-\frac{1}{2}\nu_0\sigma_0^2\gamma} \cdot \gamma^{\frac{1}{2}} e^{-\frac{1}{2}\gamma\sum_i (x_i-\theta)^2} \end{aligned}$$

- Then to find the full condition of each parameter. View this joint density as a function of that parameter, with all parameters fixed as constants.

- For example, after completion of squares (do it!), when viewed as a function of θ, it is proportional to

$$\frac{1}{\tau_n} e^{-\frac{(\theta-\mu_n)^2}{2\tau_n^2}}$$

  which corresponds to $\mathrm{N}(\mu_n, \tau_n^2)$.
- When viewed as a function of γ, it is proportional to

$$\gamma^{\frac{\nu_0+n}{2}-1} e^{-\frac{\gamma}{2}(\nu_0\sigma_0^2+\sum_i(x_i-\theta)^2)}$$

  which corresponds to $\mathrm{Gamma}\left(\frac{\nu_0+n}{2}, \frac{1}{2}(\nu_0\sigma_0^2+\sum_i(x_i-\theta)^2)\right)$.
- *Lesson:* In finding out the full conditional of each parameter, we can indeed treat quantities that does not involve that parameter as "constants" that can be ignored.
- This is in contrast to the calculation of *marginal posteriors* as we did earlier, in which case, the quanitites that involve any of the parameters must be kept! (Recall the $\gamma^{1/2}$ term.)
- In particular, here we do not have to worry about integrating out a parameter resulting in a value that depends on the other parameters.

From full conditionals to posterior samples

- So we have the full conditionals of both θ and σ^2, how to get the joint posterior?
- By a Monte Carlo strategy called *Gibbs sampling*!
- Drawing (correlated) samples from a multivariate distribution from its full conditionals.
- *Gibbs sampling*: Iteratively sample each parameter from its full conditional and repeat this process.

Example: The normal-inverse-Gamma prior

- Choose an initial value $(\theta^{(0)}, \sigma^{2(0)})$
- For $t = 1, 2, \ldots,$
  - Draw $\theta^{(t)} \sim \mathrm{N}(\mu_n^{(t)}, \tau_n^{2(t)})$
  - Draw $\sigma^{2\,(t)} \sim \mathrm{IG}\left(\frac{\nu_0+n}{2}, \frac{1}{2}(\nu_0\sigma_0^2 + \sum_i (x_i - \theta^{(t)})^2)\right).$

- In the above,

$$\mu_n^{(t)} = \left(\frac{1/\tau_0^2}{1/\tau_0^2 + n/\sigma^{2\,(t-1)}}\right)\mu_0 + \left(\frac{n/\sigma^{2\,(t-1)}}{1/\tau_0^2 + n/\sigma^{2\,(t-1)}}\right)\bar{x}$$

  and

$$\frac{1}{\tau_n^{2\,(t)}} = \frac{1}{\tau_0^2} + \frac{n}{\sigma^{2\,(t-1)}}.$$

- We can use $\gamma^{(t)}$ in place of $\frac{1}{\sigma^{(t)}}$.

A few remarks

- The samples are *dependent*—so this is not vanilla Monte Carlo.
- In particular, $(\theta^{(t)}, \sigma^{2\,(t)})$ depends on the value of $(\theta^{(t-1)}, \sigma^{2\,(t-1)})$.
- The sequence of samples

$$(\theta^{(1)}, \sigma^{2\,(1)}), (\theta^{(2)}, \sigma^{2\,(2)}), \ldots, (\theta^{(t-1)}, \sigma^{2\,(t-1)}), (\theta^{(t)}, \sigma^{2\,(t)}), \ldots$$

  form a *Markov Chain*.

Markov Chains and its convergence

- A sequence of random (possibly multi-dimensional) variables (i.e., a stochastic process)

$$\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_{t-1}, \mathbf{X}_t, \mathbf{X}_{t+1}, \ldots$$

  is a *Markov chain* if

$$p(\mathbf{X}_{t+1} \,|\, \mathbf{X}_1, \ldots, \mathbf{X}_t) = p(\mathbf{X}_{t+1} \,|\, \mathbf{X}_t).$$

- The future depends on the past only through the present.
- Check that the previous sequence of draws $(\theta^{(t)}, \sigma^{2\,(t)})$ for $t = 1, 2, \ldots$ form a (homogeneous) Markov chain.

Markov Chain convergence

- Moreover, if a Markov Chain satisfies certain conditions (namely, it is *irreducible, aperiodic, and positive recurrent*), then the marginal distribution of $\mathbf{X}_t$ *converge* to a unique stationary distribution p. (Markov chain theory is beyond the scope of this class.)
- That is, under such conditions, for large enough t, the unconditional distribution

$$\mathrm{P}(\mathbf{X}_t \in A) \approx \int_A p(x)dx \quad \text{for large enough } t.$$

where $p(A)$ is the so-called stationary distribution, that is, if $X_{t-1} \sim p$ then $X_t \sim p$, i.e.,

$$p(y) = \int p(X_t = y \,|\, X_{t-1} = x)p(x)dx.$$

- How large a t is sufficient?

Use Markov Chain for Monte Carlo

- In order to evaluate an integral

$$\mathrm{E}_p g = \int g(x)p(x)dx.$$

- If we cannot generate i.i.d. samples from p, but can construct a Markov Chain

$$X_1, X_2, \ldots$$

that converges to the stationary distribuiton p.

- It turns out that under certain conditions (called *ergodicity*) of the MC, there is a corresponding law of large number for Markov Chains that ensures

$$\frac{1}{S}\sum_{i=1}^{S} g(X_i) \to \mathrm{E}_p g \quad \text{as } S \to \infty.$$

- In practice, people will discard the X_i for small i (the "burn-in"). For example, draw 20000 X_is but only use the last 10000 values.

The Gaussian example

- The Markov chain formed $(\theta^{(t)}, \sigma^{2\,(t)})$ formed by iteratively sampling from the full conditionals of θ and σ^2 for $t = 1, 2, \ldots$ satisfies the conditions to ensure eventual convergence to the target distribution

$$p(\theta, \sigma^2 \,|\, \mathbf{x}).$$

  and the convergence of Monte Carlo estimates.
- How fast is the convergence? It depends on how strongly correlated θ and σ^2 are under the target distribution.

Gibbs sampling, more generally

- Suppose we are interested in sampling d-dimensional random vectors $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_d)$ from a multivariate probability distribuiton $p(\boldsymbol{\theta})$.
- Suppose we are able to sample from all of the d full conditionals. That is, we know how to sample from

$$p(\theta_i \,|\, \boldsymbol{\theta}_{-i})$$

  for all $i = 1, 2, \ldots, d$, where for notational simplicity, we let $\boldsymbol{\theta}_{-i} = (\theta_1, \theta_2, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_d)$.
- In Bayesian inference problems, the target distribution is usually the posterior distribution of $\boldsymbol{\theta}$ given data, $p(\boldsymbol{\theta} \,|\, \mathbf{x})$.
  - In this case the full conditionals are $p(\theta_i \,|\, \boldsymbol{\theta}_{-i}, \mathbf{x})$.
  - For example, we have applied this algorithm to a bivariate parameter (θ, σ^2), and the target distribution is $p(\theta, \sigma^2 \,|\, \mathbf{x})$.

Gibbs sampling, more generally

- The Gibbs sampler prooceeds by
  - Initialize the parameter values at $\boldsymbol{\theta}^{(0)}$.
  - For $t = 1, 2, \ldots,$
    - For $i = 1, 2 \ldots, d$, update the ith parameter θ_i while keeping all other paramters $\boldsymbol{\theta}_{-i}$ fixed.

$$\theta_i^{(t)} \sim p(\theta_i \mid \boldsymbol{\theta}_{-i}^{(t)}).$$

where $\boldsymbol{\theta}_{-i}^{(t)}$ is the latest values of all other parameters, that is,

$$\boldsymbol{\theta}_{-i}^{(t)} = (\theta_1^{(t)}, \theta_2^{(t)}, \ldots, \theta_{i-1}^{(t)}, \theta_{i+1}^{(t-1)}, \ldots, \theta_d^{(t-1)}).$$

- For large enough t, the draws $\boldsymbol{\theta}^{(t)} = (\theta_1^{(t)}, \theta_2^{(t)}, \ldots, \theta_d^{(t)})$ will have the desired marginal distribution $p(\boldsymbol{\theta})$.

The speed of convergence to the target distribution

- The speed of such convergence depends on the correlation among the d parameters under $p(\boldsymbol{\theta})$ (or $p(\boldsymbol{\theta}|\mathbf{x})$ for Bayesian inference).
- In the special case where all parameters are independent under the target, then it takes one iteration (i.e., $t = 1$) to converge!
- In the other extreme if all parameters are perfectly correlated, then the chain will never move after $t = 1$ and so will never converge!

Example: Gibbs sampling for a bivariate normal

- Suppose we want to draw samples of $\boldsymbol{\theta} = (\theta_1, \theta_2)$ from a bivariate normal distribution

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathrm{N}\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right).$$

- Of course, we can draw independent samples in R from this distribution directly. Here let's practice Gibbs sampling.
- The full conditionals are

$$\theta_1 \,|\, \theta_2 \sim \mathrm{N}(\mu_1 + \rho(\theta_2 - \mu_2), 1 - \rho^2)$$
$$\theta_2 \,|\, \theta_1 \sim \mathrm{N}(\mu_2 + \rho(\theta_1 - \mu_1), 1 - \rho^2)$$

Example: Gibbs sampling for a bivariate normal

- We initialize the Gibbs sampler at $\boldsymbol{\theta}^{(0)} = (0,0)$.
- Then for $t = 1, 2, \ldots$
  - Draw

$$\theta_1^{(t)} \mid \theta_2^{(t-1)} \sim \mathrm{N}(\mu_1 + \rho(\theta_2^{(t-1)} - \mu_2), 1 - \rho^2)$$

and

$$\theta_2^{(t)} \mid \theta_1^{(t)} \sim \mathrm{N}(\mu_2 + \rho(\theta_1^{(t)} - \mu_1), 1 - \rho^2)$$

Gibbs sampling code

```
mu <- c(2,2)
rho <- 0.5 # change this to different values and see how it works
S <- 100
theta.mc <- matrix(0,nrow=S,ncol=2)
theta <- c(0,0) # initial value

# Gibbs sampling
for (t in 1:S) {
  theta[1] <- rnorm(1,mean=mu[1]+rho*(theta[2]-mu[2]),sd=sqrt(1-rho^2))
  theta[2] <- rnorm(1,mean=mu[2]+rho*(theta[1]-mu[1]),sd=sqrt(1-rho^2))
  theta.mc[t,] <- theta
}
```

```r
library(mvtnorm)
mu <- c(2,2)
rho <- 0.5 # change this to different values
Sigma <- matrix(c(1,rho,rho,1),ncol=2);
ylim <- xlim <- c(-1,5)
x <- seq(xlim[1],xlim[2],length=200)
y <- x
xy.grid <- expand.grid(x,y)
den.grid <- matrix(dmvnorm(xy.grid,mean=mu,sigma=Sigma),nrow=length(x))

contour(x,y,den.grid,xlim=xlim,ylim=ylim,
        xlab=expression(theta[1]),ylab=expression(theta[2]))
```

```r
S <- 100
theta.mc <- matrix(0,nrow=S,ncol=2)
theta <- c(0,0) # initial value

points(x=theta[1],y=theta[2],col="red4",pch=16); Sys.sleep(1)
theta.prev <- theta
for (t in 1:S) {
  theta[1] <- rnorm(1,mean=mu[1]+rho*(theta[2]-mu[2]),sd=sqrt(1-rho^2))
  if (t<20) Sys.sleep(1)
  segments(theta.prev[1],theta.prev[2],theta[1],theta[2],col="gray") # gray line segments
  theta[2] <- rnorm(1,mean=mu[2]+rho*(theta[1]-mu[1]),sd=sqrt(1-rho^2))
  if (t<20) Sys.sleep(1)
  segments(theta[1],theta.prev[2],theta[1],theta[2],col="gray") # gray line segments
  theta.mc[t,] <- theta

  if(t < 20){
    points(x=theta[1],y=theta[2],col="red4",pch=16);
  } else {
    points(x=theta[1],y=theta[2],col="green4",pch=16); Sys.sleep(0.1)
  }

  theta.prev <- theta

}
```

Markov Chain Monte Carlo

- Gibbs sampling is an example of a Markov Chain Monte Carlo (MCMC) algorithm.
- The idea is to sample $\boldsymbol{\theta}$ through constructing a Markov Chain. As such, the draws

$$\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \ldots$$

  are dependent and form a Markov chain. So each $\boldsymbol{\theta}^{(i)}$ is generated based on only the value of $\boldsymbol{\theta}^{(i-1)}$.
- By ensuring that the Markov chain that satisfies the neccessary conditions to ensure its convergence to a desired stationary distribution, typically a posterior distribution $p(\boldsymbol{\theta}|\mathbf{x})$, as well as the convergence of Monte Carlo estimates, we are able to
  - draw these dependent samples from $p(\boldsymbol{\theta}|\mathbf{x})$;
  - evaluate integrals with respect to $p(\boldsymbol{\theta}|\mathbf{x})$.
- Thus based on this sample we can proceed with Bayesian inference as usual.

Some distinctions from sampling independent samples

- Unlike standard Monte Carlo where we draw independent samples *exactly* from some target p,
  - MCMC samples will only converge to the target p after a sufficient number of steps. So we will typically discard the first steps in the chain, which is called the *burn-in* stage.
  - The sampled values are dependent, and each is drawn based on the previous value, and so the *effective sample size* depends on how effectively that chain of values move around the parameter space to explore the distribution.

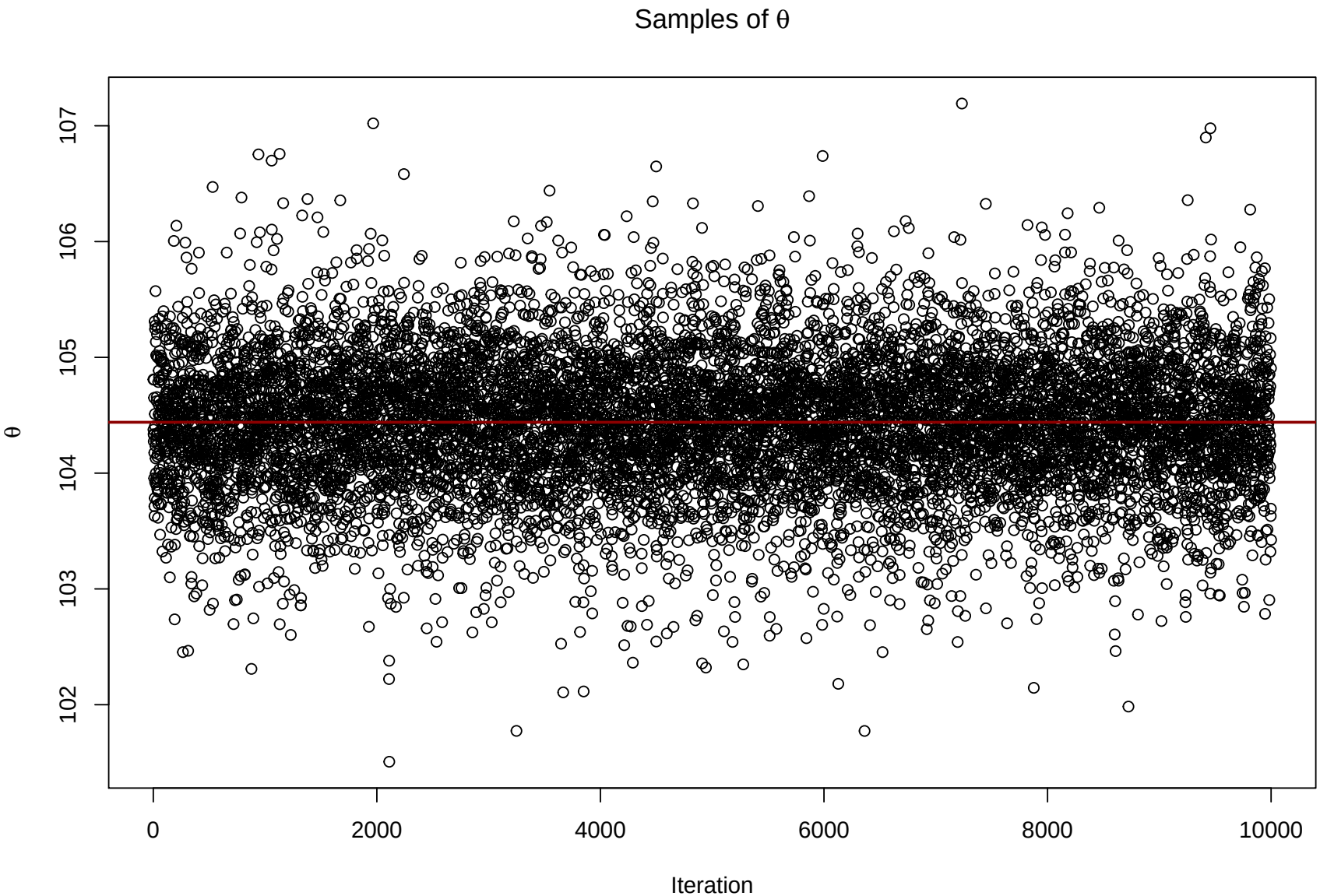
Two conditions necessary for an effective MCMC chain

- *Fast convergence*: The Markov chain needs to be long enough so that it has moved into a high-probability region of the target $p(\boldsymbol{\theta} \,|\, \mathbf{x})$.
  - This ensures that we are actually sampling from the desired posterior after the *burn-in*.
- *Good mixing*: The Markov chain should be moving across the high probability regions of $p(\boldsymbol{\theta} \,|\, \mathbf{x})$, rather than being stuck in one or a few regions, while move across to another only occassionally.
  - This ensures that the effective sample size is large so that the Monte Carlo error is small.

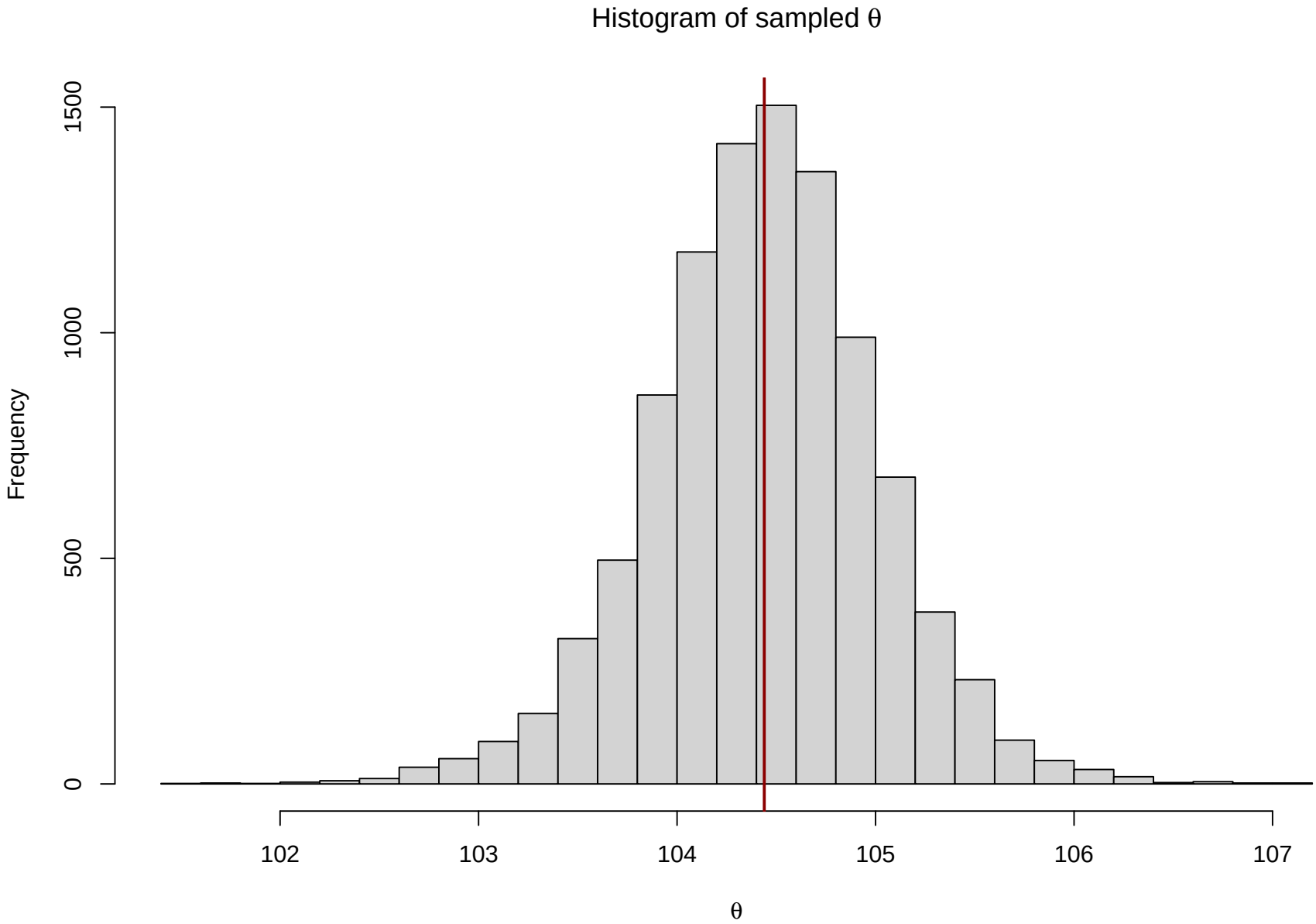
Back to air pollutant example

```
x <- c(104,105,103,102,105,107,106,104,103,106) # the data
n <- length(x) # sample size

S <- 10000
xbar <- mean(x)
s2 <- var(x)
n <- length(x)

THETA <- matrix(NA,nrow=S,ncol=2,dimnames=list(1:S,c("theta","sigma2")))
THETA.init <- c(xbar,s2) # Initial values set to the MLE
THETA.curr <- THETA.init # the parameter values at the current iteration
mu.0 <- 100; nu.0 <- 1; tau2.0 <- 25; sigma2.0 <- 4

### Start Gibbs sampling
for (t in 1:S) {
  tau2.n <- 1/(1/tau2.0 + n/THETA.curr[2])
  mu.n <- (mu.0/tau2.0 + xbar*n/THETA.curr[2])/(1/tau2.0 + n/THETA.curr[2])

  ## Update theta
  THETA.curr[1] <- rnorm(1,mean=mu.n,sd=sqrt(tau2.n))

  ## Update sigma2
  THETA.curr[2] <- 1/rgamma(1,shape=(nu.0+n)/2,
                            rate=1/2*(nu.0*sigma2.0+sum((x-THETA.curr[1])^2)))

  ## Save the current iteration
  THETA[t,] <- THETA.curr
}
```

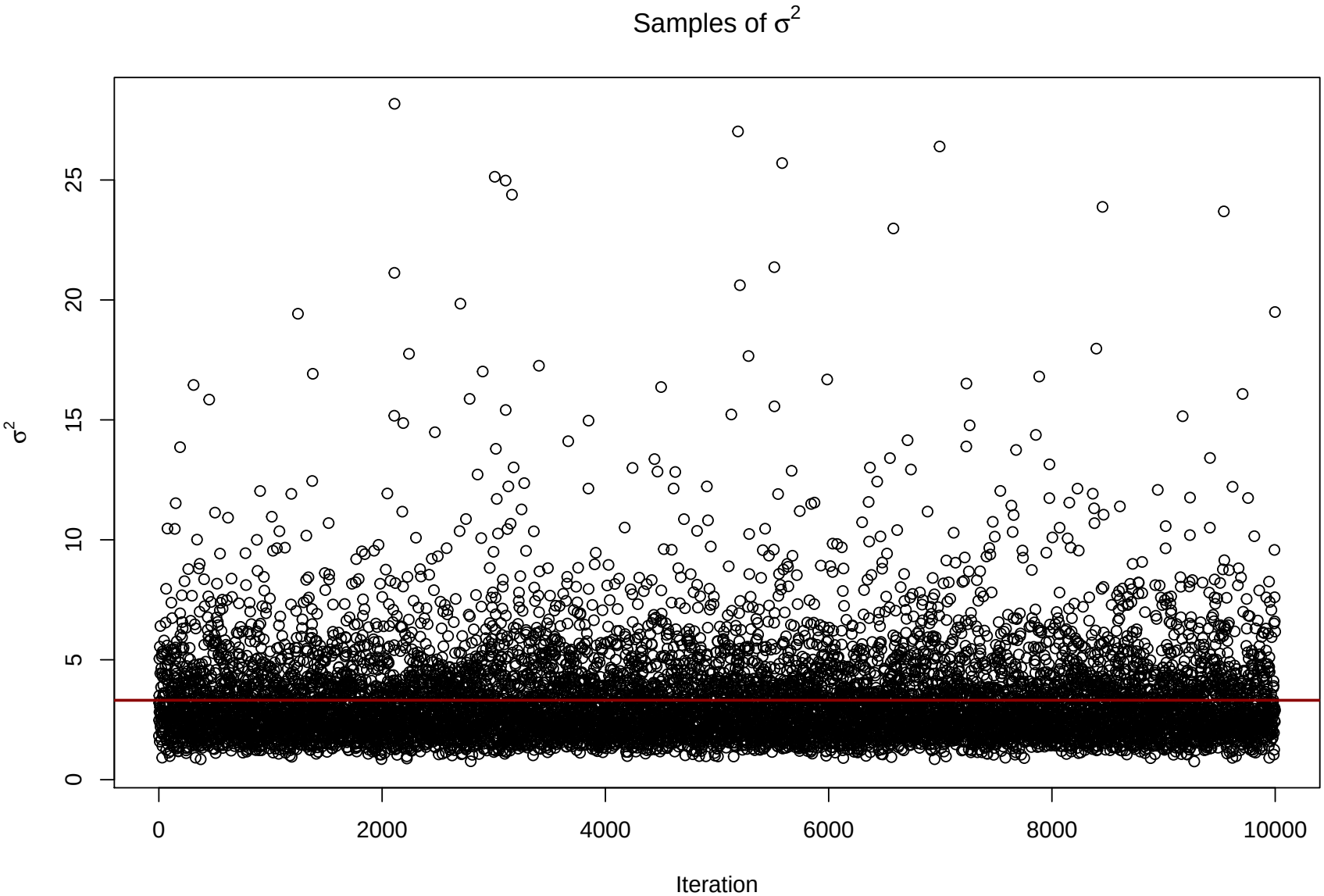
Trace plot for θ



Histogram for θ



Trace plot for σ^2



Histogram for σ^2