MAS3902: Bayesian Inference

Dr. Lee Fawcett

School of Mathematics, Statistics & Physics

Semester 2, 2022/23

Contact details

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Timetable and Administrative arrangements

- **Classes** take place on Tuesdays (3pm, Herschel LT2) and Thursdays (9am, online – fortnightly only; 12pm, Herschel LT1)
- Two of these classes will be **lectures**, and the other session will be a **problems class/drop-in**
  - Lectures will *ordinarily* take place in the in-person slots in the lecture theatres
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  - Friday 3rd February (11am, Herschel LT2)
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Assessment

Assessment is by:

- 2-hour end-of-semester exam in May/June (**80%**)
- In course assessment (**20%**), comprising four short written assignments:

Date set	Deadline	Marks/weighting
Friday 10th February	4pm, Friday 24th February	20/5%
Friday 24th February	4pm, Friday 10th March	20/5%
Friday 10th March	4pm, Friday 24th March	20/5%
Friday 24th March	4pm, Friday 5th May	20/5%

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Recommended textbooks

- "*Bayes' Rule: A Tutorial Introduction to Bayesian Analysis*" - James Stone
- "*Doing Bayesian Data Analysis: A Tutorial with R, JAGS, and Stan*" - John Krushke
- "*Bayesian Statistics: An Introduction*" - Peter Lee

"Bayes' rule" is a good introduction to the main concepts in Bayesian statistics but doesn't cover everything in this course. The other books are broader references which go well beyond the contents of this course.

Other stuff

- Notes (with gaps) will be available for use in lectures – you can fill in the gaps during lectures
- A (very!) summarised version of the notes will be used in lectures as slides
- These notes and slides will be posted on the course Canvas page after each topic is finished, along with any other course material – such as problems sheets, model solutions to assignment questions, supplementary handouts etc.

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Chapter 1

Single parameter problems

1.1 Prior and posterior distributions

Data: $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$

Model: pdf/pf $f(\boldsymbol{x}|\theta)$ depends on a single parameter θ

$\rightarrow$ Likelihood function $f(\boldsymbol{x}|\theta)$

considered as a function of θ for known $\boldsymbol{x}$

Prior beliefs: pdf/pf $\pi(\theta)$

Combine using Bayes Theorem

Posterior beliefs: pdf/pf $\pi(\theta|\boldsymbol{x})$

Posterior distribution summarises all our current knowledge about the parameter θ

Bayes Theorem

The posterior probability (density) function for θ is

$$\pi(\theta|\boldsymbol{x}) = \frac{\pi(\theta)\, f(\boldsymbol{x}|\theta)}{f(\boldsymbol{x})}$$

where

$$f(\boldsymbol{x}) = \begin{cases} \int_{\Theta} \pi(\theta)\, f(\boldsymbol{x}|\theta)\, d\theta & \text{if } \theta \text{ is continuous,} \\ \\ \sum_{\Theta} \pi(\theta)\, f(\boldsymbol{x}|\theta) & \text{if } \theta \text{ is discrete.} \end{cases}$$

As $f(\boldsymbol{x})$ is not a function of θ, Bayes Theorem can be rewritten as

$$\pi(\theta|\boldsymbol{x}) \propto \pi(\theta) \times f(\boldsymbol{x}|\theta)$$

i.e. **posterior** $\propto$ **prior** $\times$ **likelihood**

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Example 1.1

- Data

Year	1998	1999	2000	2001	2002	2003	2004	2005
Cases	2	0	0	0	1	0	2	1

Table: Number of cases of foodbourne botulism in England and Wales, 1998–2005

- Assume that cases occur at random at a constant rate θ in time
- This means the data are from a Poisson process and so are a random sample from a Poisson distribution with rate θ
- An expert was consulted to construct a suitable prior distribution for the rate θ

Example 1.1

(a) What might be an appropriate probability model for the rate θ? Why is this termed the *prior distribution*?

(b) Suppose the epidemiologist tells you that she expects around two cases of foodbourne botulism per year in England and Wales. After further discussions with the epidemiologist, you are also able to elicit that $SD(\theta) \approx \sqrt{2}$. Using your answer to part (a) find your full prior distribution for θ, and write down its density.

(c) Determine the posterior distribution for θ.

Solution

. . . Solution...

Summary

- Model: $X_i|\theta \sim Po(\theta)$, $i = 1, 2, \ldots, 8$ (independent)
- Prior: $\theta \sim Ga(2, 1)$
- Data: in Table above
- Posterior: $\theta|\boldsymbol{x} \sim Ga(8, 9)$

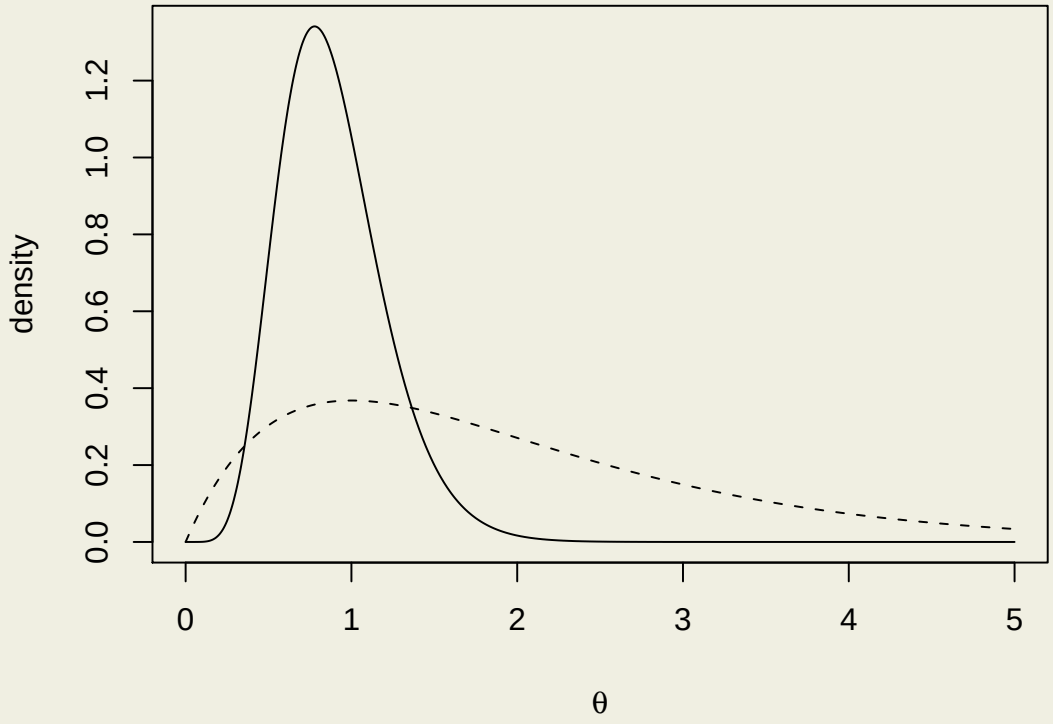


Figure: Prior (dashed) and posterior (solid) densities for θ

	Prior	Likelihood	Posterior
$Mode(\theta)$	1.00	0.75	0.78
$E(\theta)$	2.00	–	0.89
$SD(\theta)$	1.41	–	0.31

Table: Changes in beliefs about θ

- Likelihood mode $<$ prior mode $\rightarrow$ posterior mode moves in direction of likelihood mode $\rightarrow$ posterior mode $<$ prior mode
- Reduction in variability from the prior to the posterior

Example 1.2

We now consider the general case (of Example 1.1). Suppose $X_i|\theta \sim Po(\theta)$, $i = 1, 2, \ldots, n$ (independent) and our prior beliefs about θ are summarised by a $Ga(g, h)$ distribution (with g and h known), with density

$$\pi(\theta) = \frac{h^g \, \theta^{g-1} e^{-h\theta}}{\Gamma(g)}, \quad \theta > 0. \tag{1.1}$$

Determine the posterior distribution for θ.

Solution

...

(1.2)

(1.3)

Summary

- Model: $X_i|\theta \sim Po(\theta)$, $i = 1, 2, \ldots, n$ (independent)
- Prior: $\theta \sim Ga(g, h)$
- Data: observe $\boldsymbol{x}$
- Posterior: $\theta|\boldsymbol{x} \sim Ga(g + n\bar{x}, h + n)$
- Taking $g \geq 1$

	Prior (1.1)	Likelihood (1.2)	Posterior (1.3)
$Mode(\theta)$	$(g-1)/h$	$\bar{x}$	$(g + n\bar{x} - 1)/(h + n)$
$E(\theta)$	g/h	–	$(g + n\bar{x})/(h + n)$
$SD(\theta)$	$\sqrt{g}/h$	–	$\sqrt{g + n\bar{x}}/(h + n)$

Table: Changes in beliefs about θ

Comments

- Posterior mean is greater than the prior mean if and only if the likelihood mode is greater than the prior mean, that is,

$$E(\theta|\boldsymbol{x}) > E(\theta) \quad \Longleftrightarrow \quad Mode_\theta\{f(\boldsymbol{x}|\theta)\} > E(\theta)$$

- Standard deviation of the posterior distribution is smaller than that of the prior distribution if and only if the sample mean is not too large, that is

$$SD(\theta|\boldsymbol{x}) < SD(\theta) \quad \Longleftrightarrow \quad Mode_\theta\{f(\boldsymbol{x}|\theta)\} < \left(2 + \frac{n}{h}\right) E(\theta),$$

and that this will be true in large samples.

Example 1.3

Suppose we have a random sample from a normal distribution with unknown mean μ but known precision τ: $X_i|\mu \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (independent).

Suppose our prior beliefs about μ can be summarised by a $N(b, 1/d)$ distribution, with probability density function

$$\pi(\mu) = \left(\frac{d}{2\pi}\right)^{1/2} \exp\left\{-\frac{d}{2}(\mu - b)^2\right\}. \tag{1.4}$$

Determine the posterior distribution for μ.

Hint:

$$d(\mu - b)^2 + n\tau(\bar{x} - \mu)^2 = (d + n\tau)\left\{\mu - \left(\frac{db + n\tau\bar{x}}{d + n\tau}\right)\right\}^2 + c$$

where c does not depend on μ.

Solution

. . .

(1.5)

(1.6)

(1.7)

Summary

- Model: $X_i|\mu \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (independent), with τ known
- Prior: $\mu \sim N(b, 1/d)$
- Data: observe $\boldsymbol{x}$
- Posterior: $\mu|\boldsymbol{x} \sim N(B, 1/D)$, where

$$B = \frac{db + n\tau\bar{x}}{d + n\tau} \qquad \text{and} \qquad D = d + n\tau$$

	Prior (1.4)	Likelihood (1.5)	Posterior (1.7)
$Mode(\mu)$	b	$\bar{x}$	$(db + n\tau\bar{x})/(d + n\tau)$
$E(\mu)$	b	–	$(db + n\tau\bar{x})/(d + n\tau)$
$Precision(\mu)$	d	–	$d + n\tau$

Table: Changes in beliefs about μ

- Posterior mean is greater than the prior mean if and only if the likelihood mode (sample mean) is greater than the prior mean, that is

$$E(\mu|\boldsymbol{x}) > E(\mu) \quad \Longleftrightarrow \quad Mode_{\mu}\{f(\boldsymbol{x}|\mu)\} > E(\mu)$$

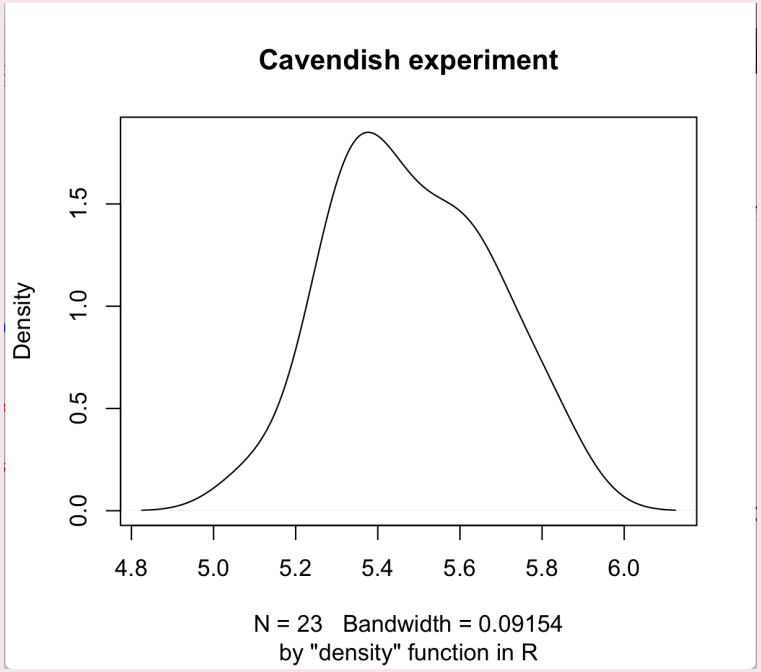
- Standard deviation of the posterior distribution is smaller than that of the prior distribution, that is

$$SD(\mu|\boldsymbol{x}) < SD(\mu)$$

Example 1.4

The 18th century physicist Henry Cavendish made 23 experimental determinations of the earth's density, and these data (in g/cm^3) are shown below.

5.36	5.29	5.58	5.65	5.57	5.53	5.62	5.29
5.44	5.34	5.79	5.10	5.27	5.39	5.42	5.47
5.63	5.34	5.46	5.30	5.78	5.68	5.85	



Example 1.4

- Cavendish asserts that the error standard deviation of these measurements is $0.2\,g/cm^3$
- Assume that they are normally distributed with mean equal to the true earth density μ, that is, $X_i|\mu \sim N(\mu, 0.2^2)$, $i = 1, 2, \ldots, 23$
- Use a normal prior distribution for μ with mean $5.41\,g/cm^3$ and standard deviation $0.4\,g/cm^3$
- Derive the posterior distribution for μ

Solution

...

Summary

- Small increase in mean from prior to posterior
- Large decrease in uncertainty from prior to posterior

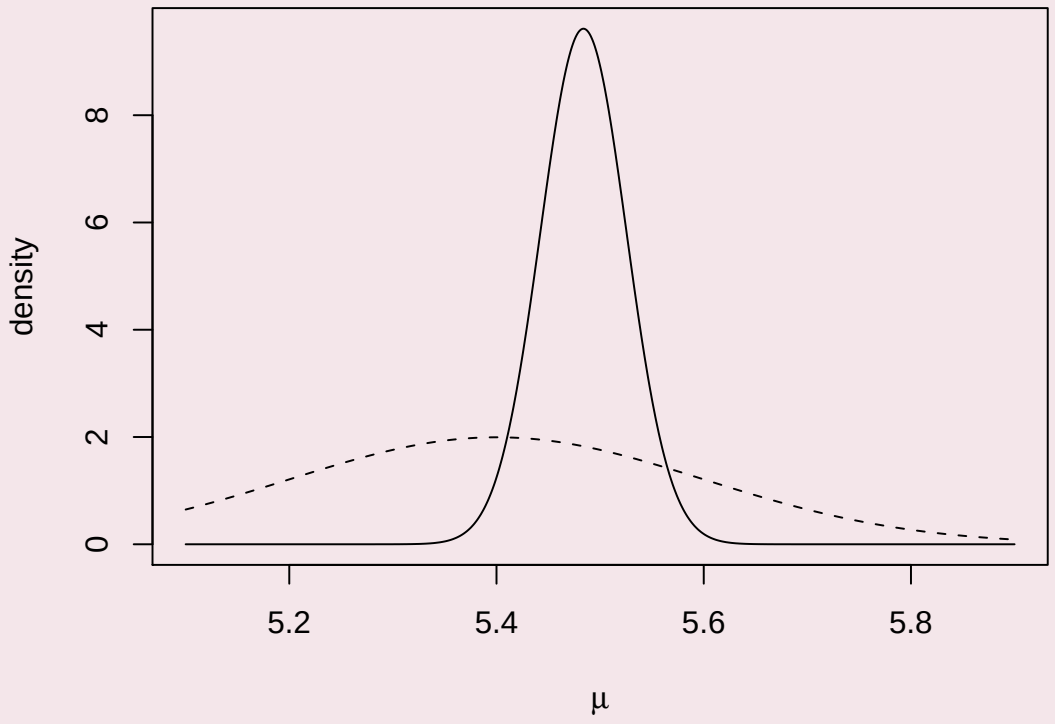


Figure: Prior (dashed) and posterior (solid) densities for the earth's density

Summary

- The actual mean density of the earth is $5.515\,g/cm^3$ (Wikipedia)
- We can determine the (posterior) probability that the mean density is within 0.1 of this value as follows...
- The posterior distribution is $\mu|\boldsymbol{x} \sim N(5.484, 0.0415^2)$ and so

$$Pr(5.415 < \mu < 5.615|\boldsymbol{x}) = 0.9510,$$

calculated using the R command

```
pnorm(5.615,5.484,0.0415)-pnorm(5.415,5.484,0.0415)
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Summary

- Without the data, the only basis for determining the earth's density is via the prior distribution
- Here the prior distribution is $\mu \sim N(5.4, 0.4^2)$ and so the (prior) probability that the mean density is within 0.1 of the (now known) true value is

$$Pr(5.415 < \mu < 5.615) = 0.1896,$$

calculated using the R command

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1.2 Different levels of prior knowledge

1.2.1 Substantial Prior Knowledge

- We have *substantial prior information* for θ when the prior distribution *dominates* the likelihood function, that is $\pi(\theta|\boldsymbol{x}) \sim \pi(\theta)$

- Difficulties:
  1. Intractability of mathematics in deriving the posterior
  2. Practical formulation of the prior distribution – coherently specifying prior beliefs in the form of a probability distribution is far from straightforward, let alone reconciling differences between experts!

1.2.2 Limited prior information

Pragmatic approach:

- Choose a distribution which makes the Bayes updating from prior to posterior mathematically straightforward
- Use what prior information is available to determine the parameters of this distribution

Previous examples:

1. Poisson random sample, Gamma prior distribution $\longrightarrow$ Gamma posterior distribution
2. Normal random sample (known variance), Normal prior distribution $\longrightarrow$ Normal posterior distribution

In these examples, the prior distribution and the posterior distribution come from the same family

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Definition 1.1 (Conjugate priors)

Suppose that data $\boldsymbol{x}$ are to be observed with distribution $f(\boldsymbol{x}|\theta)$. A family $\mathfrak{F}$ of prior distributions for θ is said to be *conjugate* to $f(\boldsymbol{x}|\theta)$ if for every prior distribution $\pi(\theta) \in \mathfrak{F}$, the posterior distribution $\pi(\theta|\boldsymbol{x})$ is also in $\mathfrak{F}$.

Comment

The conjugate family depends crucially on the model chosen for the data $\boldsymbol{x}$.

For example, the only family conjugate to the model "random sample from a Poisson distribution" is the Gamma family. Here, the likelihood is $f(\boldsymbol{x}|\theta) \propto \theta^{n\bar{x}} e^{-n\theta}$, $\theta > 0$. Therefore we need a family with density $f(\theta|\boldsymbol{a})$ and parameters $\boldsymbol{a}$ such that

$$f(\theta|\boldsymbol{A}) \propto f(\theta|\boldsymbol{a}) \times \theta^{n\bar{x}} e^{-n\theta}, \quad \theta > 0$$

$$\implies \quad f(\theta|\boldsymbol{a}) \propto \theta^{a_1} e^{-a_2\theta}, \quad \theta > 0$$

that is, the Gamma family of distributions

1.2.3 Vague prior knowledge/prior ignorance

- Have very little or no prior information about θ
- Still must choose a prior distribution
- Sensible to choose a prior distribution which is not concentrated about any particular value, that is, one with a very large variance
- Most of the information about θ will be passed through to the posterior distribution via the data, and so we have $\pi(\theta|\boldsymbol{x}) \sim f(\boldsymbol{x}|\theta)$
- Vague prior: Represent vague prior knowledge by using a prior distribution which is conjugate to the model for $\boldsymbol{x}$ and which has as large a variance as possible
- Prior ignorance: Uniform prior? Jeffreys prior?

$$I(\theta) = E_{\boldsymbol{X}|\theta}\left[-\frac{\partial^2}{\partial\theta^2}\log f(\boldsymbol{X}|\theta)\right], \tag{1.8}$$

and then:

$$\pi(\theta) \propto \sqrt{I(\theta)}. \tag{1.9}$$

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Example 1.5

In constructing the prior in Example 1.1, did we assume (i) substantial prior knowledge; (ii) limited prior knowledge; or (iii) prior ignorance?

Solution

...

Example 1.6

Suppose the parameter θ represents a probability. What might be the simplest prior to use here, if we are prior ignorant?

Solution

...

Example 1.7

Suppose we have a random sample from a $N(\mu, 1/\tau)$ distribution (with τ known). Determine the posterior distribution assuming a vague prior for μ.

Solution

...

Example 1.8

Suppose we have a random sample from an Poisson distribution, that is, $X_i|\theta \sim Po(\theta)$, $i = 1, 2, \ldots, n$ (independent). Determine the posterior distribution assuming a vague prior for θ.

Solution

- The conjugate prior distribution is a Gamma distribution
- The $Ga(g, h)$ distribution has mean $m = g/h$ and variance $v = g/h^2$
- Rearranging gives $g = m^2/v$ and $h = m/v$
- Clearly $g \to 0$ and $h \to 0$ as $v \to \infty$ (for fixed m)
- We have seen that, for this model, using a $Ga(g, h)$ prior distribution results in a $Ga(g + n\bar{x}, h + n)$ posterior distribution
- Therefore, taking a vague prior distribution will give a $Ga(n\bar{x}, n)$ posterior distribution

Note that the posterior mean is $\bar{x}$ (the likelihood mode) and that the posterior variance $\bar{x}/n \to 0$ and $n \to \infty$.

Example 1.9

Suppose we have a random sample from an exponential distribution, that is, $X_i|\theta \sim Exp(\theta)$, $i = 1, 2, \ldots, n$ (independent). Determine the Jeffreys prior for this model.

Solution

$\cdots$

What have we done so far?

1. **Posterior $\propto$ Prior $\times$ Likelihood**

   - **Example: Poisson distribution** with gamma prior (food poisoning, and generic/algebraic example)
   - **Example: Normal distribution** (known precision) with Normal prior for the mean (generic/algebraic example, and Cavendish experiment). (Memorise the results from the algebraic example!)
   - **Example: Binomial distribution** with beta prior (homework)
   - **Example: Exponential distribution** with Normal prior (homework)
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What have we done so far?

2. Different levels of prior information

- **Substantial** prior information: $\pi(\theta|\boldsymbol{x}) \sim \pi(\theta)$, but often difficult to construct
- **Limited** prior information: Use conjugate prior with parameters determined by the information provided by the expert
- **Vague** prior: Use conjugate prior with maximised variance
- **Ignorance** prior: Use a Jeffreys prior, or perhaps a $U(0,1)$?
- For vague/ignorance priors, $\pi(\theta|\boldsymbol{x}) \sim f(\boldsymbol{x}|\theta)$
- Lots of **Examples**: Examples 1.5–1.9 in notes

3. Posterior distribution when the sample is very large

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1.3 Asymptotic Posterior Distribution

Background

- There are many asymptotic results in Statistics
- The **Central Limit Theorem** is a statement about the asymptotic distribution of $\bar{X}_n$ as the sample size $n \to \infty$, where the X_i are i.i.d. with known mean μ and known (finite) variance σ^2
- Under different distributions of X_i, $\bar{X}_n$ has the same moments, $E(\bar{X}_n) = \mu$ and $Var(\bar{X}_n) = \sigma^2/n$, but its distribution varies
- The CLT says that as $n \to \infty$, regardless of the distribution of X_i,

$$\frac{\sqrt{n}(\bar{X}_n - \mu)}{\sigma} \xrightarrow{\mathcal{D}} N(0,1)$$

Theorem

Suppose we have a statistical model $f(\boldsymbol{x}|\theta)$ for data $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$, together with a prior distribution $\pi(\theta)$ for θ. Then

$$\sqrt{J(\hat{\theta})}\,(\theta - \hat{\theta})|\boldsymbol{x} \xrightarrow{\mathcal{D}} N(0,1) \qquad \text{as } n \to \infty,$$

where $\hat{\theta}$ is the likelihood mode and $J(\theta)$ is the observed information

$$J(\theta) = -\frac{\partial^2}{\partial\theta^2} \log f(\boldsymbol{x}|\theta)$$

Usage

In large samples,

$$\theta|\boldsymbol{x} \sim N\left(\hat{\theta}, J(\hat{\theta})^{-1}\right), \qquad \text{approximately.}$$

- In large samples (n large), how the prior distribution is specified does not matter.

Example 1.10

Suppose we have a random sample from a $N(\mu, 1/\tau)$ distribution (with τ known). Determine the asymptotic posterior distribution for μ.
Recall that

$$f(\boldsymbol{x}|\mu) = \left(\frac{\tau}{2\pi}\right)^{n/2} \exp\left\{-\frac{\tau}{2}\sum_{i=1}^{n}(x_i-\mu)^2\right\},$$

and therefore

$$\log f(\boldsymbol{x}|\mu) = \frac{n}{2}\log\tau - \frac{n}{2}\log(2\pi) - \frac{\tau}{2}\sum_{i=1}^{n}(x_i-\mu)^2$$

$$\Rightarrow \quad \frac{\partial}{\partial\mu}\log f(\boldsymbol{x}|\mu) = -\frac{\tau}{2}\times\sum_{i=1}^{n}-2(x_i-\mu) = \tau\sum_{i=1}^{n}(x_i-\mu) = n\tau(\bar{x}-\mu)$$

$$\Rightarrow \quad \frac{\partial^2}{\partial\mu^2}\log f(\boldsymbol{x}|\mu) = -n\tau \qquad \Rightarrow \quad J(\mu) = -\frac{\partial^2}{\partial\mu^2}\log f(\boldsymbol{x}|\mu) = n\tau.$$

Solution

...

1.4 Bayesian inference

- The posterior distribution $\pi(\theta|\boldsymbol{x})$ summarises all our information about θ to date
- It can answer the questions: How to estimate the value of θ, and what is the uncertainty of the estimator?

1.4.1 Estimation

Point estimates

Many useful summaries, such as

- the mean: $E(\theta|\boldsymbol{x})$
- the mode: $Mode(\theta|\boldsymbol{x})$
- the median: $Median(\theta|\boldsymbol{x})$

Interval Estimates

- A more useful summary of the posterior distribution is one which also reflects its variation
- A $100(1-\alpha)\%$ *Bayesian confidence interval* for θ is any region C_α that satisfies $Pr(\theta \in C_\alpha | \boldsymbol{x}) = 1 - \alpha$
- If θ is continuous with posterior density $\pi(\theta|\boldsymbol{x})$ then

$$\int_{C_\alpha} \pi(\theta|\boldsymbol{x})\, d\theta = 1 - \alpha$$

- The usual correction is made for discrete θ, that is, we take the largest region C_α such that $Pr(\theta \in C_\alpha | \boldsymbol{x}) \leq 1 - \alpha$
- Bayesian confidence intervals are sometimes called *credible regions* or *plausible regions*
- Clearly these intervals are not unique, since there will be many intervals with the correct probability coverage for a given posterior distribution

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Highest density intervals

- A $100(1-\alpha)\%$ *highest density interval* (HDI) for θ is the region

$$C_\alpha = \{\theta : \ \pi(\theta|\boldsymbol{x}) \geq \gamma\}$$

  where γ is chosen so that $Pr(\theta \in C_\alpha|\boldsymbol{x}) = 1-\alpha$
- It is a $100(1-\alpha)\%$ Bayesian confidence interval but only includes the most likely values of θ
- This region is sometimes called a *most plausible Bayesian confidence interval*
- If the posterior distribution has many modes then it is possible that the HDI will be the union of several disjoint regions

Highest density intervals

- If the posterior distribution is unimodal (has one mode) and symmetric about its mean then the HDI is an equi-tailed interval, that is, takes the form $C_\alpha = (a, b)$, where

$$Pr(\theta < a|\boldsymbol{x}) = Pr(\theta > b|\boldsymbol{x}) = \alpha/2$$

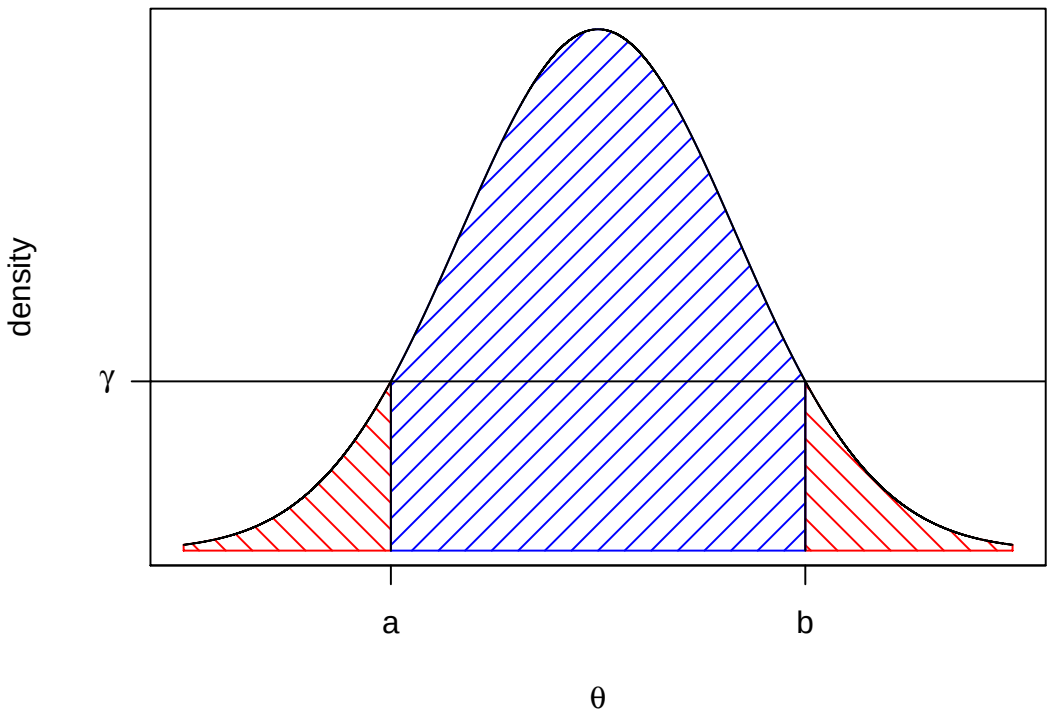

Figure: HDI for θ

Example 1.11

Suppose we have a random sample $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$ from a $N(\mu, 1/\tau)$ distribution (where τ is known). We have seen that, assuming vague prior knowledge, the posterior distribution is $\mu|\boldsymbol{x} \sim N\{\bar{x}, 1/(n\tau)\}$. Determine the $100(1-\alpha)\%$ HDI for μ.

Solution

...

Comment

Note that this interval is numerically identical to the 95% frequentist confidence interval for the (population) mean of a normal random sample with known variance. However, the interpretation is very different.

Interpretation of confidence intervals

C_B is a 95% Bayesian confidence interval for θ

C_F is a 95% frequentist confidence interval for θ

These intervals do not have the same interpretation:

- the probability that C_B contains θ is 0.95
- the probability that C_F contains θ is either 0 or 1
- the interval C_F covers the true value θ on 95% of occasions — in repeated applications of the formula

Example 1.12

Recall Example 1.1 on the number of cases of foodbourne botulism in England and Wales. The data were modelled as a random sample from a Poisson distribution with mean θ. Using a $Ga(2, 1)$ prior distribution, we found the posterior distribution to be $\theta|\boldsymbol{x} \sim Ga(8, 9)$, with density

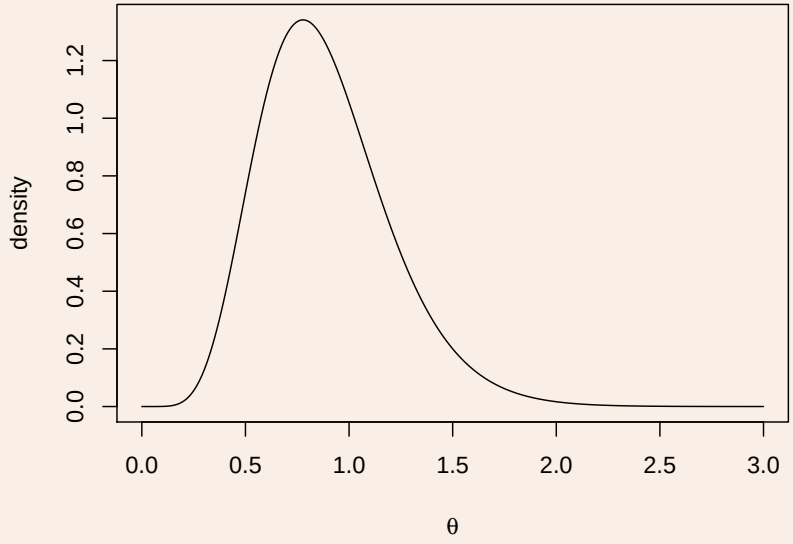

Figure: Posterior density for θ

Determine the 95% HDI for θ.

Solution

. . .

Simple way to calculate the HDI

- Use the `R` function `hdiGamma` in the package `nclbayes`
- It calculates the HDI for any Gamma distribution
- Here we use

```
library(nclbayes)
hdiGamma(p=0.95,a=8,b=9)
```

- The package also has functions
  - `hdiBeta` for the Beta distribution
  - `hdiInvchi` for the Inv-Chi distribution (introduced in Chapter 3)

1.4.2 Prediction

- Much of statistical inference (both Frequentist and Bayesian) is aimed towards making statements about a parameter θ
- Often the inferences are used as a yardstick for similar future experiments
- For example, we may want to predict the outcome when the experiment is performed again

Predicting the future

- There will be uncertainty about the future outcome of an experiment
- Suppose this future outcome Y is described by a probability (density) function $f(y|\theta)$
- If θ were known, say θ_0, then any prediction can do no better than one based on $f(y|\theta = \theta_0)$
- What if θ is unknown?

Frequentist solution

- Get estimate $\hat{\theta}$ and use $f(y|\theta = \hat{\theta})$ but this ignores uncertainty on $\hat{\theta}$
- Better: use $E_{\hat{\theta}}\{f(y|\theta = \hat{\theta})\}$ to average over uncertainty on $\hat{\theta}$

Bayesian solution

- Use the *predictive distribution*, with density

$$f(y|\boldsymbol{x}) = \int_{\Theta} f(y|\theta)\,\pi(\theta|\boldsymbol{x})\,d\theta$$

  when θ is a continuous quantity
- Notice this could be rewritten as

$$f(y|\boldsymbol{x}) = E_{\theta|\boldsymbol{x}}\{f(y|\theta)\}$$

- Uses $f(y|\theta)$ but weights each θ by our posterior beliefs

Prediction interval

- Useful range of plausible values for the outcome of a future experiment
- Similar to a HDI interval
- A $100(1-\alpha)\%$ *prediction interval* for Y is the region

$$C_\alpha = \{y : \ f(y|\boldsymbol{x}) \geq \gamma\}$$

where γ is chosen so that $Pr(Y \in C_\alpha|\boldsymbol{x}) = 1-\alpha$

Example 1.13

Recall Example 1.1 on the number of cases of foodbourne botulism in England and Wales.

The data for 1998–2005 were modelled as a random sample from a Poisson distribution with mean θ.

Using a $Ga(2, 1)$ prior distribution, we found the posterior distribution to be $\theta|\boldsymbol{x} \sim Ga(8, 9)$.

Determine the predictive distribution for the number of cases for the following year (2006).

Solution

...

Comments

- This predictive probability function is related to that of a negative binomial distribution
- If $Z \sim NegBin(r, p)$ then

$$Pr(Z = z) = \binom{z-1}{r-1} p^r (1-p)^{z-r}, \quad z = r, r+1, \ldots$$

and so $W = Z - r$ has probability function

$$Pr(W = w) = Pr(Z = w+r) = \binom{w+r-1}{r-1} p^r (1-p)^w, \quad w = 0, 1, \ldots$$

- This is the same probability function as our predictive probability function, with $r = 8$ and $p = 0.9$
- Therefore $Y|\mathbf{x} \sim NegBin(8, 0.9) - 8$
- Note that, unfortunately, `R` also calls the distribution of W a negative binomial distribution with parameters r and p: `dnbinom(y,r,p)`

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Comparison between predictive and naive predictive distributions

- Can compare the predictive distribution $Y|\boldsymbol{x}$ with a naive predictive $Y|\theta = \hat{\theta} \sim Po(0.75)$ where

$$f(y|\theta = \hat{\theta}) = \frac{0.75^y \, e^{-0.75}}{y!}, \quad y = 0, 1, \ldots \ .$$

- Probability functions:

y `y = 0:5`	correct $f(y\|\boldsymbol{x})$ `dnbinom(y,8,0.9)`	naive $f(y\|\theta = \hat{\theta})$ `dpois(y,0.75)`
0	0.430	0.472
1	0.344	0.354
2	0.155	0.133
3	0.052	0.033
4	0.014	0.006
5	0.003	0.001
≥ 6	0.005	0.002

- The naive predictive distribution is a predictive distribution which uses a degenerate posterior distribution $\pi^*(\theta|\boldsymbol{x})$
- Here $Pr_{\pi^*}(\theta = 0.75|\boldsymbol{x}) = 1$ and standard deviation $SD_{\pi^*}(\theta|\boldsymbol{x}) = 0$
- The correct posterior standard deviation of θ is $SD_{\pi}(\theta|\boldsymbol{x}) = \sqrt{8}/9 = 0.314$
- Using a degenerate posterior distribution results in the naive predictive distribution having too small a standard deviation:

$$SD(Y|x = 1) = \begin{cases} 0.994 & \text{using the correct } \pi(\theta|\boldsymbol{x}) \\ 0.866 & \text{using the naive } \pi^*(\theta|\boldsymbol{x}), \end{cases}$$

  these values being calculated from $NegBin_{\mathrm{R}}(8, 0.9)$ and $Po(0.75)$ distributions
- $\{0, 1, 2\}$ is a 92.9% prediction set/interval
- $\{0, 1, 2\}$ is a 95.9% prediction set/interval using the the more "optimistic" naive predictive distribution

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Predictive distribution (general case)

- Generally requires calculation of a non-trivial integral (or sum)

$$f(y|\boldsymbol{x}) = \int_{\Theta} f(y|\theta)\,\pi(\theta|\boldsymbol{x})\,d\theta$$

- Easier method available when using a conjugate prior distribution
- Suppose θ is a continuous quantity and $\boldsymbol{X}$ and Y are independent given θ
- Using Bayes Theorem, the posterior distribution for θ given $\boldsymbol{x}$ and y is

$$\begin{aligned}
\pi(\theta|\boldsymbol{x}, y) &= \frac{\pi(\theta) f(\boldsymbol{x}, y|\theta)}{f(\boldsymbol{x}, y)} \\
&= \frac{\pi(\theta) f(\boldsymbol{x}|\theta) f(y|\theta)}{f(\boldsymbol{x}) f(y|\boldsymbol{x})} \qquad \text{since } \boldsymbol{X} \text{ and } Y \text{ are indep given } \theta \\
&= \frac{\pi(\theta|\boldsymbol{x})\, f(y|\theta)}{f(y|\boldsymbol{x})}.
\end{aligned}$$

Rearranging, we obtain ...

Predictive distribution (general case)

- Generally requires calculation of a non-trivial integral (or sum)

$$f(y|\boldsymbol{x}) = \int_{\Theta} f(y|\theta)\,\pi(\theta|\boldsymbol{x})\,d\theta$$

- Easier method available when using a conjugate prior distribution
- Suppose θ is a continuous quantity and $\boldsymbol{X}$ and Y are independent given θ
- Using Bayes Theorem, the posterior distribution for θ given $\boldsymbol{x}$ and y is

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&= \frac{\pi(\theta|\boldsymbol{x})\, f(y|\theta)}{f(y|\boldsymbol{x})}.
\end{aligned}$$

Rearranging, we obtain ...

Candidate's formula

- The predictive p(d)f is

$$f(y|\boldsymbol{x}) = \frac{f(y|\theta)\pi(\theta|\boldsymbol{x})}{\pi(\theta|\boldsymbol{x}, y)}$$

- The RHS looks as if it depends on θ but it doesn't: all terms in θ cancel
- For this formula to be useful, we have to be able to work out $\theta|\boldsymbol{x}$ and $\theta|\boldsymbol{x}, y$ fairly easily
- This is the case when using conjugate priors

Example 1.14

Rework Example 1.13 using Candidate's formula to determine the number of cases in 2006.

Solution

...

1.5 Sequential Bayesian Updating

- Last year, and so far this year: Bayes Theorem to update beliefs about θ after observing a single sample $\boldsymbol{x}$
- Real-world: New samples of data coming online continuously!
- First sample $\boldsymbol{x}^{(1)} + \pi(\theta) \longrightarrow \pi(\theta|\boldsymbol{x}^{(1)})$
- New sample $\boldsymbol{x}^{(2)}$?
  - Use $\pi(\theta|\boldsymbol{x}^{(1)})$ as the "new prior"
  - Update once again to obtain the "new posterior" $\pi(\theta|\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)})$

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1.5 Sequential Bayesian Updating

In other words, we might replace the usual mantra

$$\text{Posterior} \propto \text{Prior} \times \text{Likelihood}$$

with

$$\text{Revised} \propto \text{Current} \times \text{New likelihood},$$

with the ability to update our likelihood function with each new sample of data. Why does this work?

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Suppose we have data assumed drawn from a probability distribution with parameter θ

1. Before we make any observations at all, our prior beliefs about θ are represented by $\pi(\theta)$. We might refer to this as our "original prior"
2. Now we observe a sample $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$; our posterior is then

$$\pi(\theta|\boldsymbol{x}) \propto \pi(\theta) \times f(\boldsymbol{x}|\theta) = \pi(\theta) \times \prod_{i=1}^{n} f(x_i|\theta),$$

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1.5 Sequential Bayesian Updating

3. Now suppose we make a new observation x_{n+1} assumed from the same probability distribution as $\boldsymbol{x}$
   - Beforehand our *current* beliefs about θ are represented by $\pi(\theta|\boldsymbol{x})$; re-label this $\pi_n(\theta)$, our "new prior"
   - Assume the *new likelihood* has the same form as the likelihood for $\boldsymbol{x}$
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Example 1.15

Table 1.6 provides an update to table 1.1, giving the number of cases of foodbourne botulism in England and Wales between 2006 and 2010.
Use your solution to Example 1.1, and sequential Bayesian updating, to obtain your new posterior distribution for θ.

Year	2006	2007	2008	2009	2010
Cases	1	0	0	1	1

Table: Number of cases of foodbourne botulism in England and Wales, 2006–2010

Solution

. . .

Example 1.16

Devise a generic sequential Bayesian updating plan for successive random samples from a Poisson distribution, assuming a conjugate prior specification.

Solution

...

1.6 Learning objectives

By the end of this chapter, you should be able to:

1. Determine the likelihood function using a random sample from **any** distribution
2. Combine this likelihood function with **any** prior distribution to obtain the posterior distribution
3. Name the posterior distribution if it is a "standard" distribution listed in these notes or on the exam paper – this list may well include distributions that are standard within the subject but which you have not met before. If the posterior is not a "standard" distribution then it is okay just to give its density (or probability function) up to a constant.
4. Do all the above for a particular data set or for a general case with random sample $x_1, \ldots, x_n$

5. Describe the different levels of prior information; determine and use conjugate priors and vague priors
6. Determine the asymptotic posterior distribution
7. Determine the predictive distribution, particularly when having a random sample from any distribution and a conjugate prior via Candidate's formula
8. Describe and calculate the confidence intervals, HDIs and prediction intervals
9. Operate sequential Bayesian updating schemes

Chapter 2

Inference for a Normal population

2.1 Bayes Theorem for many parameters

Data: $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$

Model: depends on many parameters $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)^T$
pdf/pf $f(\boldsymbol{x}|\boldsymbol{\theta}) \rightarrow$ Likelihood function $f(\boldsymbol{x}|\boldsymbol{\theta})$

Prior beliefs: pdf/pf $\pi(\boldsymbol{\theta})$

Combine using Bayes Theorem

Posterior beliefs: pdf/pf $\pi(\boldsymbol{\theta}|\boldsymbol{x})$

Posterior distribution summarises all our current knowledge about the parameter $\boldsymbol{\theta}$

Bayes Theorem

The posterior probability (density) function for $\boldsymbol{\theta}$ is

$$\pi(\boldsymbol{\theta}|\boldsymbol{x}) = \frac{\pi(\boldsymbol{\theta})\, f(\boldsymbol{x}|\boldsymbol{\theta})}{f(\boldsymbol{x})}$$

where

$$f(\boldsymbol{x}) = \begin{cases} \int_{\Theta} \pi(\boldsymbol{\theta})\, f(\boldsymbol{x}|\boldsymbol{\theta})\, d\boldsymbol{\theta} & \text{if } \boldsymbol{\theta} \text{ is continuous,} \\ \\ \sum_{\Theta} \pi(\boldsymbol{\theta})\, f(\boldsymbol{x}|\boldsymbol{\theta}) & \text{if } \boldsymbol{\theta} \text{ is discrete.} \end{cases}$$

As before, this can be rewritten as

$$\pi(\boldsymbol{\theta}|\boldsymbol{x}) \propto \pi(\boldsymbol{\theta}) \times f(\boldsymbol{x}|\boldsymbol{\theta})$$

$$i.e. \quad \text{posterior} \propto \text{prior} \times \text{likelihood}$$

Generalised t distribution: $X \sim t_a(b, c)$

- Density for $x \in \mathbb{R}$

$$f(x|a, b, c) = \frac{\Gamma\left(\frac{a+1}{2}\right)}{\sqrt{ac\pi}\,\Gamma\left(\frac{a}{2}\right)} \left\{1 + \frac{(x-b)^2}{ac}\right\}^{-\frac{a+1}{2}}$$

- Parameters: $a > 0$, $b \in \mathbb{R}$, $c > 0$
- $E(X) = Mode(X) = b$ and $Var(X) = \dfrac{ac}{a-2}$, if $a \geq 2$
- Generalisation of the standard t-distribution since $(X - b)/\sqrt{c} \sim t_a$
- $t_a(0, 1) \equiv t_a$
- $\lim_{a\to\infty} t_a(b, c) = N(b, c)$

Example 2.1

- If $X \sim t_a(b, c)$ then show that $Y = (X - b)/\sqrt{c} \sim t_a$, with density

$$f(y) = \frac{\Gamma\left(\frac{a+1}{2}\right)}{\sqrt{a\pi}\,\Gamma\left(\frac{a}{2}\right)} \left\{1 + \frac{y^2}{a}\right\}^{-\frac{a+1}{2}}, \qquad -\infty < y < \infty,$$

Recall the general result: if X is a random variable with probability density function $f_X(x)$ and g is a bijective (1–1) function then the random variable $Y = g(X)$ has probability density function

$$f_Y(y) = f_X\left\{g^{-1}(y)\right\} \left| \frac{d}{dy} g^{-1}(y) \right|. \tag{2.1}$$

Solution

...

Comments

- `R` functions `pgt` and `dgt` in the package `nclbayes` give values for $F_X(x)$ and $f_X(x)$ when $X \sim t_a(b, c)$
- Relationship between the generalised t distribution and the standard t distribution is similar to that of the normal distribution and the standard normal distribution:

$$X \sim N(b, c) \quad \Longrightarrow \quad \frac{X - b}{\sqrt{c}} \sim N(0, 1)$$

$$X \sim t_a(b, c) \quad \Longrightarrow \quad \frac{X - b}{\sqrt{c}} \sim t_a$$

Inverse Chi distribution: $Y \sim Inv\text{-}Chi(a, b)$

- Density

$$f(y|a, b) = \frac{2b^a y^{-2a-1} e^{-b/y^2}}{\Gamma(a)}, \quad y > 0$$

- Parameters: $a > 0$, $b > 0$
- $E(Y) = \dfrac{\sqrt{b}\,\Gamma(a - 1/2)}{\Gamma(a)}$
- $Var(Y) = \dfrac{b}{a-1} - E(Y)^2$, if $a \geq 1$
- The name of the distribution comes from the fact that $1/Y^2 \sim Ga(a, b) \equiv \chi^2_{2a}/(2b)$

2.2 Prior to posterior analysis

- Data: $X_i|\mu,\tau \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (indep)
- Prior: $\mu|\tau \sim N\left(b, \frac{1}{c\tau}\right)$, $\tau \sim Ga(g, h)$, with joint density, for $\mu \in \mathbb{R}$, $\tau > 0$

$$\begin{aligned}
\pi(\mu,\tau) &= \pi(\mu|\tau)\pi(\tau) \\
&= \left(\frac{c\tau}{2\pi}\right)^{1/2} \exp\left\{-\frac{c\tau}{2}(\mu-b)^2\right\} \times \frac{h^g \tau^{g-1} e^{-h\tau}}{\Gamma(g)} \\
&\propto \tau^{g-\frac{1}{2}} \exp\left\{-\frac{\tau}{2}\left[c(\mu-b)^2 + 2h\right]\right\} \qquad (2.2)
\end{aligned}$$

- We write $\begin{pmatrix}\mu \\ \tau\end{pmatrix} \sim NGa(b, c, g, h)$
- Determine the posterior distribution for $\begin{pmatrix}\mu \\ \tau\end{pmatrix}$

  Hint:

$$c(\mu-b)^2 + n(\bar{x}-\mu)^2 = (c+n)\left\{\mu - \left(\frac{cb+n\bar{x}}{c+n}\right)\right\}^2 + \frac{nc(\bar{x}-b)^2}{c+n}$$

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Solution

$$\cdots \tag{2.3}$$

2.2.1 Marginal distributions

- If $\begin{pmatrix} \mu \\ \tau \end{pmatrix} \sim NGa(b, c, g, h)$ then $\tau \sim Ga(g, h)$
- The (marginal) density for μ is, for $\mu \in \mathbb{R}$

$$
\begin{aligned}
\pi(\mu) &= \int_0^\infty \pi(\mu, \tau)\, d\tau \\
&\propto \int_0^\infty \tau^{g-\frac{1}{2}} \exp\left\{-\frac{\tau}{2}\left[c(\mu-b)^2 + 2h\right]\right\} d\tau \\
&\propto \int_0^\infty \tau^{g+\frac{1}{2}-1} \exp\left\{-\frac{\tau}{2}\left[c(\mu-b)^2 + 2h\right]\right\} d\tau \\
&\propto \frac{\Gamma\left(g+\frac{1}{2}\right)}{[\{c(\mu-b)^2+2h\}/2\}]^{g+\frac{1}{2}} \quad \text{using } \int_0^\infty \theta^{a-1} e^{-b\theta}\, d\theta = \frac{\Gamma(a)}{b^a} \\
&\propto h^{-g-1/2}\left\{1 + \frac{c(\mu-b)^2}{2h}\right\}^{-g-1/2} \\
&\propto \left\{1 + \frac{c(\mu-b)^2}{2h}\right\}^{-\frac{2g+1}{2}} \\
&\text{i.e.} \quad \mu \sim t_{2g}\left(b, \frac{h}{gc}\right)
\end{aligned}
\tag{2.4}
$$

Summary of marginal distributions

- The data: $X_i|\mu,\tau \sim N(\mu, 1/\tau)$
- Priors: $\mu|\tau \sim N(b, 1/c\tau)$, $\tau \sim Ga(g,h)$
- The joint prior $\begin{pmatrix}\mu\\ \tau\end{pmatrix} \sim NGa(b,c,g,h)$ has marginal distributions
  - $\mu \sim t_{2g}\left(b, \frac{h}{gc}\right)$ (Exactly the same proof as for $\mu|\boldsymbol{x}$)
  - $\tau \sim Ga(g,h)$

  Also $\sigma = 1/\sqrt{\tau} \sim Inv\text{-}Chi(g,h)$ (One for you in assignment 3!)
- The posterior $\left.\begin{pmatrix}\mu\\ \tau\end{pmatrix}\right| \boldsymbol{x} \sim NGa(B,C,G,H)$ has marginal distributions
  - $\mu|\boldsymbol{x} \sim t_{2G}\left(B, \frac{H}{GC}\right)$ (Proven in yesterday's lecture)
  - $\tau|\boldsymbol{x} \sim Ga(G,H)$

  Also $\sigma|\boldsymbol{x} \sim Inv\text{-}Chi(G,H)$ (One for you in assignment 3!)

Example 2.2

- The 18th century physicist Henry Cavendish made 23 experimental determinations of the earth's density, and these data (in g/cm^3) are

5.36	5.29	5.58	5.65	5.57	5.53	5.62	5.29
5.44	5.34	5.79	5.10	5.27	5.39	5.42	5.47
5.63	5.34	5.46	5.30	5.78	5.68	5.85	

  with sufficient statistics $n = 23$, $\bar{x} = 5.4848$, $s = 0.1882$
- We consider $X|\mu, \tau \sim N(\mu, 1/\tau)$, with τ unknown
- In Example 1.4 we assumed $X_i|\mu \sim N(\mu, 0.2^2)$ with $\mu \sim N(5.41, 0.4^2)$ and τ known with $\tau = 1/0.2^2 = 25$.
- Must specify the parameters in the $NGa(b, c, g, h)$ prior distribution for $(\mu, \tau)^T$. Suppose we choose $Var(\tau) = 250$.
- Choice of b and c: the NGa prior distribution has $\mu|\tau \sim N\{b, 1/(c\tau)\}$. Matching the prior for $\mu|\tau = 25$ gives $b = 5.41$ and $c = 0.25$

  Choice of g and h: the NGa prior distribution has $\tau \sim Ga(g, h)$. Choose $E(\tau) = 25$, giving $g = 2.5$ and $h = 0.1$

- Summary: take prior

$$\begin{pmatrix} \mu \\ \tau \end{pmatrix} \sim NGa(b = 5.41, c = 0.25, g = 2.5, h = 0.1)$$

- Is the marginal prior distribution for μ close to what we used in Example 1.4? Yes, see plot below

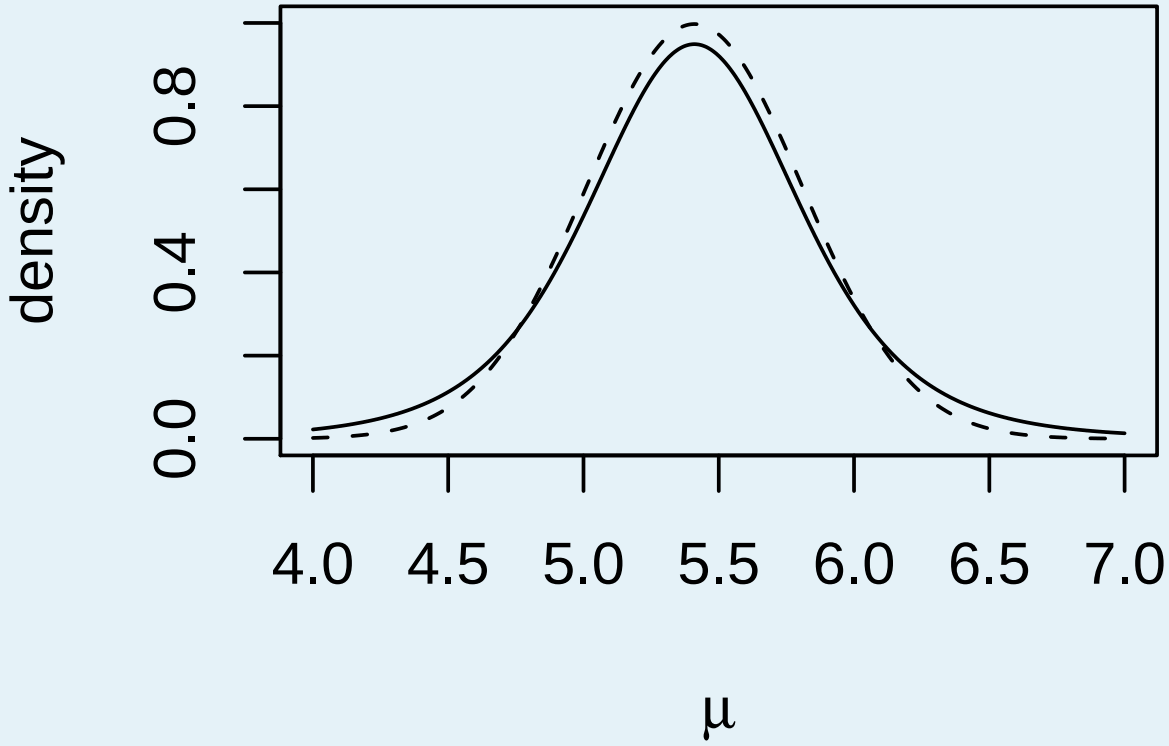


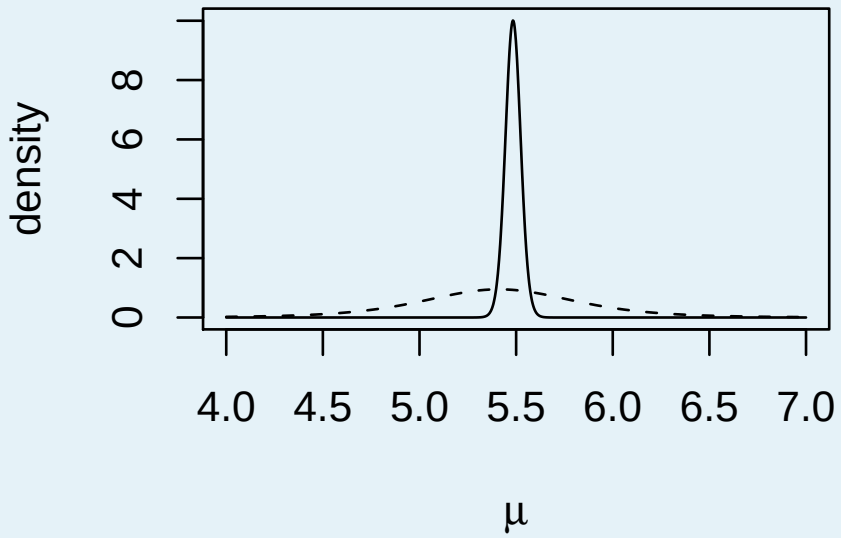
Figure: Marginal prior density for μ: new version (solid) and previous version (dashed)

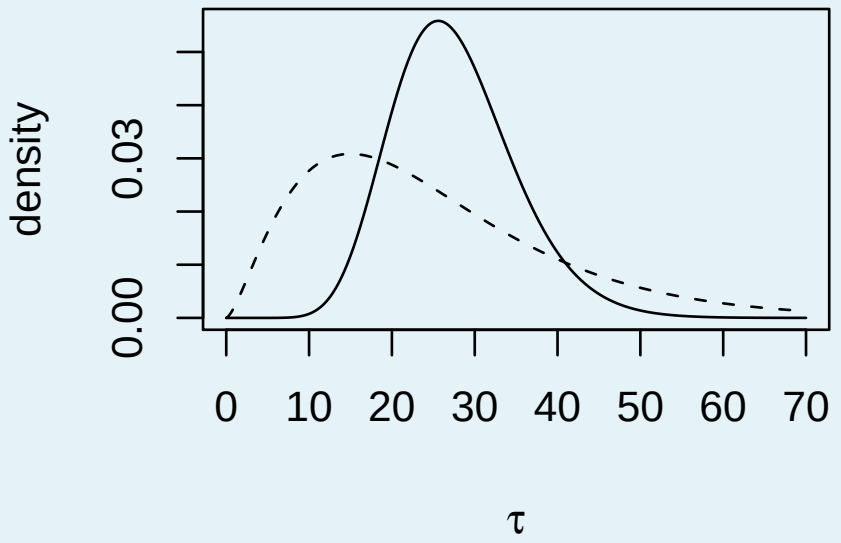
- Determine the posterior distribution for $(\mu, \tau)^T$. Also determine the marginal prior distribution for τ and for σ, and the marginal posterior distribution for each of μ, τ and σ.

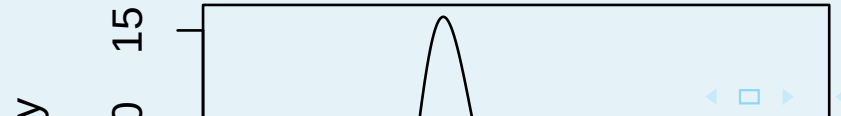
Solution

...

Comparison of prior and posterior marginal distributions







Review of contour plots for bivariate distribution

- Bivariate normal: $\begin{pmatrix} X \\ Y \end{pmatrix} \sim N\left\{\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix}\right\}$, with density $\frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \exp\left\{-\frac{1}{2(1-\rho^2)}\left(\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} - 2\rho\frac{xy}{\sigma_x\sigma_y}\right)\right\}$.

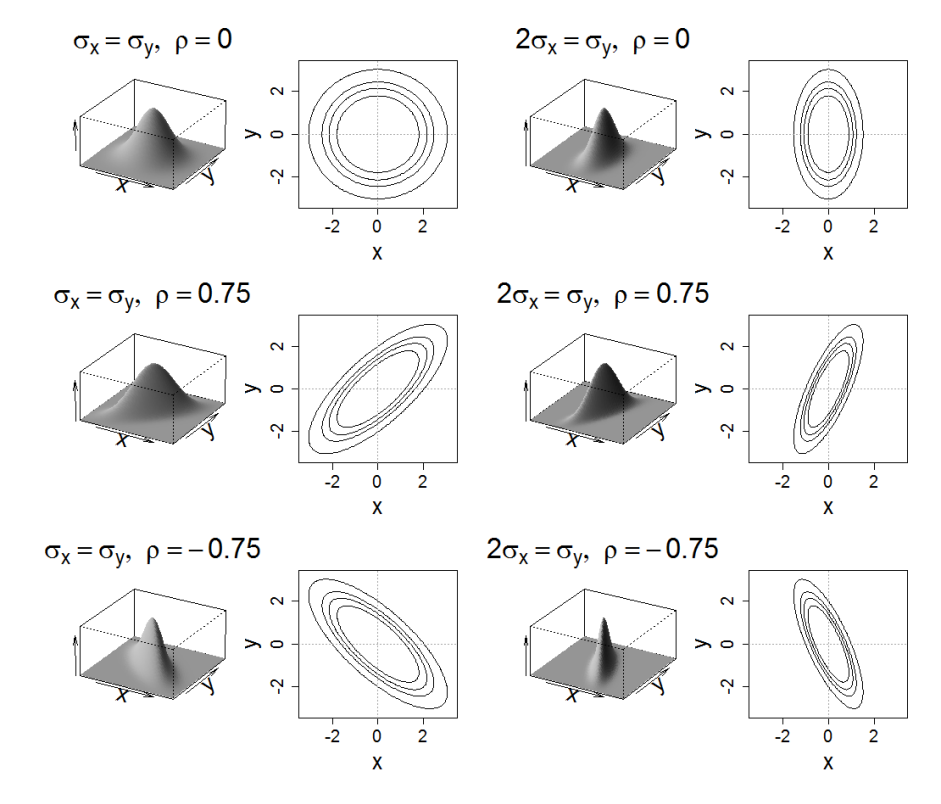


Figure: Contour plots for different bivariate normal densities

Comparison of prior and posterior distributions

- Can plot their contours using R command NGacontour:

```
mu=seq(4.5,6.5,len=1000); tau=seq(0,71,len=1000)
NGacontour(mu,tau,b,c,g,h,lty=3); NGacontour(mu,tau,B,C,G,H,add=TRUE)
```

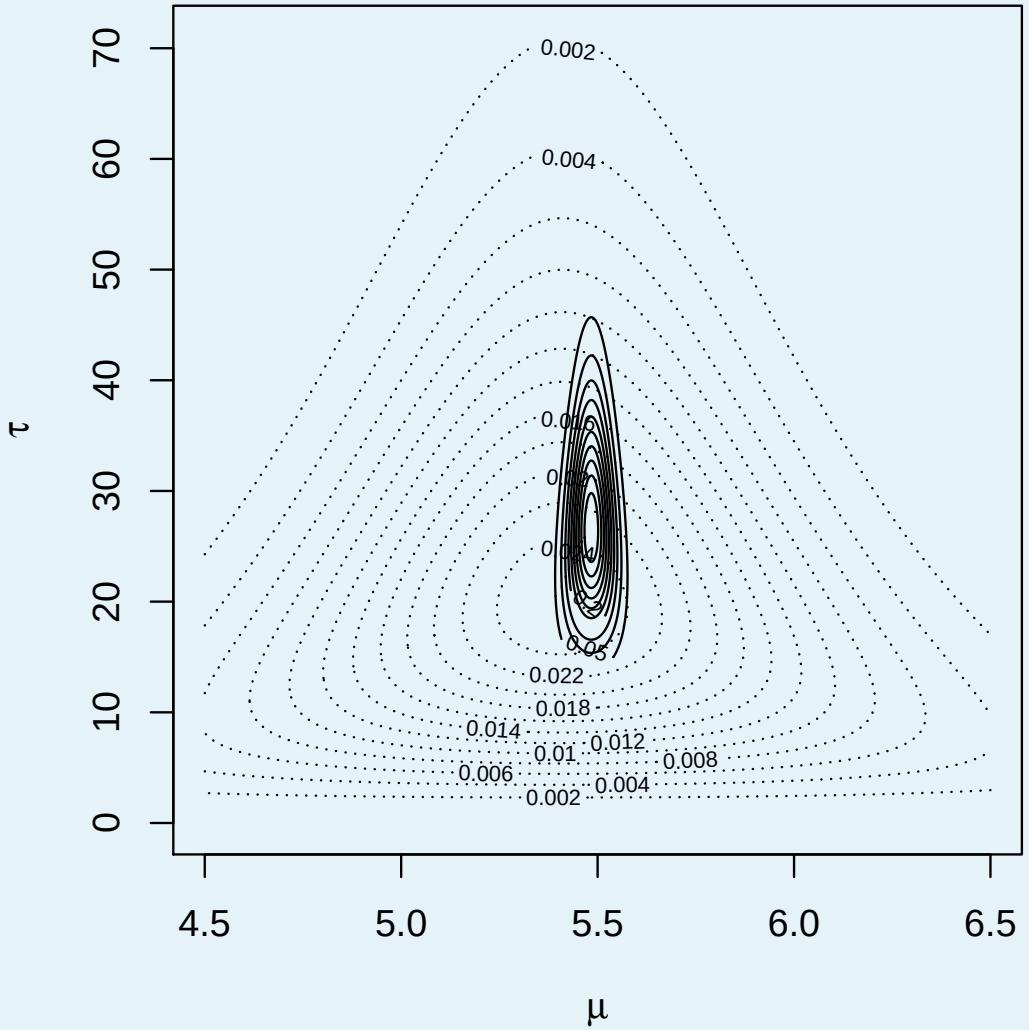


Figure: Contour plot of the prior (dashed) and posterior (solid) densities for $(\mu, \tau)^T$.

Comments

- Wikipedia tells us that the actual mean density of the earth is $5.515\, g/cm^3$
- What is the (posterior) probability that the mean density is within 0.1 of this value?

$$\mu|\boldsymbol{x} \sim t_{28}(5.484, 0.001561) \quad \Rightarrow \quad Pr(5.415 < \mu < 5.615|\boldsymbol{x}) = 0.9529$$

using
`pgt(5.615,28,5.484,0.001561)-pgt(5.415,28,5.484,0.001561)`

- Without the data, the only basis for determining the earth's density is via the prior distribution

$$\mu \sim t_5(5.41, 0.16) \quad \Rightarrow \quad Pr(5.415 < \mu < 5.615) = 0.1802$$

using `pgt(5.615,5,5.41,0.16)-pgt(5.415,5,5.41,0.16)`

- These probability calculations demonstrate that the data have been very informative and changed our beliefs about the earth's density

Comments

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using `pgt(5.615,5,5.41,0.16)-pgt(5.415,5,5.41,0.16)`

- These probability calculations demonstrate that the data have been very informative and changed our beliefs about the earth's density

Example 2.3

Determine the $100(1-\alpha)\%$ highest density interval (HDI) for the population mean μ in terms of quantiles of the standard t-distribution

Solution

...

Calculating 95% posterior confidence intervals using R

- $\mu|\boldsymbol{x} \sim t_{2G}\{B, H/(GC)\}$
  Symmetric distribution $\rightarrow$ HDI and equi-tailed intervals are the same
  `c(qgt(0.025,2*G,B,H/(G*C)),qgt(0.975,2*G,B,H/(G*C)))`

- $\tau|\boldsymbol{x} \sim Ga(G, H)$
  Skewed distribution $\rightarrow$ HDI and equi-tailed intervals are different
  `hdiGamma(0.95,G,H)`
  `c(qgamma(0.025,G,H),qgamma(0.975,G,H))`

- $\sigma|\boldsymbol{x} \sim \textit{Inv-Chi}(G, H)$
  Skewed distribution $\rightarrow$ HDI and equi-tailed intervals are different
  `hdiInvchi(0.95,G,H)`
  `c(qinvchi(0.025,G,H),qinvchi(0.975,G,H))`

Results from this data analysis . . .

	Prior	Posterior	
μ:	$(4.3818, 6.4382)$	$(5.4031, 5.5649)$	
τ:	$(1.4812, 55.9573)$	$(14.0193, 42.2530)$	$\leftarrow$ HDI
	$(4.1561, 64.1625)$	$(15.0674, 43.7625)$	
σ:	$(0.1062, 0.4246)$	$(0.1466, 0.2505)$	$\leftarrow$ HDI
	$(0.1248, 0.4905)$	$(0.1512, 0.2576)$	

- Posterior HDI and equi-tailed intervals for τ are fairly similar but prior intervals are not
- Ditto for σ
- Why?

  The prior distributions are quite skewed but the posterior distributions are fairly symmetric

Results from this data analysis . . .

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μ:	$(4.3818, 6.4382)$	$(5.4031, 5.5649)$	
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- Ditto for σ
- Why?

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Confidence regions

- We have looked at (marginal) HDIs
- Can be useful to also look at (joint) confidence regions

Example 2.4

Determine a joint α confidence region for $(\mu, \tau)^T$ by calculating k satisfying $P(\pi(\mu, \tau) > k) = \alpha$ or $P(\pi(\mu, \tau) > k \mid \boldsymbol{x}) = \alpha$.

Solution

...

- Can plot these regions using `NGacontour` by using the appropriate value for the contour level

```
mu=seq(3.5,7.5,len=1000)
tau=seq(0,80,len=1000)
NGacontour(mu,tau,b,c,g,h,p=c(0.95,0.9,0.8),lty=3)
NGacontour(mu,tau,B,C,G,H,p=c(0.95,0.9,0.8),add=TRUE)
```

Confidence regions for $(\mu, \tau)^T$

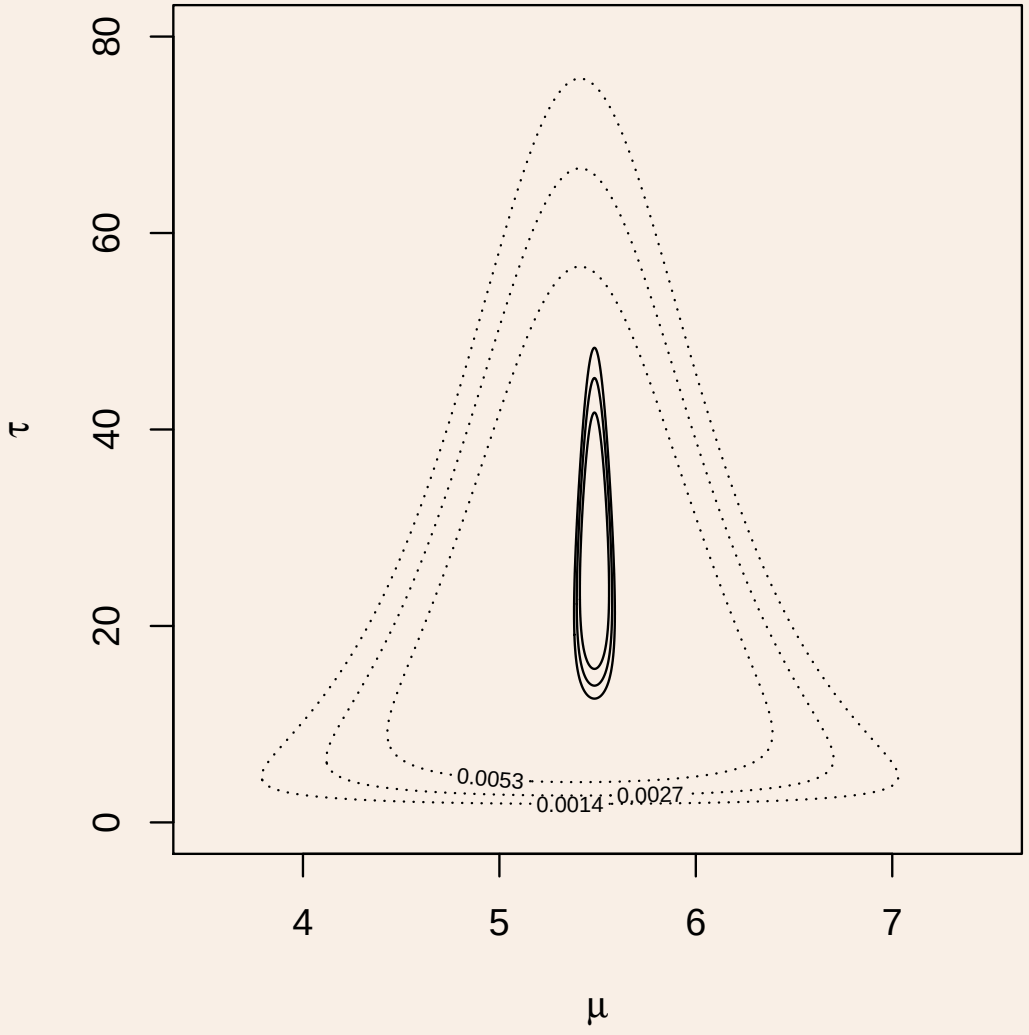

Figure: 95%, 90% and 80% prior (dashed) and posterior (solid) confidence regions for $(\mu, \tau)^T$; 95% (outer), 80% (inner).

Focusing on central part of plot . . .

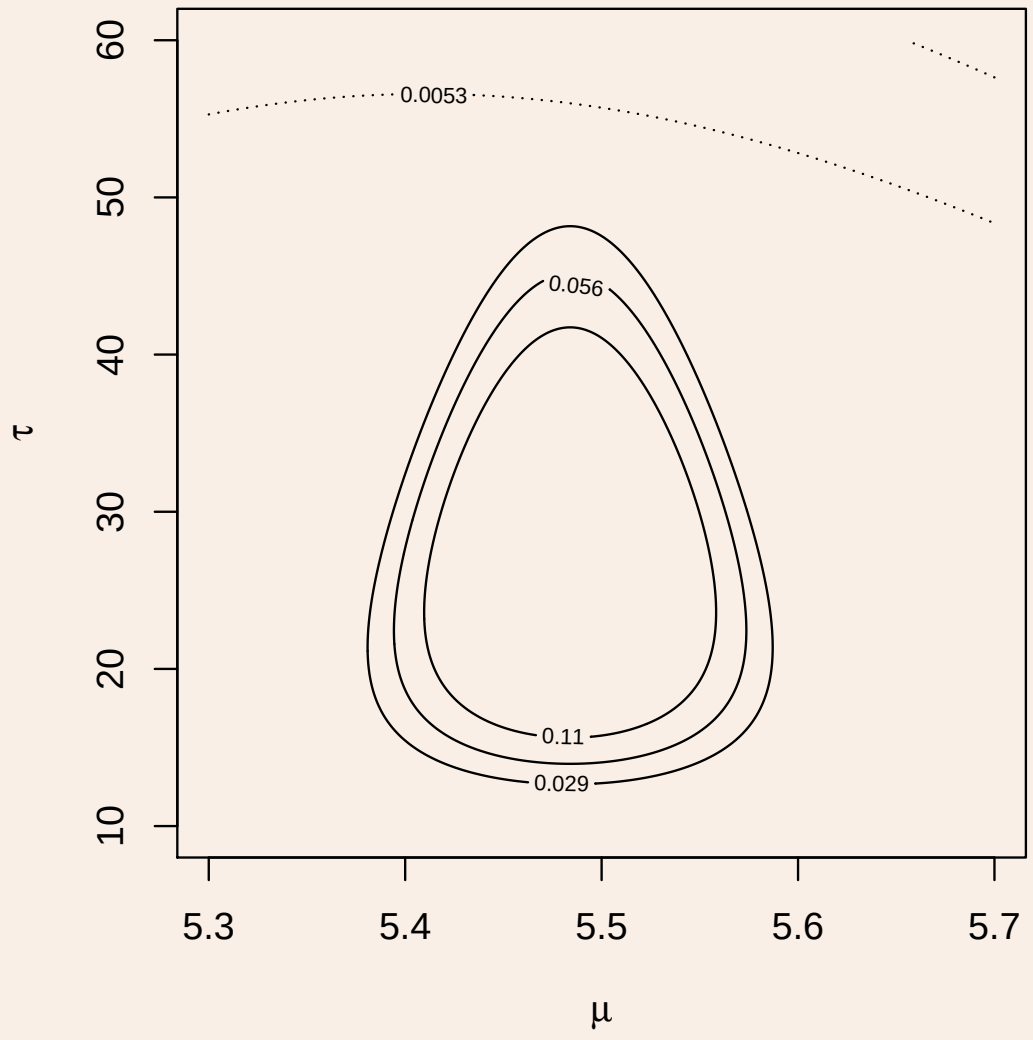

Figure: 95%, 90% and 80% prior (dashed) and posterior (solid) confidence regions for $(\mu, \tau)^T$; 95% (outer), 80% (inner).

2.4 Predictive distributions

- In this model we can determine the predictive distribution via

$$f(y|\boldsymbol{x}) = \int f(y|\mu,\tau)\,\pi(\mu,\tau|\boldsymbol{x})\,d\mu\,d\tau$$

  or by using Candidate's formula (as this is a conjugate analysis)
- But, for this model, there is a more straightforward way

. . .

- These predictive intervals can be calculated easily using the R function qgt
- In Example 2.2, the prior and posterior predictive HDIs for a new value Y from the population are $(4.2604, 6.5596)$ and $(5.0855, 5.8825)$ respectively, calculated using

```
c(qgt(0.025,2*g,b,h*(c+1)/(g*c)),qgt(0.975,2*g,b,h*(c+1)/(g*c)))
c(qgt(0.025,2*G,B,H*(C+1)/(G*C)),qgt(0.975,2*G,B,H*(C+1)/(G*C)))
```

2.4 Predictive distributions

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c(qgt(0.025,2*g,b,h*(c+1)/(g*c)),qgt(0.975,2*g,b,h*(c+1)/(g*c)))
c(qgt(0.025,2*G,B,H*(C+1)/(G*C)),qgt(0.975,2*G,B,H*(C+1)/(G*C)))
```

2.5 Summary

Suppose we have a normal random sample with $X_i|\mu,\tau \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (independent)

(i) $(\mu,\tau)^T \sim NGa(b, c, g, h)$ is a conjugate prior distribution

(ii) The posterior distribution is $(\mu,\tau)^T|\boldsymbol{x} \sim NGa(B, C, G, H)$ where the posterior parameters are given in the proof in Section 2.2.

(iii) The marginal prior distributions are $\mu \sim t_{2g}\{b, h/(gc)\}$, $\tau \sim Ga(g, h)$, $\sigma = 1/\sqrt{\tau} \sim \textit{Inv-Chi}(g, h)$

(iv) The marginal posterior distributions are $\mu|\boldsymbol{x} \sim t_{2G}\{B, H/(GC)\}$, $\tau|\boldsymbol{x} \sim Ga(G, H)$, $\sigma|\boldsymbol{x} \sim \textit{Inv-Chi}(G, H)$

(v) Prior and posterior means and standard deviations for μ, τ and σ can be calculated from the properties of the t, *Gamma* and *Inv-Chi* distributions

(vi) Prior and posterior probabilities and densities for μ, τ and σ can be calculated using the `R` functions `pgt, dgt, pgamma, dgamma, pinvchi, dinvchi`

Suppose we have a normal random sample with $X_i|\mu,\tau \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (independent)

(vii) HDIs or equi-tailed CIs for μ, τ and σ can be calculated using `qgt`, `hdiGamma`, `hdiInvchi`, `qgamma`, `qinvchi`

(viii) Contour plots of the prior and posterior densities for $(\mu, \tau)^T$ can be plotted using the `NGacontour` function

(ix) Prior and posterior confidence regions for $(\mu, \tau)^T$ can be plotted using the `NGacontour` function

(x) The predictive distribution for a new observation Y from the population is $Y|\boldsymbol{x} \sim t_{2G}\{B, H(C+1)/(GC)\}$ and its HDI can be calculated using the `qgt` function

2.6 Why do we have so many different distributions?

- So far we have used many distributions, some you will have met before and some will be new
- After a while the variety and sheer number of different distributions can become overwhelming
- Why do we need so many distributions and why do we name so many of them?

Justification

- Statistics studies the random variation in experiments, samples and processes
- The variety of applications leads to their randomness being described by many different distributions
- In many applications, bespoke distributions need to be formulated
- However, some distributions come up time and time again for modelling random variation in data and for describing prior beliefs

Justification (continued)

- It is helpful for us to be able to refer to these distributions – and so we give each one a name – and be able to quote known results for these distributions such as their mean and variance
- For example, in this chapter you have been introduced to
  - a generalisation of the t-distribution
  - the inverse chi distribution
  - The Normal-Gamma distribution
- We have been able to use results for their mean and variance to study prior and posterior distributions and have been able to plot these distributions using functions in the `R` package
- You will meet several other new distributions in the remainder of the module

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Justification (continued)

- Obviously it's useful to have a working knowledge of each of these distributions but not vital to remember all their properties
- The exam paper will contain a list of all the distributions used in the exam, together with their density (or probability function) and any useful proprieties such as their mean and variance (as needed for the exam)

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- The exam paper will contain a list of all the distributions used in the exam, together with their density (or probability function) and any useful proprieties such as their mean and variance (as needed for the exam)

2.7 Learning objectives

By the end of this chapter, you should be able to:

1. Determine the posterior distribution for $(\mu, \tau)^T$
2. Determine and use the univariate prior and posterior distributions
3. Determine confidence intervals, HDIs and confidence regions
4. Determine the predictive distribution of another value from the population, and its predictive interval
5. Determine the predictive distribution of the mean of another random sample from the population

both in general and for a particular prior and data set.

Also you should be able to:

6. Appreciate the benefit of naming distributions and for having lists of properties for these distributions

Chapter 3

General results for multi-parameter problems

3.1 Different levels of prior knowledge

- Substantial prior information: $\pi(\boldsymbol{\theta}|\boldsymbol{x}) \sim \pi(\boldsymbol{\theta})$
- Limited prior knowledge: use conjugate prior where possible and determine its parameter(s) by prior knowledge
- Vague prior information: use conjugate prior where possible and make them diffuse
- Prior ignorant – use 'flat' prior? Problem?
  1. Have $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)^T$ and we are prior ignorant
  2. Use $\pi(\boldsymbol{\theta}) = constant$?
  3. Let $\phi_i = g_i(\theta), i = 1, \ldots, p$ and $\boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_p)^T$
  4. Prior density for $\boldsymbol{\phi}$ is not constant!
  5. But if we are ignorant about $\boldsymbol{\theta}$ we must be ignorant about $\boldsymbol{\phi}$...

Example 3.1

Suppose $0 < \theta_1 < 1$ and $0 < \theta_2 < 1$. If we are ignorant about $\boldsymbol{\theta} = (\theta_1, \theta_2)^T$ then show that $\theta_1\theta_2$ does not have constant prior density.

Solution

...

Example 3.2

Suppose we have a random sample from a $N(\mu, 1/\tau)$ distribution (with τ unknown). Determine the Jeffreys prior for this model.

Hint: We have already seen that the likelihood function can be written as

$$f(\boldsymbol{x}|\mu,\tau) = \left(\frac{\tau}{2\pi}\right)^{n/2} \exp\left[-\frac{n\tau}{2}\left\{s^2 + (\bar{x}-\mu)^2\right\}\right]$$

where

$$s^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

Solution

...

3.2 Asymptotic posterior distribution

$p = 1$ case : $\sqrt{J(\hat{\theta})}\,(\theta - \hat{\theta})\Big|\,\boldsymbol{x} \xrightarrow{\mathcal{D}} N(0,1)$ as $n \to \infty$

Suppose we have a statistical model $f(\boldsymbol{x}|\boldsymbol{\theta})$ for data $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$, where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)^T$, together with a prior distribution $\pi(\boldsymbol{\theta})$ for $\boldsymbol{\theta}$. Then

$$J(\hat{\boldsymbol{\theta}})^{1/2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})|\boldsymbol{x} \xrightarrow{\mathcal{D}} N_p(\underline{0}, \mathrm{I}_p) \qquad \text{as } n \to \infty,$$

where $\hat{\boldsymbol{\theta}}$ is the likelihood mode, I_p is the $p \times p$ identity matrix and $J(\boldsymbol{\theta})$ is the observed information matrix, with $(i,j)^{th}$ element

$$J_{ij} = -\frac{\partial^2}{\partial\theta_i \partial\theta_j} \log f(\boldsymbol{x}|\boldsymbol{\theta}),$$

Comments

When n is large, $\boldsymbol{\theta} \mid \boldsymbol{x} \sim N_p(\hat{\boldsymbol{\theta}}, J(\hat{\boldsymbol{\theta}})^{-1})$ approximately. . . .

Example 3.3

Suppose we now have a random sample from a $N(\mu, 1/\tau)$ distribution (with τ unknown). Determine the asymptotic posterior distribution for (μ, τ).

Hint: we have already seen that the likelihood function can be written as

$$f(\boldsymbol{x}|\mu, \tau) = \left(\frac{\tau}{2\pi}\right)^{n/2} \exp\left[-\frac{n\tau}{2}\left\{s^2 + (\bar{x} - \mu)^2\right\}\right]$$

where $s^2 = \sum_{i=1}^{n}(x_i - \bar{x})^2/n$

Solution

...

3.3 Learning objectives

By the end of this chapter, you should be able to:

1. describe the different levels of prior information; determine and use vague priors
2. determine the asymptotic posterior distribution when the data are a random sample from **any** distribution
3. explain the similarities and differences between the asymptotic posterior distribution and the asymptotic distribution of the maximum likelihood estimator

Chapter 4

Non-conjugate multi-parameter problems

Consequences of strike action for MAS3902

- Probably won't get all of Chapter 4 covered :-(
- Will get enough done to make sure you're OK for the exam
- No time to start revision early – will have three revision classes in teaching week 11 (w/b 8th May)
- Assignment 4: Due **4pm, Friday 5th May**
- Specimen paper already on Canvas: Solutions posted soon

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Chapter 4. Non-conjugate multi-parameter problems

- Here we will study some multi-parameter problems in which the prior distribution does not have to be conjugate
- Inferences are made by using techniques which simulate realisations from the posterior distribution
- These methods are generally referred to as Markov Chain Monte Carlo techniques, and often abbreviated to MCMC
- Two main MCMC techniques:
  1. the Gibbs sampler – at the forefront of the recent MCMC revolution
  2. Metropolis-Hastings sampling
- MCMC schemes based on the combination of these two fundamental techniques are still at the forefront of MCMC research

4.1 Why is inference not straightforward in non-conjugate problems?

Example 4.1

- Consider again the problem in section 2.2

  $X_i|\mu, \tau \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (independent)
- Here we showed that a NGa prior for $(\mu, \tau)^T$ was conjugate
- But what if a $NGa(b, c, g, h)$ prior distribution does not adequately represent our prior beliefs?
- Suppose instead that our prior beliefs are represented by independent priors for the parameters

$$\mu \sim N\left(b, \frac{1}{c}\right) \qquad \text{and} \qquad \tau \sim Ga(g, h)$$

What is the posterior distribution for $(\mu, \tau)^T$?

Solution

...

In this case . . .

- What is the posterior mean of μ and of τ?
- What are their marginal distributions?
- How can we calculate the moments $E(\mu^{m_1}\tau^{m_2}|\boldsymbol{x})$ of this posterior distribution?

Marginal posterior density for μ

$$\pi(\mu|\boldsymbol{x}) = \int_0^\infty \pi(\mu,\tau|\boldsymbol{x})\,d\tau$$

$$= \frac{\displaystyle\int_0^\infty \tau^{g+\frac{n}{2}-1}\exp\left\{-\frac{c}{2}(\mu-b)^2 - h\tau - \frac{n\tau}{2}\left[s^2+(\bar{x}-\mu)^2\right]\right\}d\tau}{\displaystyle\int_{-\infty}^\infty\int_0^\infty \tau^{g+\frac{n}{2}-1}\exp\left\{-\frac{c}{2}(\mu-b)^2 - h\tau - \frac{n\tau}{2}\left[s^2+(\bar{x}-\mu)^2\right]\right\}d\tau\,d\mu}$$

In this case ...

- What is the posterior mean of μ and of τ?
- What are their marginal distributions?
- How can we calculate the moments $E(\mu^{m_1}\tau^{m_2}|\boldsymbol{x})$ of this posterior distribution?

Marginal posterior density for μ

$$\pi(\mu|\boldsymbol{x}) = \int_0^\infty \pi(\mu,\tau|\boldsymbol{x})\,d\tau$$

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Marginal posterior density for τ

$$\pi(\tau|\boldsymbol{x}) = \int_{-\infty}^{\infty} \pi(\mu, \tau|\boldsymbol{x})\, d\mu$$

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General moments

$$E(\mu^{m_1}\tau^{m_2}|\boldsymbol{x})$$

$$= \int_{-\infty}^{\infty}\int_{0}^{\infty} \mu^{m_1}\tau^{m_2}\pi(\mu, \tau|\boldsymbol{x})\, d\tau\, d\mu$$

$$= \frac{\displaystyle\int_{-\infty}^{\infty}\int_{0}^{\infty} \mu^{m_1}\tau^{m_2} \times \tau^{g+\frac{n}{2}-1} \exp\left\{-\frac{c}{2}(\mu-b)^2 - h\tau - \frac{n\tau}{2}\left[s^2 + (\bar{x}-\mu)^2\right]\right\} d\tau\, d\mu}{\displaystyle\int_{-\infty}^{\infty}\int_{0}^{\infty} \tau^{g+\frac{n}{2}-1} \exp\left\{-\frac{c}{2}(\mu-b)^2 - h\tau - \frac{n\tau}{2}\left[s^2 + (\bar{x}-\mu)^2\right]\right\} d\tau\, d\mu}$$

Marginal posterior density for τ

$$\pi(\tau|\boldsymbol{x}) = \int_{-\infty}^{\infty} \pi(\mu, \tau|\boldsymbol{x})\, d\mu$$

$$= \frac{\displaystyle\int_{-\infty}^{\infty} \tau^{g+\frac{n}{2}-1} \exp\left\{-\frac{c}{2}(\mu-b)^2 - h\tau - \frac{n\tau}{2}\left[s^2 + (\bar{x}-\mu)^2\right]\right\} d\mu}{\displaystyle\int_{-\infty}^{\infty}\int_{0}^{\infty} \tau^{g+\frac{n}{2}-1} \exp\left\{-\frac{c}{2}(\mu-b)^2 - h\tau - \frac{n\tau}{2}\left[s^2 + (\bar{x}-\mu)^2\right]\right\} d\tau\, d\mu}$$

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Comments

- These integrals cannot be determined analytically
- It is possible to use numerical integration methods or approximations (for large n)
- However, in general, the accuracy of the numerical approximation to the integral deteriorates as the dimension of the integral increases
- How do we analyse models with a large number of parameters?

Comment

- Not using a conjugate prior distribution can cause many basic problems such as difficulty in plotting the marginal posterior density or determining posterior moments
- But having to use conjugate priors is far too restrictive for many real data analyses:
  - (i) our prior beliefs may not be captured using a conjugate prior
  - (ii) most models for complex data do not have conjugate priors
- Until relatively recently, practical Bayesian inference for real complex problems was either not feasible or only undertaken by the dedicated few prepared to develop bespoke computer code to numerically evaluate all the integrals etc.

Examples

- Poisson distribution for our data, $X_i|\lambda \sim Po(\lambda)$:

$$\lambda \sim Ga(g,h) \quad \longrightarrow \quad \lambda|\boldsymbol{x} \sim Ga(g+n\bar{x}, h+n)$$

$$\lambda \sim Weibull(a,b) \quad \longrightarrow \quad \lambda|\boldsymbol{x} \sim \mathbf{??}$$

- Normal distribution for our data, $X_i|\mu,\tau \sim N(\mu, 1/\tau)$:

$$\mu|\tau \sim N\left(b, \frac{1}{c\tau}\right), \tau \sim Ga(g,h)$$

$$\longrightarrow (\mu,\tau)^T \sim NGa(b,c,g,h) \quad \longrightarrow \quad (\mu,\tau)^T|\boldsymbol{x} \sim NGa(B,C,G,H)$$

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All hell breaks loose.

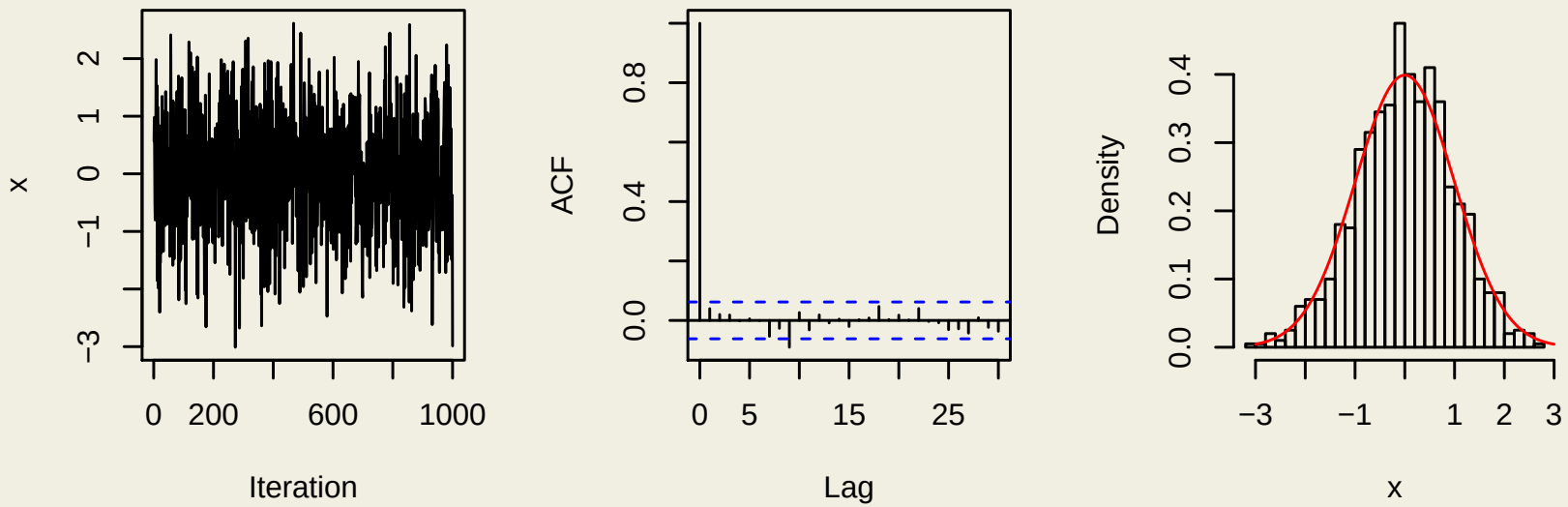
4.2 Simulation-based inference

- Can get around the problem of having to work out integrals
- Base inferences on simulated realisations from the posterior distribution
- This is the fundamental idea behind **Markov Chain Monte Carlo** (MCMC) methods
- If we could simulate from the posterior distribution then we could use a very large sample of realisations to determine posterior means, standard deviations, correlations, joint densities, marginal densities etc.

Black box simulator demo in R

(Ignore the upcoming slides if you'd rather try out the R code!)

- Imagine you wanted to know about the standard normal distribution – its shape, its mean, its standard deviation
- But didn't know any mathematics so that you couldn't derive say the distribution's zero mean and unit variance
- However you've been given a "black box" which can simulate realisations from this distribution
- Here we'll use the `R` function `rnorm()` as the black box simulator
- If you decide to generate 1K realisations the output might look something like



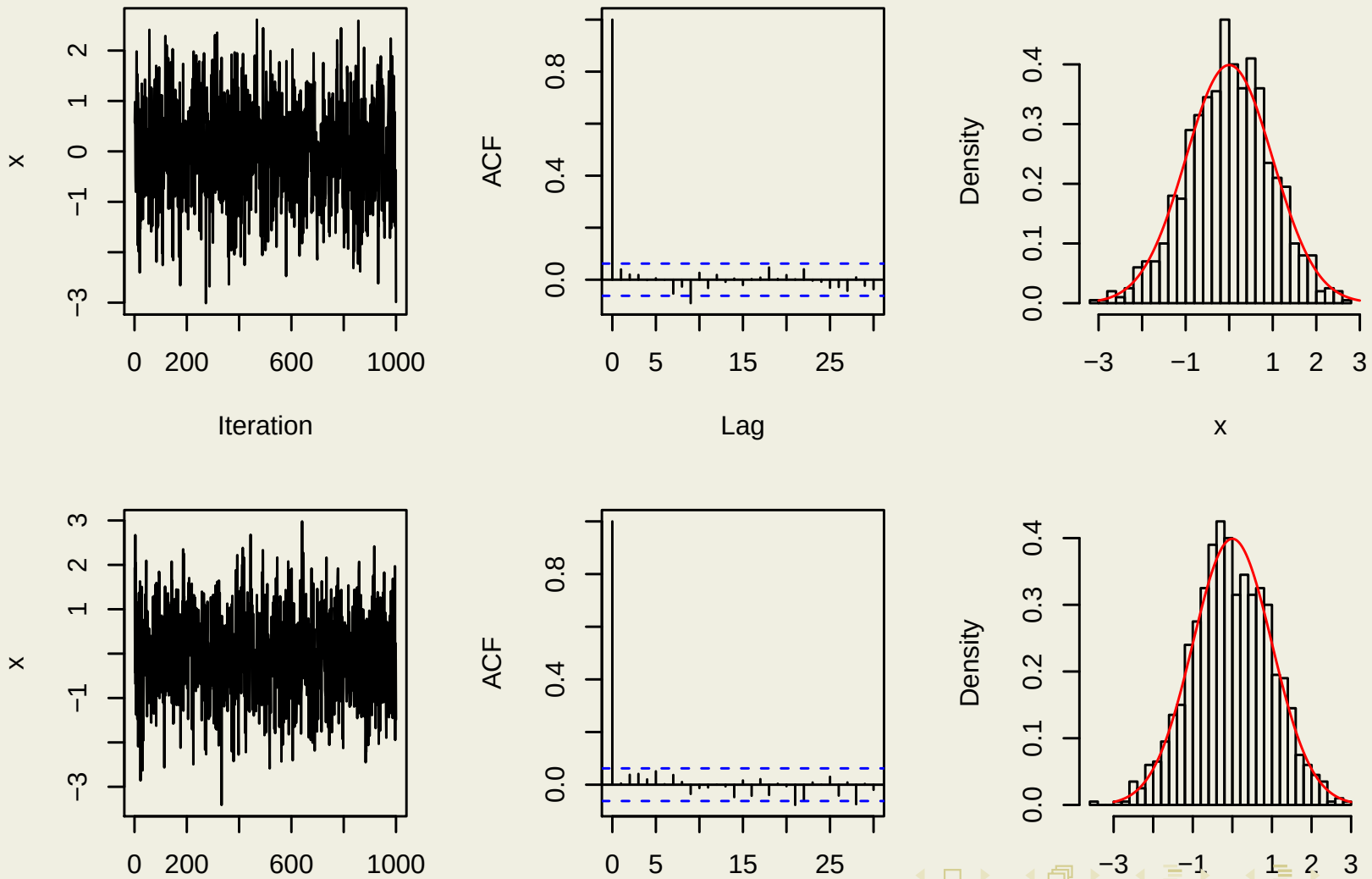
In these plots

Left: the trace plot of the output – the realisations from the black box sampler in the order they are produced

Mid: the autocorrelation (ACF) plot – shows the correlation between $\{x_1, \ldots, x_{N-k}\}$ and $\{x_{k+1}, \ldots, x_N\}$ for $k \geq 0$. Call k as the lag. It shows how correlated the realisations are at different lags. The lag 0 autocorrelation $corr(x_i, x_i)$ must be one (by definition). Here the (sample) correlation between say consecutive values $corr(x_i, x_{i+1})$ will be almost zero, which shows that the simulator `rnorm()` produces independent realisations. This is also the case for correlations at all positive lags. This sample ACF plot tells that the simulator generates independent sample.

Right: the density histogram of the realisations. This tells that what the standard normal distribution is like.

- If you simulate another 1K realisations then the output you get will be a different set of realisations but from the same distribution
- Both sets of realisations might look like



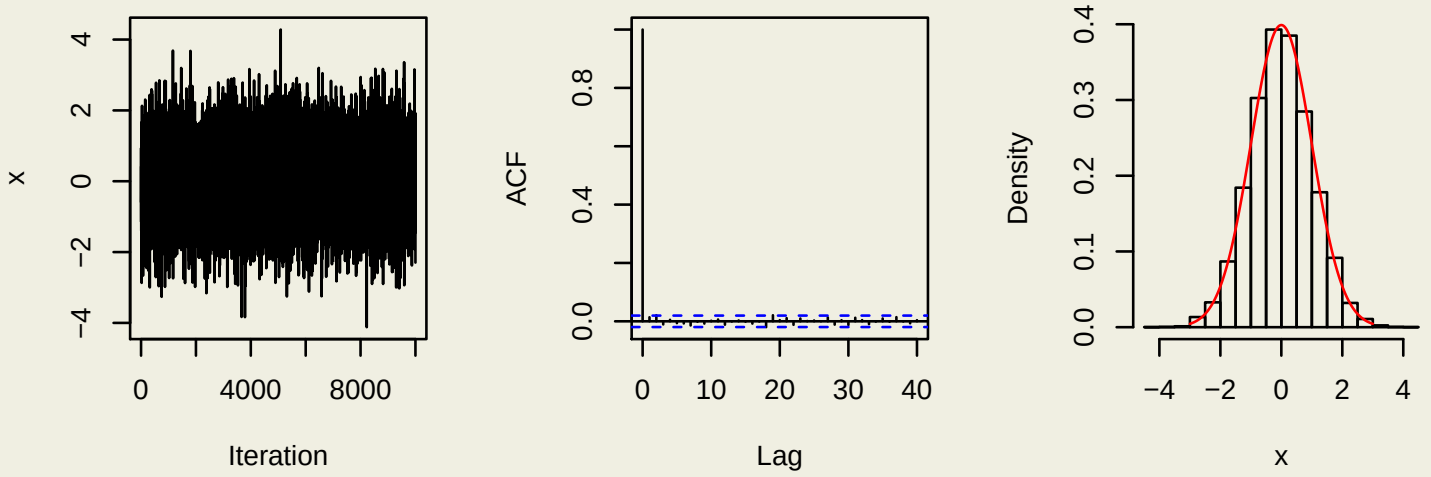
- We can also estimate various quantities of the standard normal distribution from these simulated datasets of 1K realisations

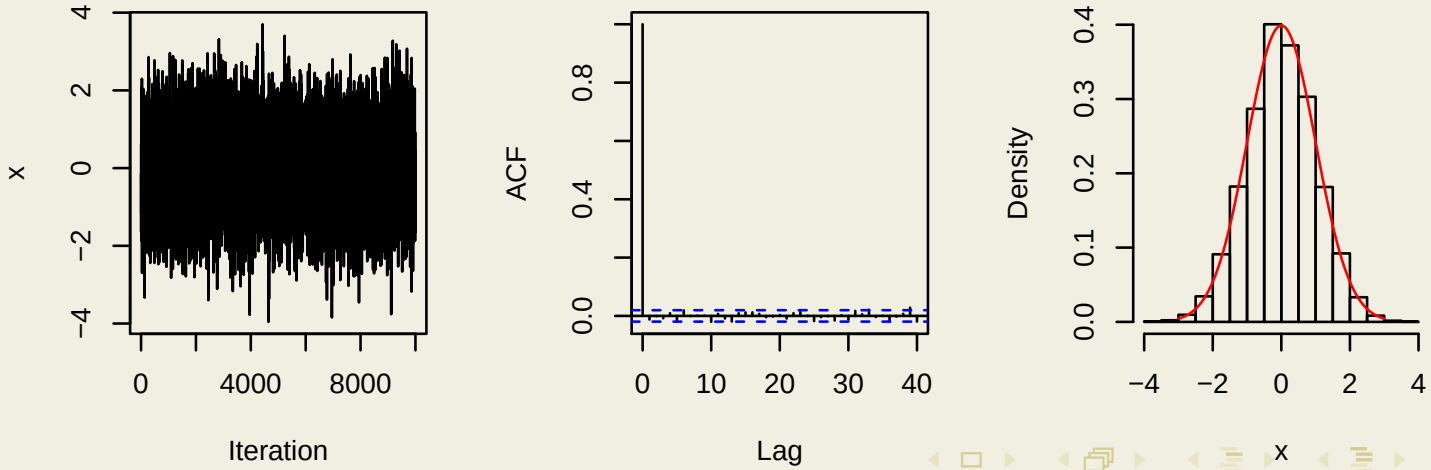
	1st Qu.	Median	Mean	3rd Qu.	St.Dev.
Dataset 1	-0.65240	-0.00130	-0.00192	0.64810	0.96049
Dataset 2	-0.69880	-0.09637	-0.03274	0.67330	0.99599

- The numerical summaries are slightly different but essentially tell the same story
- In each Dataset, the mean and median are around zero and the standard deviation is around one.
- We know from previous modules that there is sample variability in estimates of means from random samples

- Now look at two datasets with 10K simulated realisations:

	1st Qu.	Median	Mean	3rd Qu.	St.Dev.
Dataset 3	-0.66820	-0.00048	0.00370	0.68070	0.99593
Dataset 4	-0.67130	0.01354	0.01008	0.67920	1.00691





- Now estimates have much less sampling variability due to the larger sample size
- In fact we can estimate any "population" quantity to any required accuracy simply by simulating a large enough collection of realisations

- These analyses show how we can make inferences, calculate means, variances, densities etc by using realisations from a distribution. In the rest of this chapter, we will look into how we can construct algorithms for simulating from (complex) posterior distributions, from which we can then make inferences

4.3 Motivation for MCMC methods

- We consider a generic case where we want to simulate realisations of two random variables X and Y with joint density $f(x, y)$
- This joint density can be factorised as

$$f(x, y) = f(x)\, f(y|x)$$

  and so we can simulate from $f(x, y)$ by first simulating $X = x$ from $f(x)$, and then simulating $Y = y$ from $f(y|x)$
- On the other hand, we can write

$$f(x, y) = f(y)\, f(x|y)$$

  and so simulate $Y = y$ from $f(y)$ and then $X = x$ from $f(x|y)$
- Assume that simulating from $f(y|x)$ and $f(x|y)$ is straightforward

Example from MAS2906

Suppose $X \sim U(0.1, 0.5)$ and

$$f_{Y|X}(Y|X = x) = \begin{cases} xe^{-xy}, & \text{when } y \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Write an R function to generate a $2 \times n$ matrix of samples from this distribution, and produce a scatter plot.
Note that

$$Y|X = x \sim Exp(x).$$

```
example.sim = function(n) {
    output = matrix(0, 2, n)
    x = runif(n, 0.1, 0.5)
    y = rexp(n, rate = x)
    output[1, ] = x
    output[2, ] = y
    output
}
```

Another example from MAS2906

Suppose $(X, Y)^T \sim N_2(\boldsymbol{\mu}, \Sigma)$;

- $\boldsymbol{\mu} = (\mu_x, \mu_y)^T$
- $\Sigma = \begin{pmatrix} \sigma_x^2 & \sigma_{xy}^2 \\ \sigma_{xy}^2 & \sigma_y^2 \end{pmatrix}$

What does the theory tell us about X, Y, $X|Y$ and $Y|X$?

1. $X \sim N(\mu_x, \sigma_x^2)$, $Y \sim N(\mu_y, \sigma_y^2)$
2. $X|Y = y \sim N\left(\mu_x + \rho\frac{\sigma_x}{\sigma_y}(y - \mu_y), \sigma_x^2(1 - \rho^2)\right)$ (same for $Y|X = x$)

Recall that the correlation, ρ, is

$$\rho = \frac{\sigma_{xy}^2}{\sigma_x \sigma_y} \longrightarrow \sigma_{xy}^2 = \rho\sigma_x\sigma_y.$$

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Another example from MAS2906

- Suppose we want to investigate the marginal distributions of X and Y
- Suppose further that we did not know much theory about the bivariate Normal; we simply knew the results in (2) telling us about the conditional distributions
- Could use a **Gibbs sampler**, in place of statistical theory, to investigate the marginals for X and Y!
- Example:

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N_2\left(\begin{bmatrix} 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}\right).$$

- We see that $\mu_x = 2, \mu_y = 3; \sigma_x = 1, \sigma_y = 1, \sigma_{xy}^2 = 0.5 \rightarrow \rho = 0.5$
- From result 2, we can write down that

$$\begin{aligned} X|Y = y &\sim N(2 + 0.5(y - 3), 0.75) \quad \text{and} \\ Y|X = x &\sim N(3 + 0.5(x - 2), 0.75). \end{aligned}$$

- What about the marginals for X and Y?

Recall that we know from the theory that $X \sim N(2, 1)$ and $Y \sim N(3, 1)$.

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$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N_2\left(\begin{bmatrix} 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}\right).$$

- We see that $\mu_x = 2, \mu_y = 3; \sigma_x = 1, \sigma_y = 1, \sigma_{xy}^2 = 0.5 \rightarrow \rho = 0.5$
- From result 2, we can write down that

$$\begin{aligned} X|Y = y &\sim N(2 + 0.5(y-3), 0.75) \quad \text{and} \\ Y|X = x &\sim N(3 + 0.5(x-2), 0.75). \end{aligned}$$

- What about the marginals for X and Y?

Recall that we know from the theory that $X \sim N(2, 1)$ and $Y \sim N(3, 1)$.

Another example from MAS2906

- Suppose we want to investigate the marginal distributions of X and Y
- Suppose further that we did not know much theory about the bivariate Normal; we simply knew the results in (2) telling us about the conditional distributions
- Could use a **Gibbs sampler**, in place of statistical theory, to investigate the marginals for X and Y!
- Example:

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N_2\left(\begin{bmatrix} 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}\right).$$

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- What about the marginals for X and Y?

Recall that we know from the theory that $X \sim N(2,1)$ and $Y \sim N(3,1)$.

Another example from MAS2906

Bivariate Normal demo in R

- The key problem: in general, we can't simulate from the marginal distribution, $f(x)$ and $f(y)$
- Suppose we have a single simulated sample point from the marginal distribution for X, that is, we have an $X = x$ from $f(x)$. We can now simulate a $Y = y$ from $f(y|x)$ to give a pair (x, y) from the bivariate density $f(x, y)$.
- Given that this pair is from the bivariate density, the y value must be from the marginal $f(y)$, and so we can simulate an $X = x'$ from $f(x|y)$ to give a new pair (x', y) also from the joint density $f(x, y)$.
- But now x' is from the marginal $f(x)$, and so we can simulate a $Y = y'$ from $f(y|X = x')$ to give a new pair (x', y') also from the joint density $f(x, y)$.
- And we can keep going.
- This alternate sampling from conditional distributions defines a bivariate Markov chain, and it can be shown that $f(x, y)$ is its stationary distribution.

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- But now x' is from the marginal $f(x)$, and so we can simulate a $Y = y'$ from $f(y|X = x')$ to give a new pair (x', y') also from the joint density $f(x, y)$.
- And we can keep going.
- This alternate sampling from conditional distributions defines a bivariate Markov chain, and it can be shown that $f(x, y)$ is its stationary distribution.

4.4 The Gibbs sampler

- Suppose we want to generate realisations from the posterior density $\pi(\boldsymbol{\theta}|\boldsymbol{x})$, where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)^T$, and that we can simulate from the full conditional distributions (FCDs)

$$\pi(\theta_i|\theta_1, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_p, \boldsymbol{x}) = \pi(\theta_i|\cdot), \qquad i = 1, 2, \ldots, p$$

- The Gibbs sampler follows the following algorithm:
  1. Initialise the iteration counter to $j = 1$.
     Initialise the state of the chain to $\boldsymbol{\theta}^{(0)} = (\theta_1^{(0)}, \ldots, \theta_p^{(0)})^T$.
  2. Obtain a new value $\boldsymbol{\theta}^{(j)}$ from $\boldsymbol{\theta}^{(j-1)}$ by successive generation of values

$$\begin{aligned}
\theta_1^{(j)} &\sim \pi(\theta_1|\theta_2^{(j-1)}, \theta_3^{(j-1)}, \ldots, \theta_p^{(j-1)}, \boldsymbol{x}) \\
\theta_2^{(j)} &\sim \pi(\theta_2|\theta_1^{(j)}, \theta_3^{(j-1)}, \ldots, \theta_p^{(j-1)}, \boldsymbol{x}) \\
\vdots \qquad & \qquad \vdots \qquad\qquad \vdots \\
\theta_p^{(j)} &\sim \pi(\theta_p|\theta_1^{(j)}, \theta_2^{(j)}, \ldots, \theta_{p-1}^{(j)}, \boldsymbol{x})
\end{aligned}$$

  3. Change counter j to $j + 1$, and return to step 2.

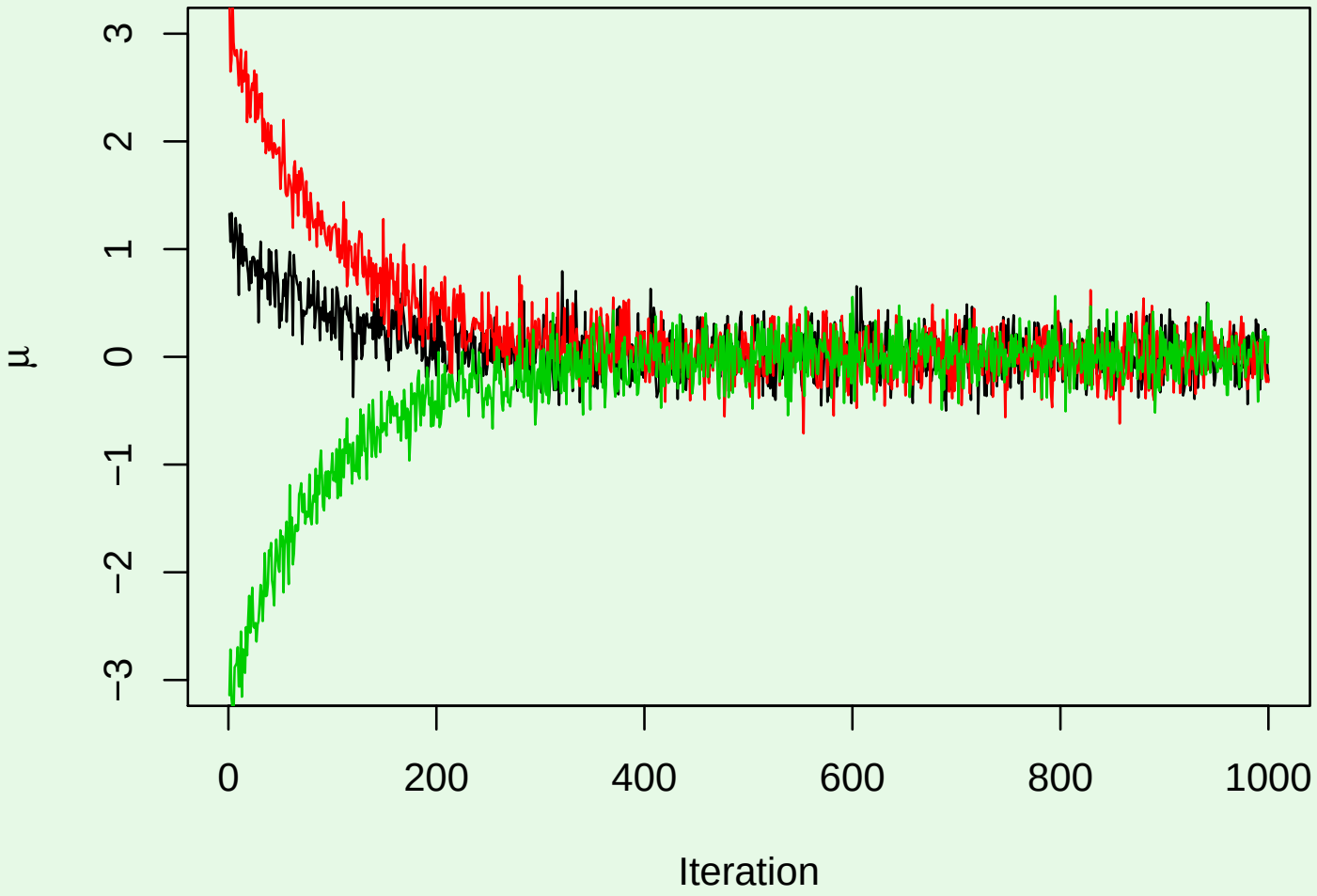
Comments

- This algorithm defines a homogeneous Markov chain as each simulated value depends only on the previous simulated value and not on any other previous values or the iteration counter j
- It can be shown that $\pi(\boldsymbol{\theta}|\boldsymbol{x})$ is the stationary distribution of this chain and so if we simulate realisations by using a Gibbs sampler, eventually the Markov chain will converge to the required posterior distribution

More comments

- This is an iterative scheme
- It needs a period to get to convergence: the *burn-in* period
- As it is a Markov chain, successive iterates are not independent
- We can get accurate values for $E(\boldsymbol{\theta}|\boldsymbol{x})$, $SD(\boldsymbol{\theta}|\boldsymbol{x})$ or even $\pi(\boldsymbol{\theta}|\boldsymbol{x})$ by running the sampler for a long time

Illustration of burn-in



- Different starting points
- But distributions of the realisations after iteration 500 are the "same"

Illustration of burn-in in two dimensions

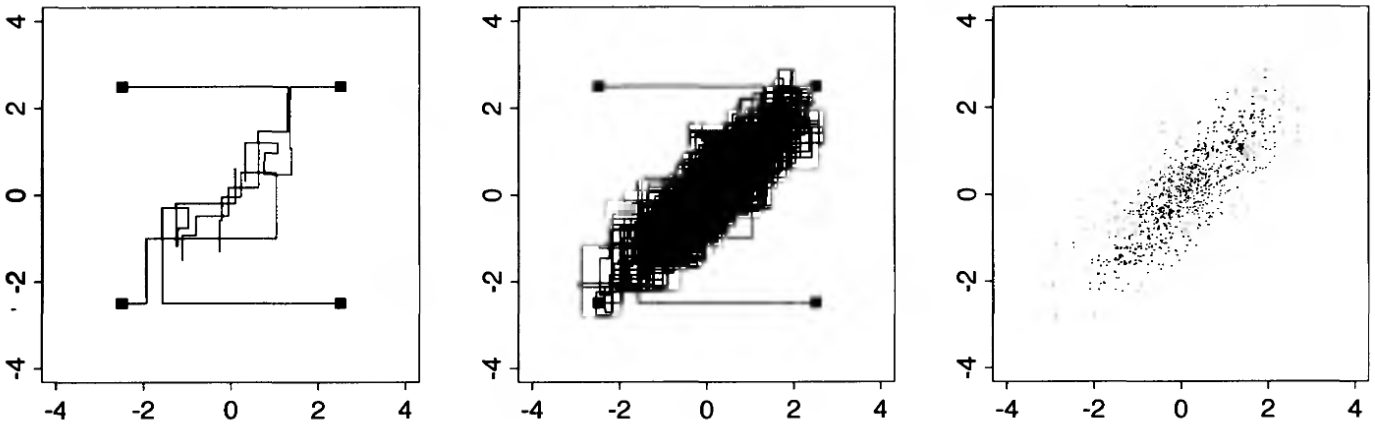


Figure 11.3 *Four independent sequences of the Gibbs sampler for a bivariate normal distribution with correlation $\rho = 0.8$, with overdispersed starting points indicated by solid squares. (a) First 10 iterations, showing the component-by-component updating of the Gibbs iterations. (b) After 500 iterations, the sequences have reached approximate convergence. Figure (c) shows the iterates from the second halves of the sequences.*

- Different starting points
- Chains converge to the "same" distribution

4.4.1 Processing output from a Gibbs sampler: Burn-in

- Consider a $p = 2$ parameter problem, with $\boldsymbol{\theta} = (\mu, \tau)^T$
- Run Gibbs sampler for N iterations after burn-in, giving

$$\{(\mu^{(1)}, \tau^{(1)}), (\mu^{(2)}, \tau^{(2)}), \ldots, (\mu^{(N)}, \tau^{(N)})\}$$

- Can calculate features of the posterior distribution using their sample equivalents: $\bar{\mu}$, $\bar{\tau}$, s_μ^2, s_τ^2 and $r_{\mu\tau}$

How accurate are these "estimates"?

- Difficult to determine exactly as they are not a *random sample*
- If it was a random sample then (for large N) approximate 95% CI for μ is

$$\bar{\mu} \pm \frac{1.96 s_\mu}{\sqrt{N}}$$

- But we don't have a random sample! What to do?

4.4.1 Processing output from a Gibbs sampler: Burn-in

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- But we don't have a random sample! What to do?

4.4.1 Processing output from a Gibbs sampler: autocorrelation

- **Method one:** Assume the output follows some Markov chain model, and use CI of this model to approximate the true CI.
- E.g. the autoregressive model with order 1, AR(1), is

$$\mu^{(t)} - \mu = \theta(\mu^{(t-1)} - \mu) + \varepsilon_t, \text{ where } \varepsilon_t \sim N(0,1).$$

  The approximate 95% CI of μ depends on the sample autocorrelation $r(1) = Corr(\mu^{(t)}, \mu^{(t+1)})$, and is

$$\bar{\mu} \pm \frac{1.96 s_\mu}{\sqrt{N\{1 - r(1)\}^2}}.$$

  Effective sample size: $N_{eff} = N\{1 - r(1)\}^2$.
- In general, MCMC output with positive autocorrelations has $N_{eff} < N$.

How to deal with autocorrelation

- **Method two (more popular):** `thin` the output – don't take every iterate
- Sample autocorrelation function with lag k for μ is

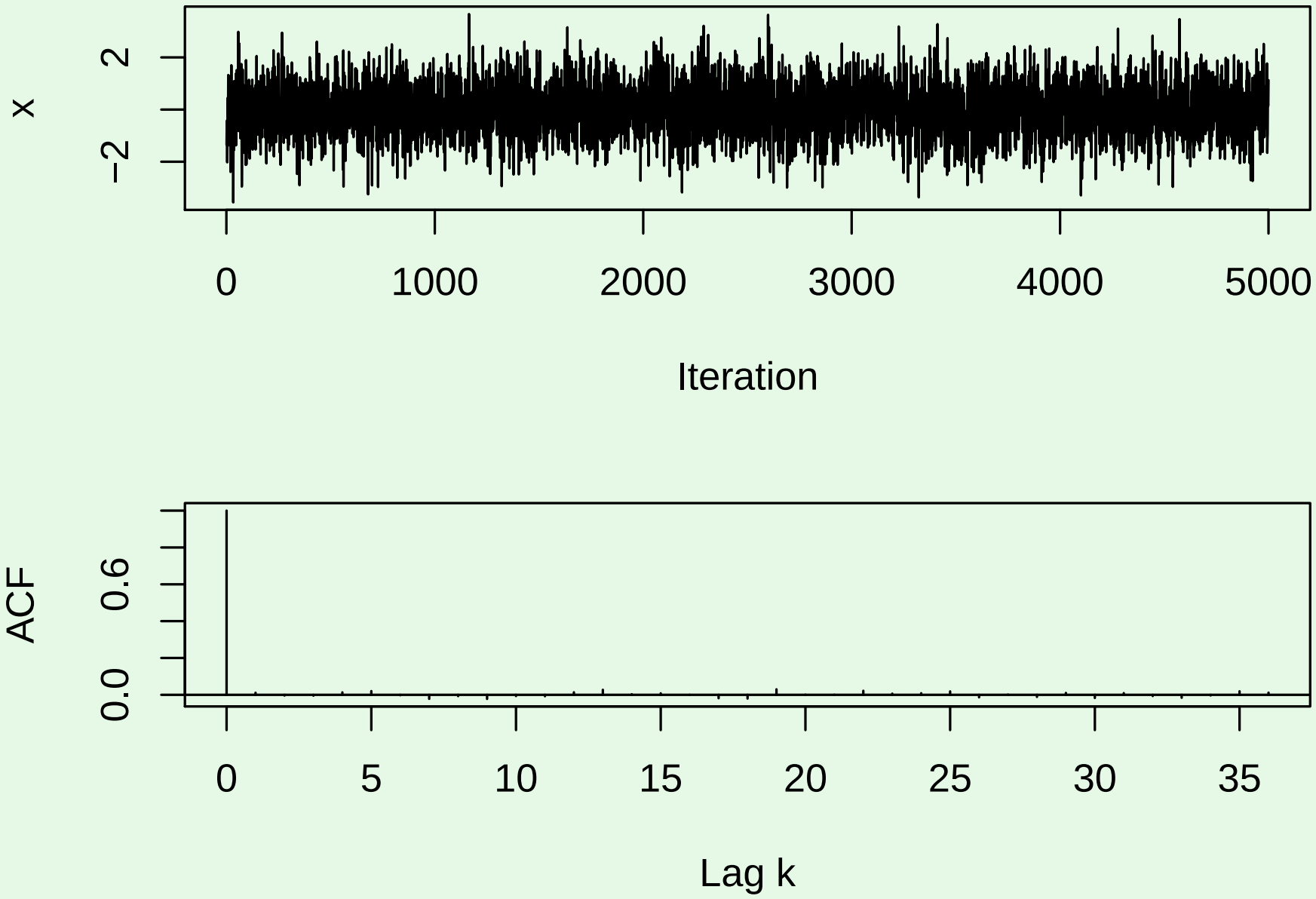
$$r(k) = Corr(\mu^{(j)}, \mu^{(j+k)}).$$

- For example, if $r(k) \simeq 0$, $k \geq 2$ then taking every 2nd iterate would give a posterior sample

$$\{(\mu^{(1)}, \tau^{(1)}), (\mu^{(3)}, \tau^{(3)}), \ldots, (\mu^{(2j+1)}, \tau^{(2j+1)}, \ldots)\}$$

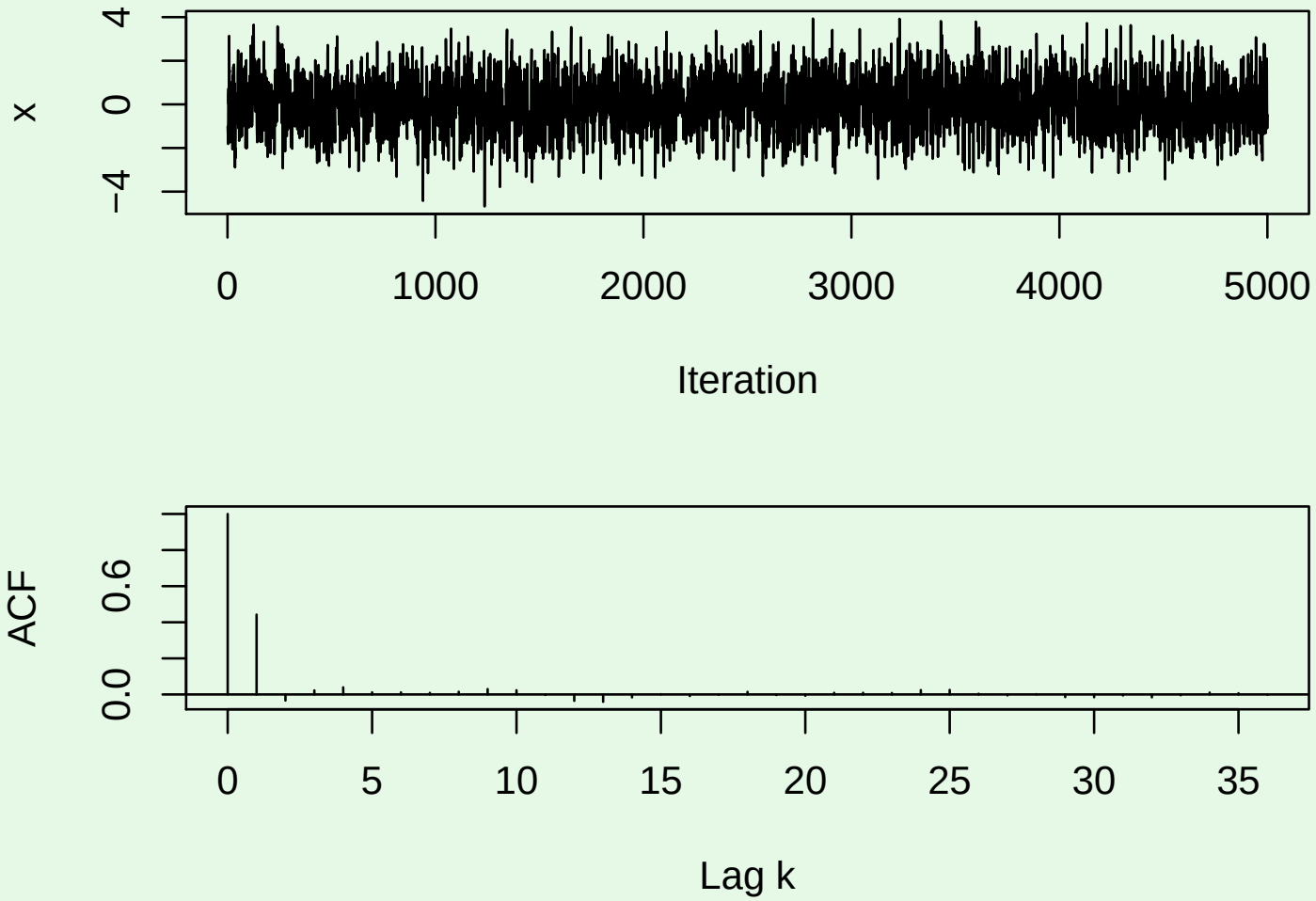
  with autocorrelation function $r^*(k) = 0$, $k \geq 1$, that is, this output has very low autocorrelation
- Generally we look at the ACF plot and choose the level of thinning needed to give low autocorrelations
- We will see how this works in some examples

$N(0,1)$ random sample

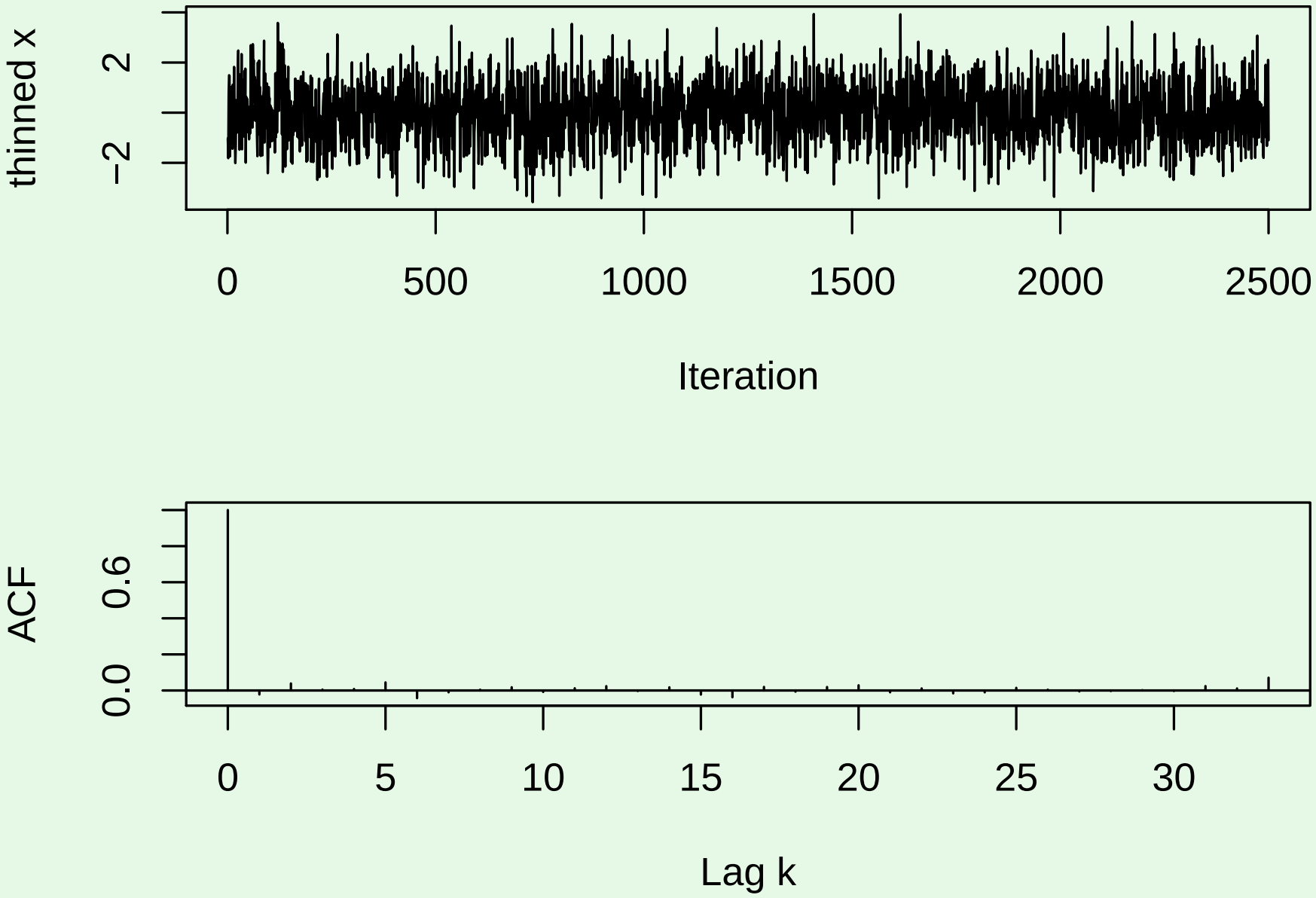


Sample from a $MA(1)$ process

$$x_t = \varepsilon_t + \theta\varepsilon_{t-1}, \text{ where } \varepsilon_t \sim N(0,1), \text{and } r(1) = \theta, r(k) = 0, k \geq 2.$$

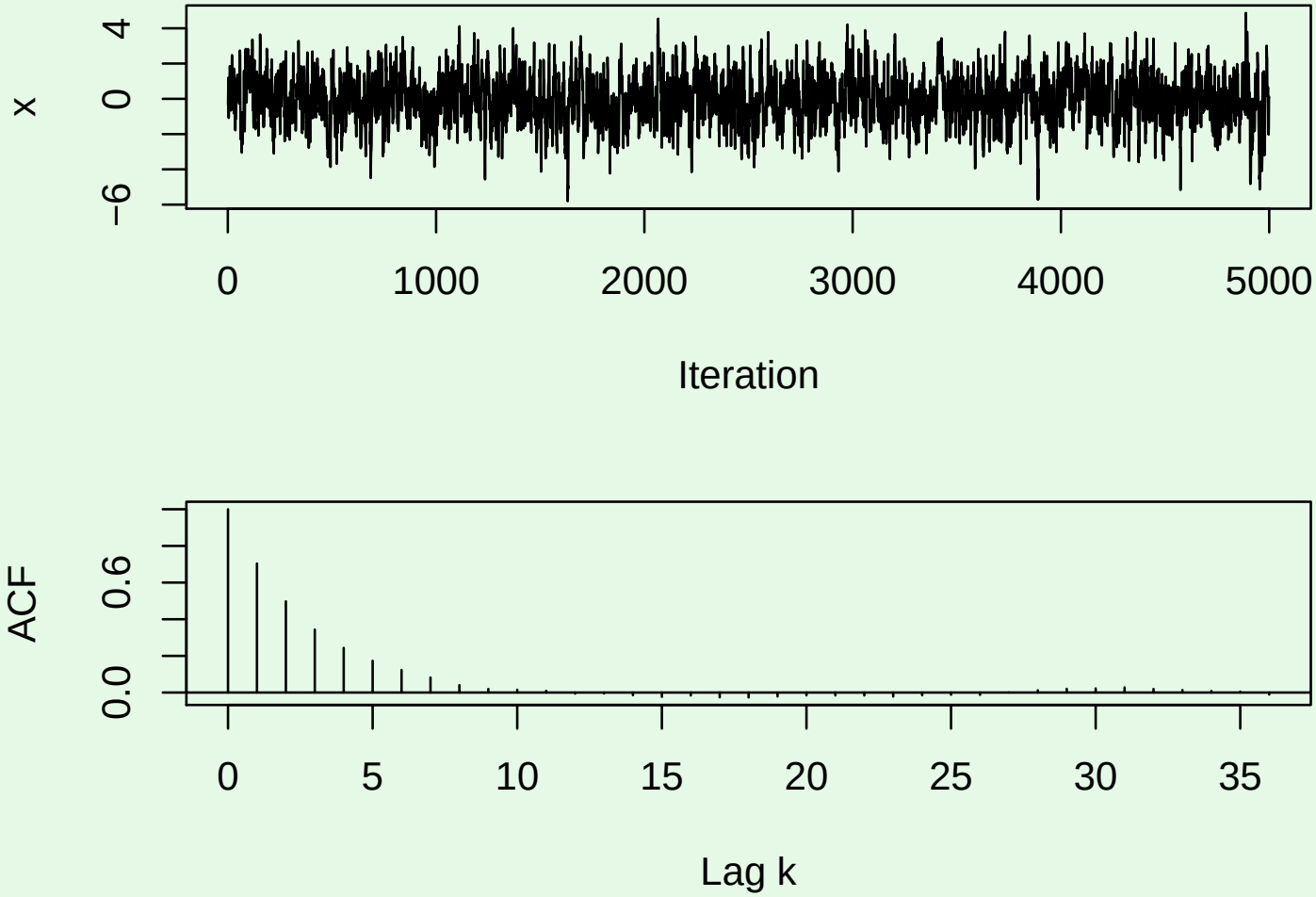


Thinned sample from a $MA(1)$ process ($\texttt{thin} = 2$)

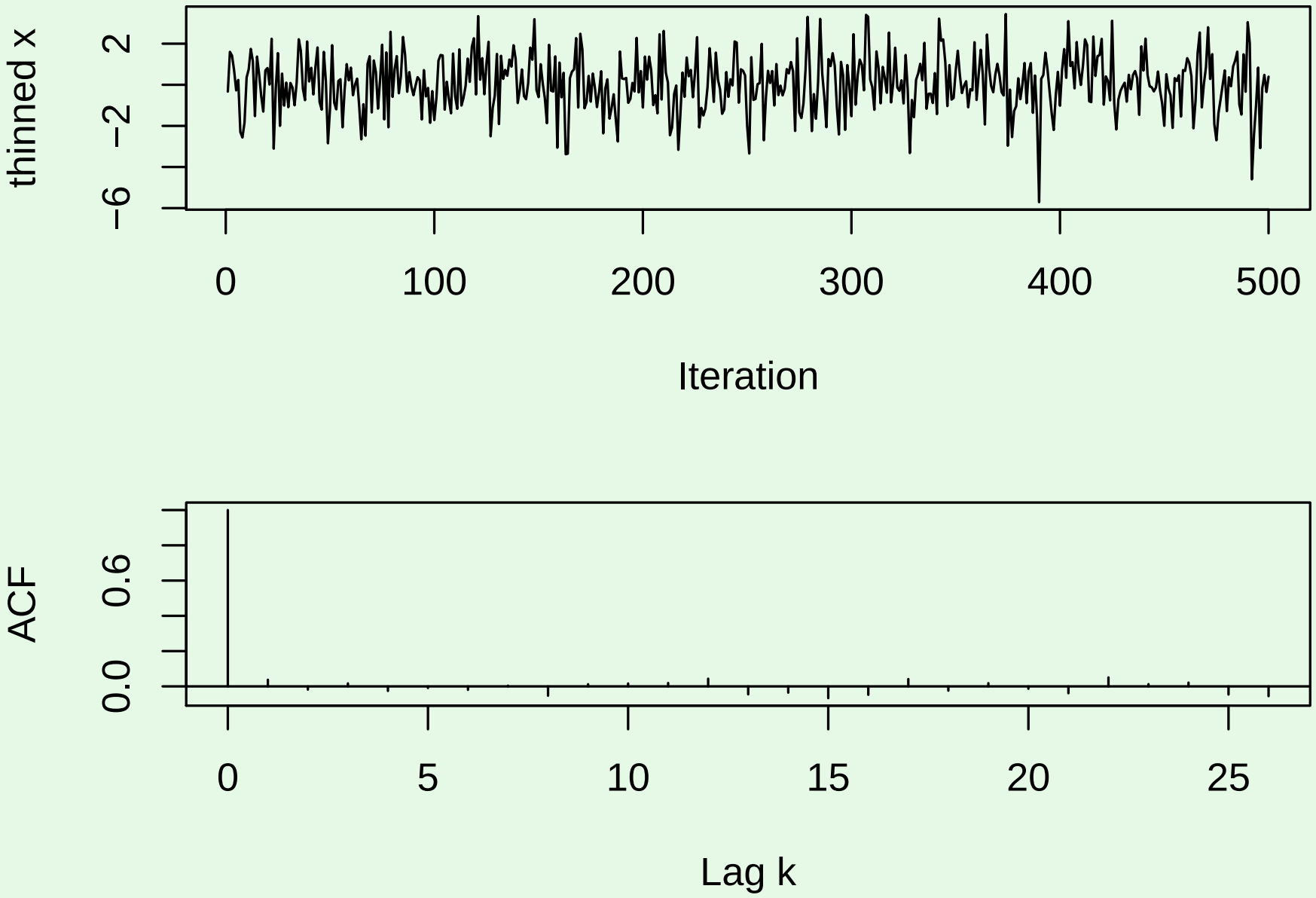


Sample from a $AR(1)$ process

$$x_t = \theta x_{t-1} + \varepsilon_t, \text{ where } \varepsilon_t \sim N(0,1), \text{and } r(k) \simeq r(1)^k, k \geq 2.$$



Thinned sample from a $AR(1)$ process ($\texttt{thin} = 10$)



Strategy

1. Determine the *burn-in* period, after which the Gibbs sampler has reached its stationary distribution
   This may involve thinning the posterior sample as slowly snaking trace plots may be due to high autocorrelations rather than a lack of convergence
2. After this, determine the level of thinning to obtain a posterior sample whose autocorrelations are roughly zero
3. Repeat steps 1 and 2 several times using different initial values to make sure that the sample really is from the posterior distribution

4.4.2 Bayesian inference using a Gibbs sampler

Example 4.2

Construct a Gibbs sampler for the posterior distribution in Example 4.1:

- Data: $X_i|\mu, \tau \sim N(\mu, 1/\tau)$, $i = 1, 2, \ldots, n$ (independent)
- Prior:

$$\mu \sim N\left(b, \frac{1}{c}\right) \qquad \text{and} \qquad \tau \sim Ga(g, h), \qquad \text{independent}$$

Solution

...

R functions in the nclbayes library

- `gibbsNormal` – implements this algorithm
- `mcmcProcess` – used to remove the `burn-in` and `thin` the output
- `mcmcAnalysis` – analyses the MCMC output

Look at a particular numerical example

- Data: $n = 100$, $\bar{x} = 15$ and $s = 4.5$
- Prior: $\mu \sim N(10, 1/100)$ and $\tau \sim Ga(3, 12)$, independently
- Initialise Gibbs sampler at $(10, 0.25)$

Gibbs sampler demo in R

(Ignore the upcoming slides if you'd rather try out the R code!)

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- Initialise Gibbs sampler at $(10, 0.25)$

Gibbs sampler demo in R

(Ignore the upcoming slides if you'd rather try out the R code!)

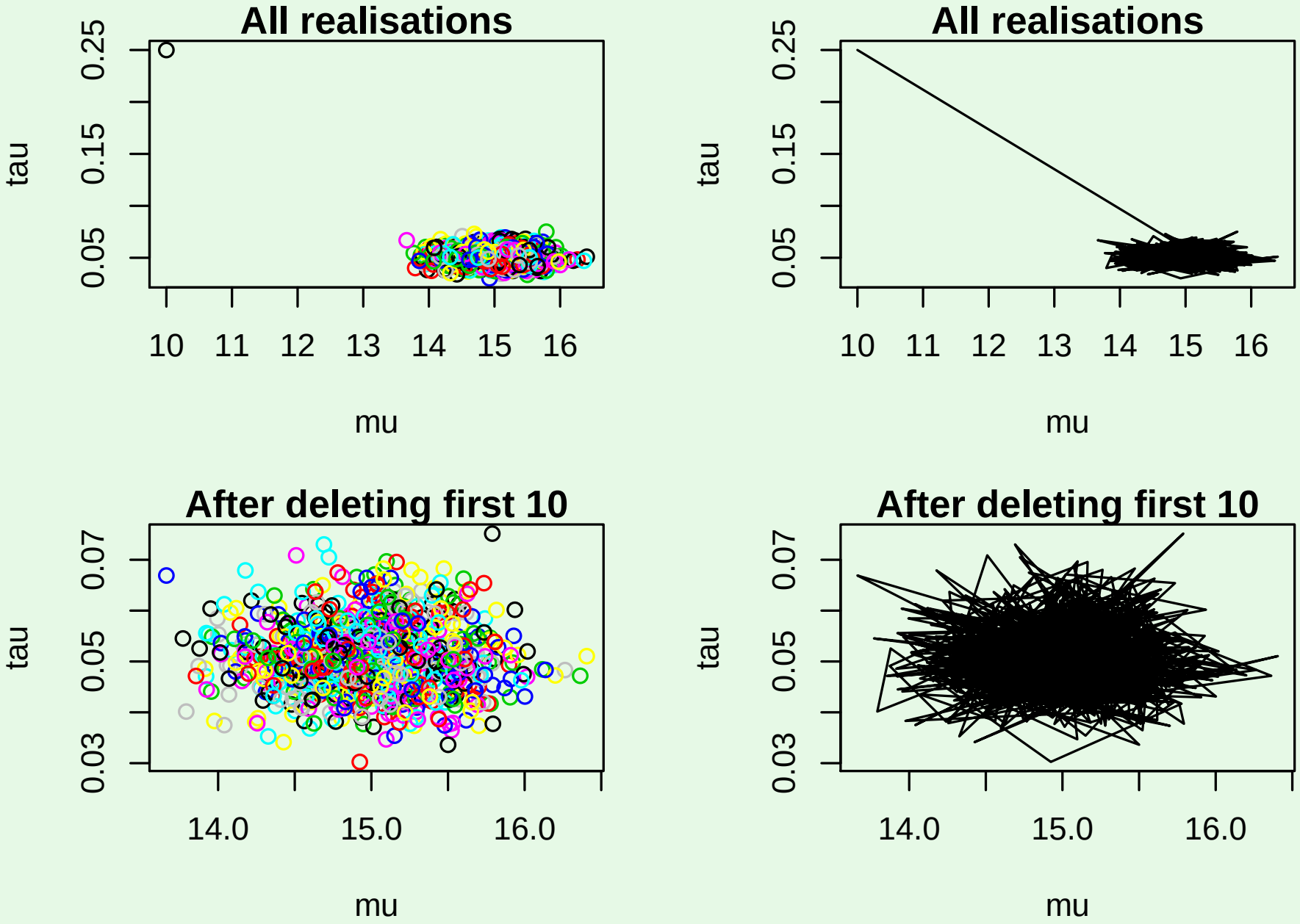
R commands used

```
library(nclbayes)
posterior=gibbsNormal(N=2000,initial=c(10,0.25),
    priorparam=c(10,1/100,3,12),n=100,xbar=15,s=4.5)
posterior2=mcmcProcess(input=posterior,burnin=1000,thin=1)

op=par(mfrow=c(2,2))
plot(posterior,col=c(1:length(posterior)),
    main="All realisations")
plot(posterior,type="l",main="All realisations")
plot(posterior2,col=c(1:length(posterior2)),
    main="After deleting first 1000")
plot(posterior2,type="l",main="After deleting first 1000")
par(op)

mcmcAnalysis(posterior,rows=2,show=F)
mcmcAnalysis(posterior2,rows=2,show=F)
```

Progress of the MCMC scheme



Analysis of MCMC output (all realisations)

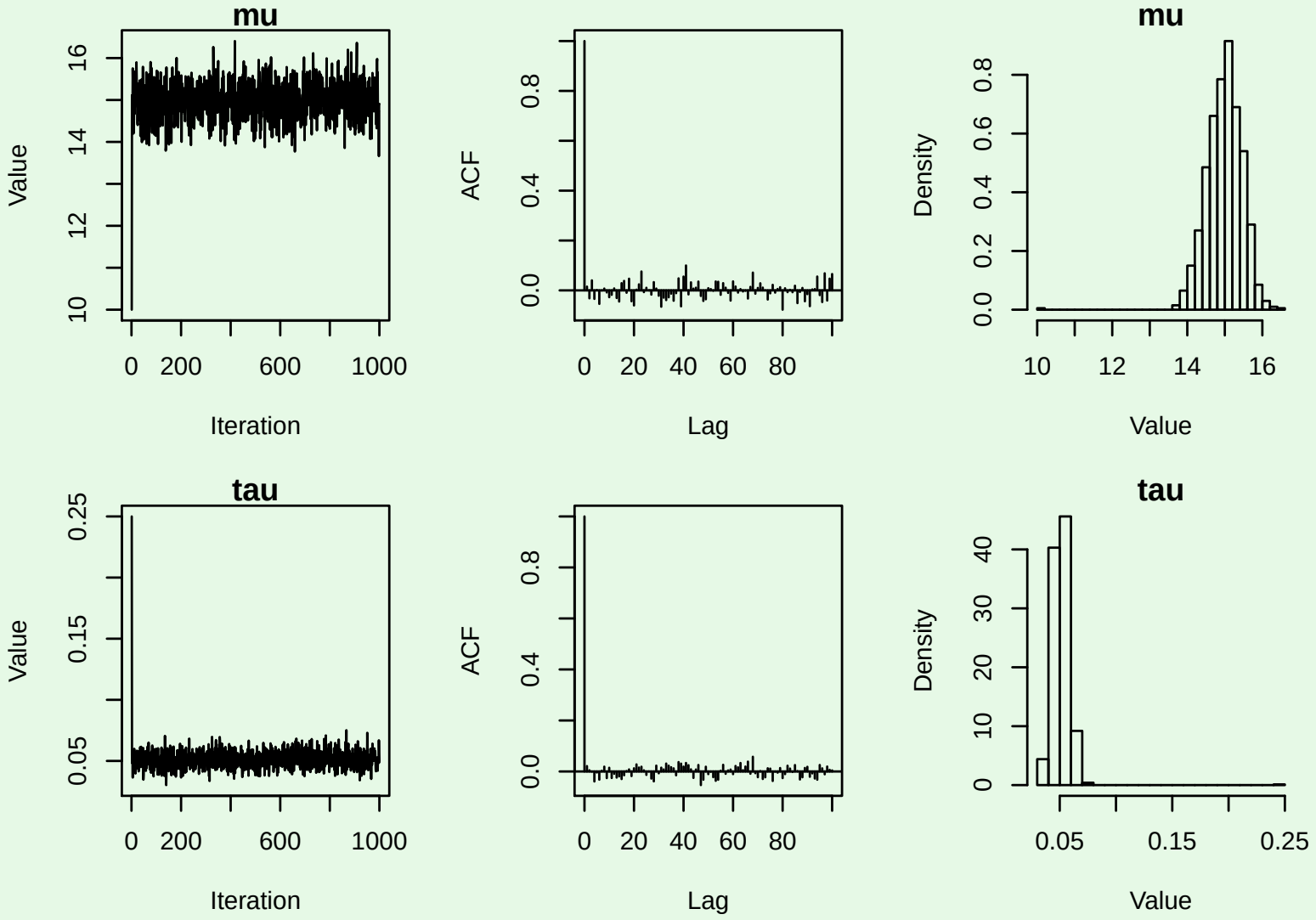


Figure: Trace plots, autocorrelation plots and histograms of the Gibbs sampler output

Analysis of MCMC output (after deleting the first 10 iterations)

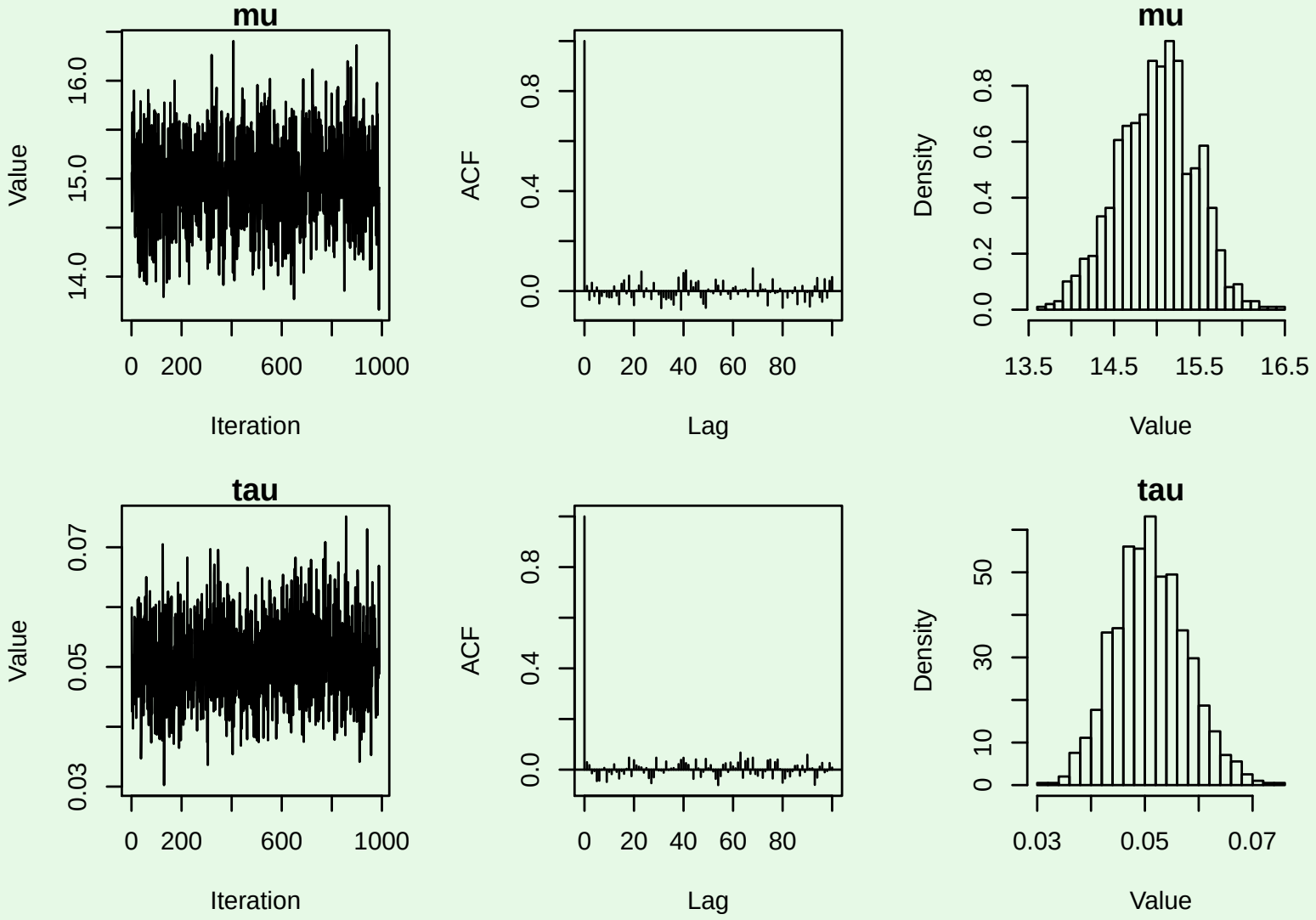


Figure: Trace plots, autocorrelation plots and histograms of the Gibbs sampler output

- Summaries of the output (after deleting the first 10 iterations)

```
N = 1000 iterations
       mu              tau
 Min.   :13.54   Min.   :0.03017
 1st Qu.:14.69   1st Qu.:0.04595
 Median :15.01   Median :0.05089
 Mean   :14.99   Mean   :0.05110
 3rd Qu.:15.28   3rd Qu.:0.05562
 Max.   :16.52   Max.   :0.07253
Standard deviations:
         mu          tau
0.444299473 0.007124057
```

- Also $Corr(\mu, \tau|\boldsymbol{x}) = -0.02153$

- Equi-tailed confidence intervals are calculated as follows:
  - MCMC output has N realisations $(\mu^{(j)}, \tau^{(j)})$
  - Sort the $\mu^{(j)}$ and the $\tau^{(j)}$ into increasing order
  - CI end-points will be the $N\alpha/2$th and the $N(1-\alpha/2)$th values
  - Use `mcmcCi` command in the `nclbayes` package
  - Gives 95% confidence intervals

$$\begin{aligned} \mu: &\quad (14.123,\ 15.847) \\ \tau: &\quad (0.037949,\ 0.065571) \end{aligned}$$

Distributions of functions of the parameters

- Now we have a sample from the posterior distribution, we can determine the posterior distribution for any function of the parameters
- For example, if we want the posterior distribution for $\sigma = 1/\sqrt{\tau}$ then we can easily obtain realisations of σ as

$$\sigma^{(j)} = 1 \Big/ \sqrt{\tau^{(j)}}$$

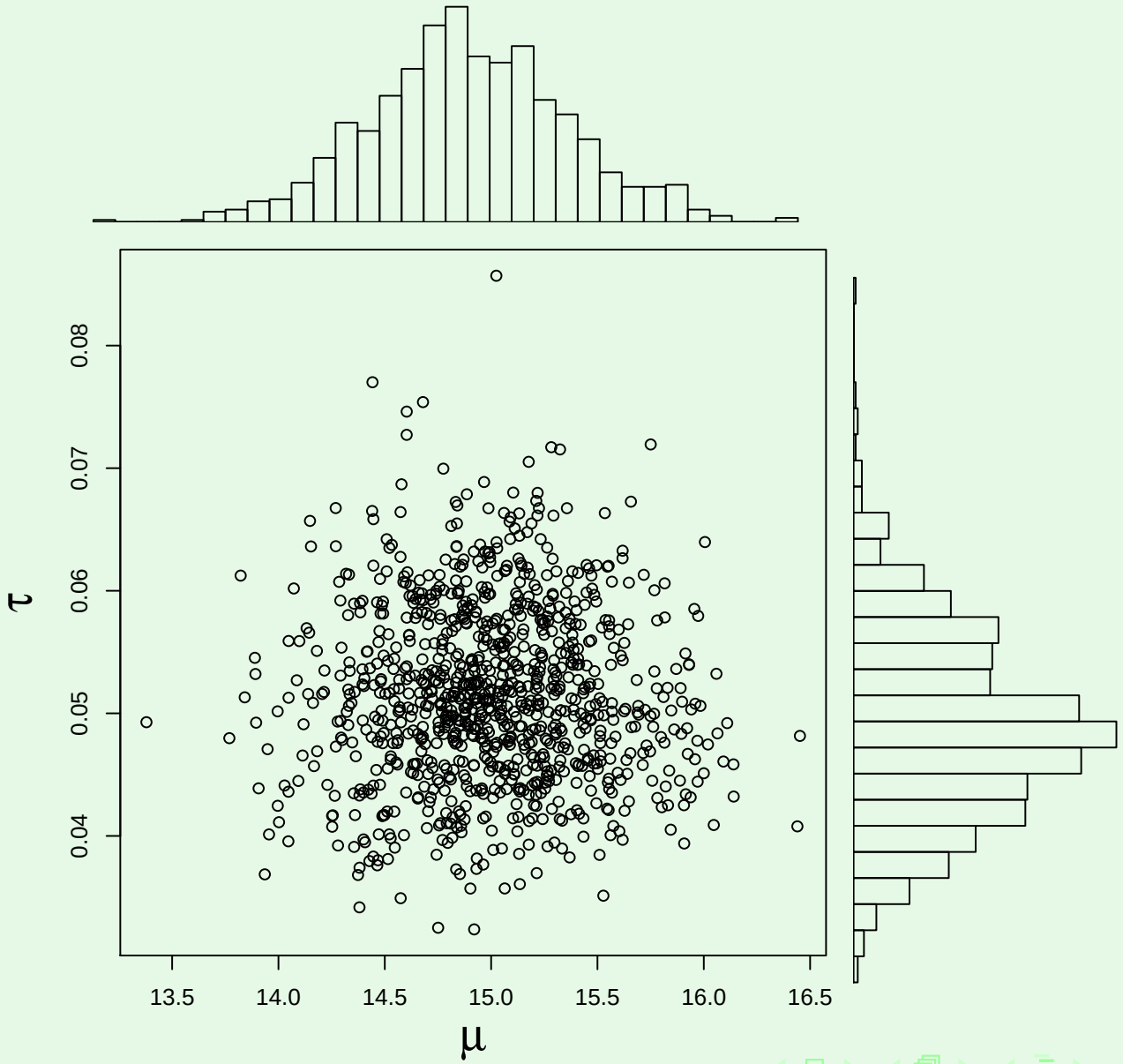
- Summaries of the output for σ

```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  3.713   4.240   4.433   4.457   4.665   5.758
```

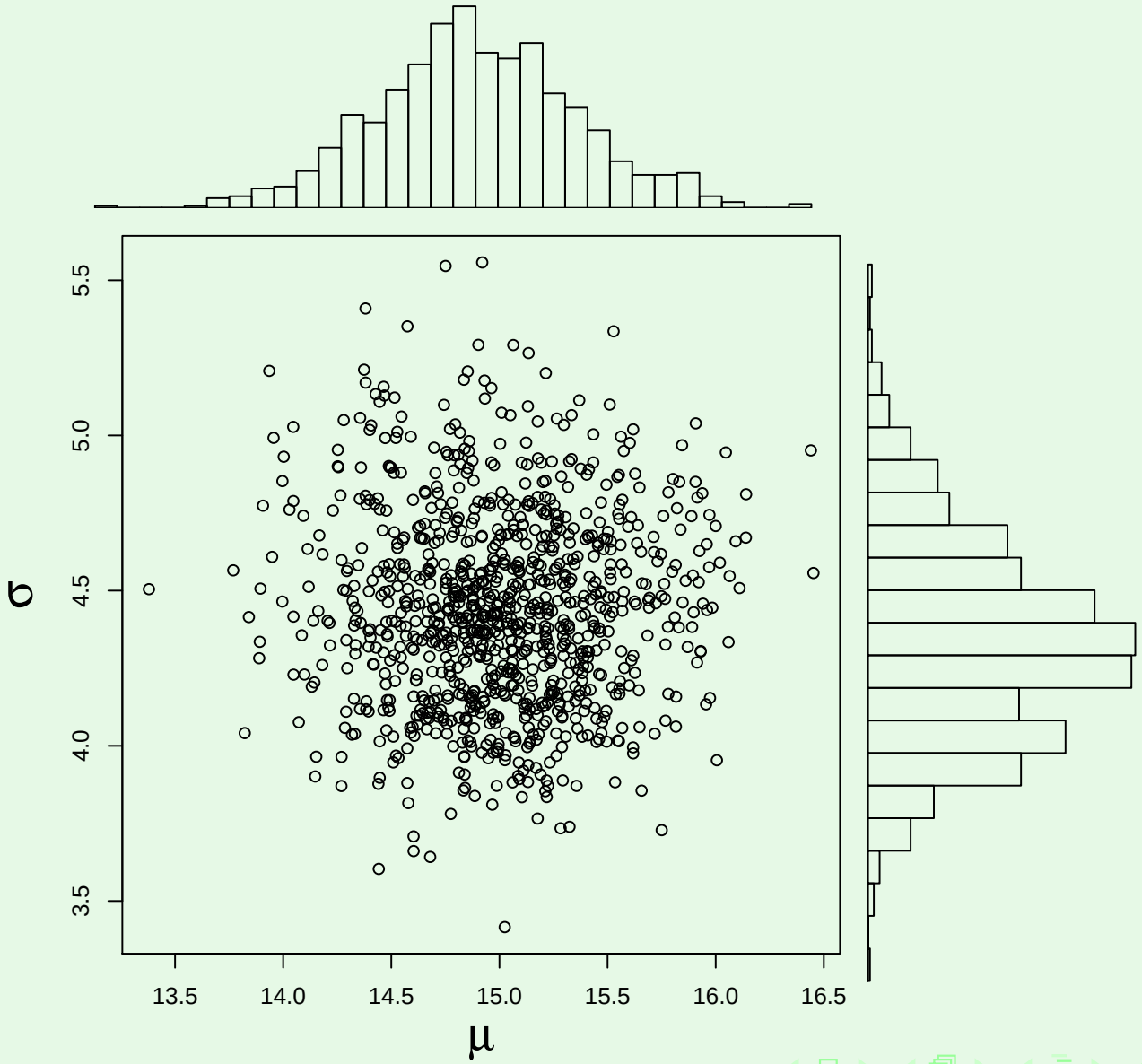
st.dev. 0.3178429

Equi-tailed 95% confidence interval for σ is (3.9001, 5.1192).

Joint and marginal distributions of $(\mu, \tau)^T$



Joint and marginal distributions of $(\mu, \sigma)^T$



R commands used

```
library(nclbayes)
posterior=gibbsNormal(N=2000,initial=c(10,0.25),
    priorparam=c(10,1/100,3,12),n=100,xbar=15,s=4.5)
posterior2=mcmcProcess(input=posterior,burnin=1000,thin=1)

mcmcAnalysis(posterior,rows=2,show=F)
mcmcAnalysis(posterior2,rows=2,show=F)

cor(posterior2)
mcmcCi(posterior2,level=0.95)

sigma=1/sqrt(posterior2[,2])
summary(sigma)
sd(sigma)
```

Summary

We can use the (converged and thinned) MCMC output to do the following

- Obtain the posterior distribution for any (joint) functions of the parameters (such as $\sigma = 1/\sqrt{\tau}$ or $(\theta_1 = \mu - \tau, \theta_2 = e^{\mu+\tau/2})^T$)
- Look at bivariate posterior distributions via scatter plots
- Look at univariate marginal posterior distributions via histograms or boxplots
- Obtain numerical summaries such as the mean, standard deviation and confidence intervals for single variables and correlations between variables

Example 4.3

- Gibbs sampling can also be used when using a conjugate prior
- Construct a Gibbs sampler for the problem in Example 3.2: Cavendish's data on the earth's density
- Data: random sample from a normal distribution with unknown mean μ and precision τ, that is

$$X_i|\mu,\tau \sim N(\mu, 1/\tau), \quad i = 1, 2, \ldots, n \quad \text{(independent)}$$

- Prior: *NGa* distribution for $(\mu, \tau)^T$

Solution

...

R function in the nclbayes library

- `gibbsNormal2` – implements this algorithm

Reanalysis of Cavendish's data

- Data: $n = 23$, $\bar{x} = 5.4848$, $s = 0.1882$
- Prior: $NGa(b = 5.41, c = 0.25, g = 2.5, h = 0.1)$
- Have seen in Example 3.2 that
  - posterior is $NGa(B = 5.4840, C = 23.25, G = 14, H = 0.5080)$
  - marginals are

$$\mu|\boldsymbol{x} \sim t_{2G=28}(B = 5.4840, H/(GC) = 0.001561)$$

$$\tau|\boldsymbol{x} \sim Ga(G = 14, H = 0.5080)$$

- We now analyse this problem using the Gibbs sampler
- Can check that the Gibbs sampler is producing realisations from the correct distribution by comparing its output with the above theoretical marginal distributions

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- We now analyse this problem using the Gibbs sampler
- Can check that the Gibbs sampler is producing realisations from the correct distribution by comparing its output with the above theoretical marginal distributions

Main R commands used

```
library(nclbayes)
posterior=gibbsNormal2(N=2000,initial=c(5.41,25),
    priorparam=c(5.41,0.25,2.5,0.1),n=23,xbar=5.4848,s=0.1882)
posterior2=mcmcProcess(input=posterior,burnin=1000,thin=1)

mcmcAnalysis(posterior,rows=2,show=F)
mcmcAnalysis(posterior2,rows=2,show=F)
```

Analysis of MCMC output (after deleting the first 1000 iterations)

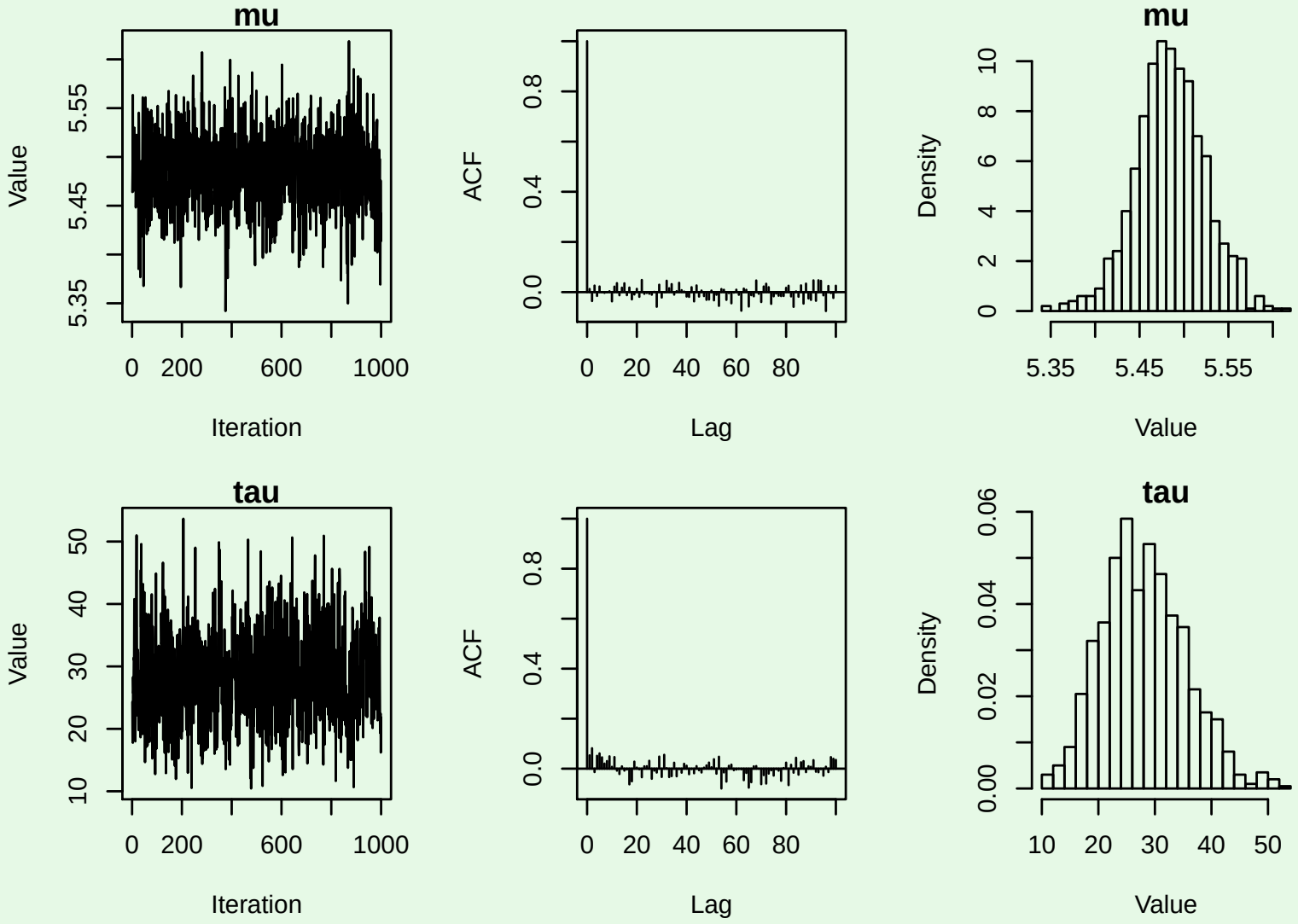


Figure: Trace plots, autocorrelation plots and histograms of the Gibbs sampler output

- Summaries of the output (after deleting the first 1000 iterations)

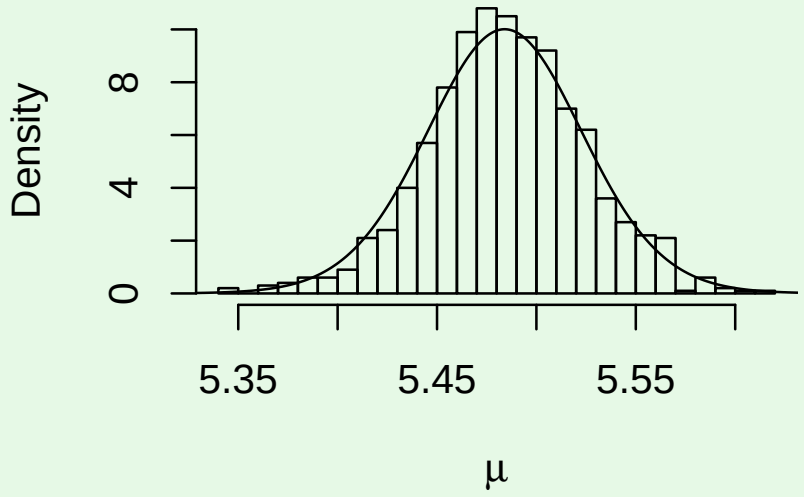
```
N = 1000 iterations
       mu              tau
 Min.   :5.376   Min.   :11.01
 1st Qu.:5.456   1st Qu.:22.09
 Median :5.483   Median :27.06
 Mean   :5.484   Mean   :27.66
 3rd Qu.:5.512   3rd Qu.:32.60
 Max.   :5.605   Max.   :56.16
Standard deviations:
        mu        tau
0.04090114 7.47836536
```

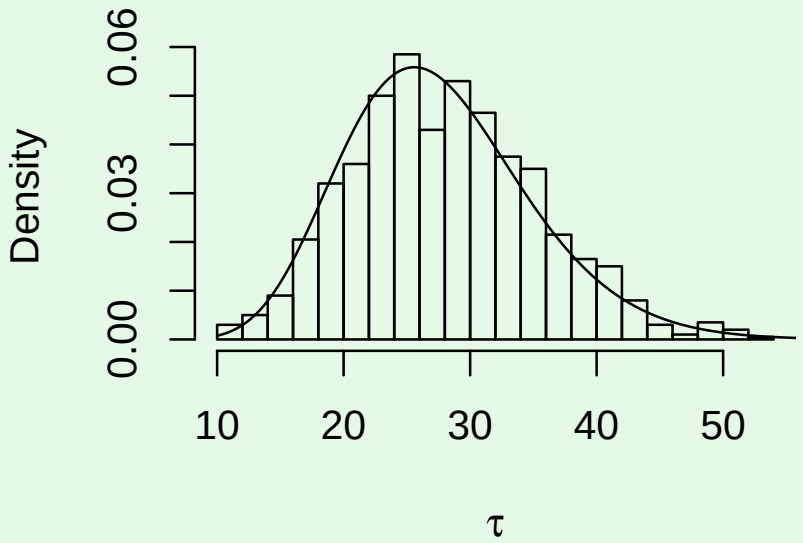
- Check:

$$E(\mu|\boldsymbol{x}) = B = 5.4840, \qquad SD(\mu|\boldsymbol{x}) = \sqrt{\frac{H}{(G-1)C}} = 0.04100$$

$$E(\tau|\boldsymbol{x}) = \frac{G}{H} = 27.559, \qquad SD(\tau|\boldsymbol{x}) = \frac{\sqrt{G}}{H} = 7.3655$$

Marginal posterior distributions of μ and σ

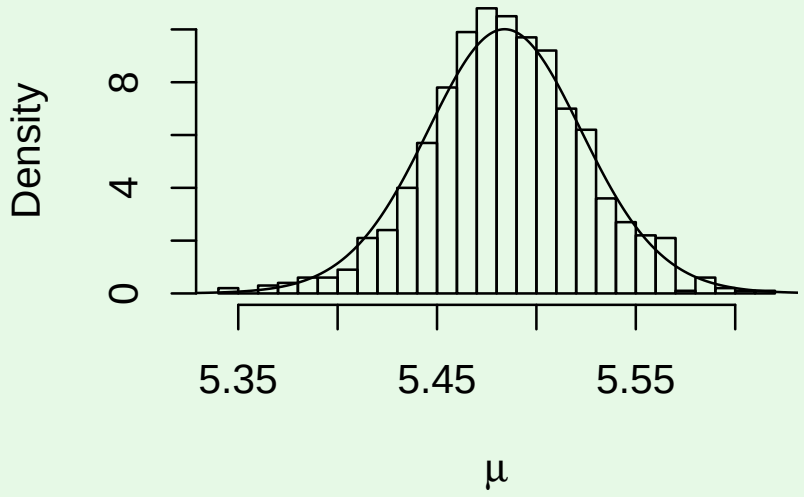


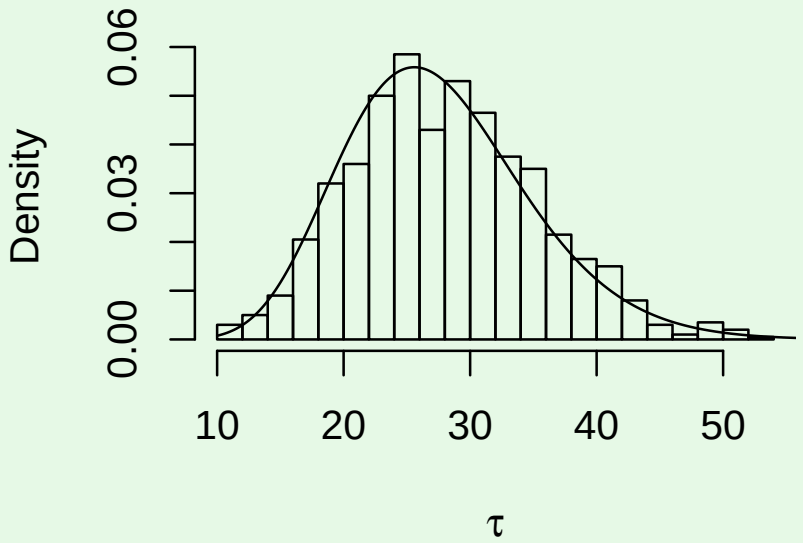


Conclusion

- Posterior means match pretty closely
- Posterior standard deviations match pretty closely
- Marginal posterior denisties match pretty closely
- They are close enough within sampling error – but could run sampler for more iterations if we wanted more accurate estimates
- This confirms that the Gibbs sampler does indeed produce realisations from the correct posterior distribution

Marginal posterior distributions of μ and σ





Conclusion

- Posterior means match pretty closely
- Posterior standard deviations match pretty closely
- Marginal posterior denisties match pretty closely
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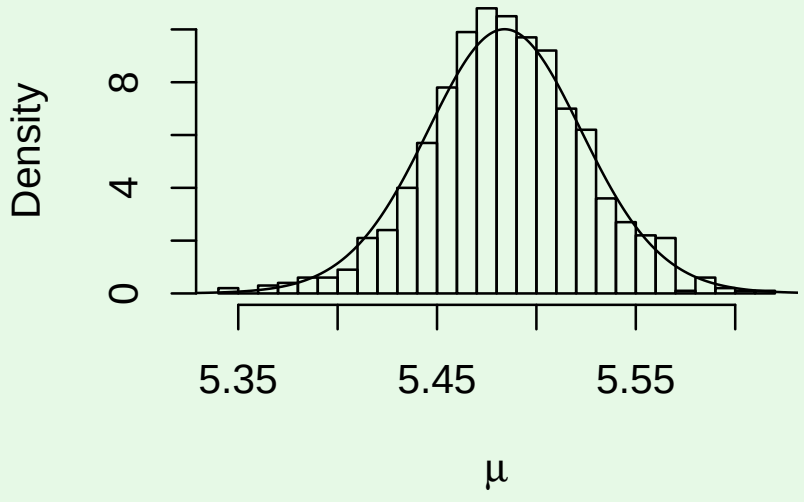

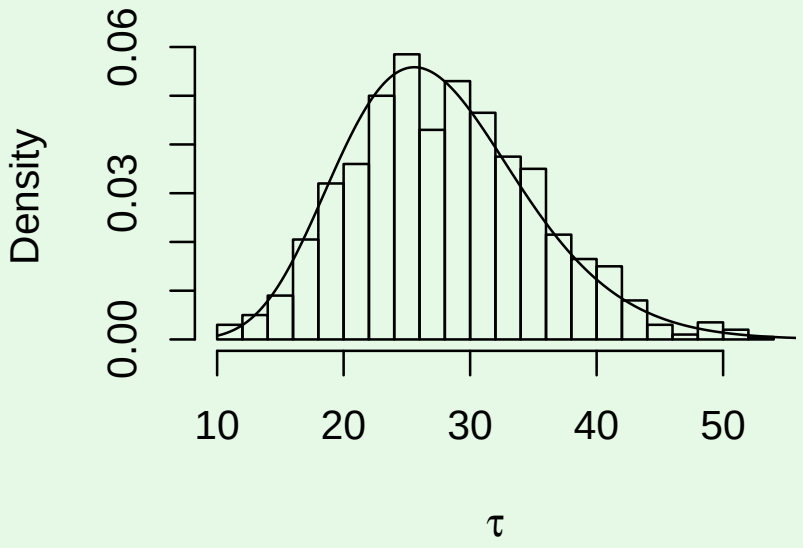

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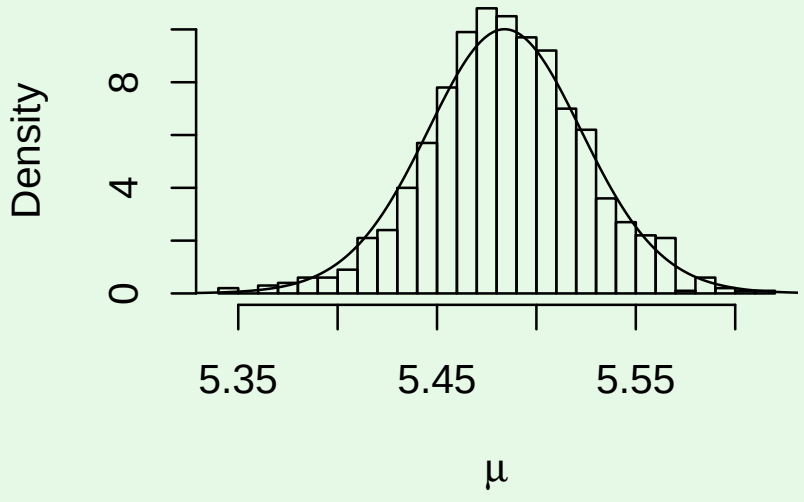

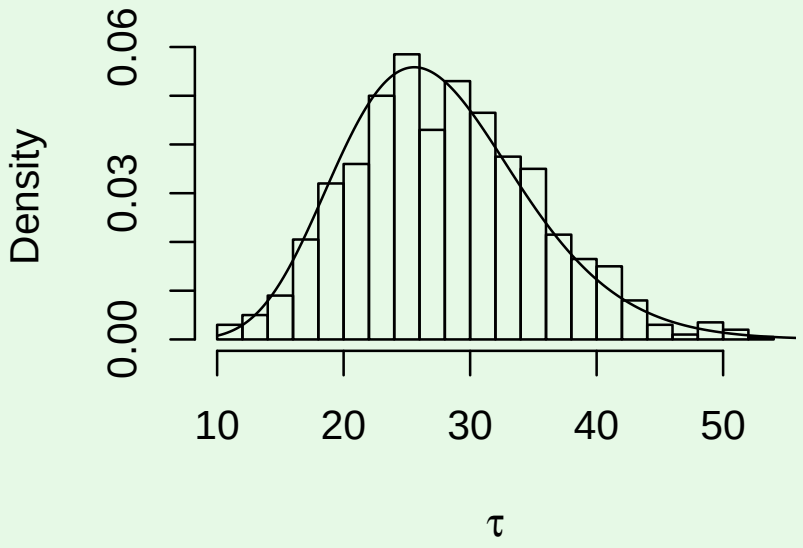

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Accuracy of posterior estimates

- Posterior output: sample mean $\bar{\mu}$, standard deviation s_μ
- How accuracte are these estimates of $M = E(\mu|\boldsymbol{x})$ and $\Sigma = SD(\mu|\boldsymbol{x})$?

- Each time we run an MCMC scheme, we obtain a different sample from the posterior distribution
- Suppose we have a large sample with effective sample size N
- It's easiest to think of this as being a sample which has been thinned so that it has N values, say $\mu_1, \ldots, \mu_N$ (and effective sample size N)
- To quantify accuracy, we need to make an assumption about the posterior distribution
- If the data sample size n is large then the posterior distribution will be approximately normal
- Think of the MCMC output as being a random sample from a normal distribution

- When the random sample $\theta_1, \ldots, \theta_N$ is from the normal $N(a, 1/d)$, from example 3.1, the asymptotic posterior distribution about the mean and precision $(a, d)^T$ is

$$a|\boldsymbol{\theta} \sim N(\bar{\theta}, s^2/N), \qquad d|\boldsymbol{\theta} \sim N\{1/s^2, 2/(Ns^4)\}, \qquad \text{independently}$$

- If the Gibbs outputs $\mu_1, \ldots, \mu_N$ come from a normal distribution $N(M, \Sigma^2)$, rewriting this result in terms of the MCMC sample mean $\bar{\mu}$, standard deviation s_μ and the parameters they estimate gives posterior distributions

$$M \sim N(\bar{\mu}, s_\mu^2/N), \qquad \Sigma^{-2} \sim N\{1/s_\mu^2, 2/(Ns_\mu^4)\}, \qquad \text{independently}$$

- Therefore an approximate 95% HDI for M is

$$\bar{\mu} \pm z_{0.025} \frac{s_\mu}{\sqrt{N}} \simeq \bar{\mu} \pm \frac{2s_\mu}{\sqrt{N}}$$

since $z_{0.025} \simeq 2$.

- Also, from the posterior distribution for Σ^{-2}, we have

$$P\left(\frac{1}{s_\mu^2} - 2\sqrt{\frac{2}{Ns_\mu^4}} < \Sigma^{-2} < \frac{1}{s_\mu^2} + 2\sqrt{\frac{2}{Ns_\mu^4}}\right) \simeq 0.95$$

$$\Longrightarrow \quad P\left(\frac{1 - 2\sqrt{2/N}}{s_\mu^2} < \Sigma^{-2} < \frac{1 + 2\sqrt{2/N}}{s_\mu^2}\right) \simeq 0.95$$

$$\Longrightarrow \quad P\left(\frac{s_\mu}{\sqrt{1 + 2\sqrt{2/N}}} < \Sigma < \frac{s_\mu}{\sqrt{1 - 2\sqrt{2/N}}}\right) \simeq 0.95.$$

  Therefore a 95% confidence interval for Σ is

$$s_\mu\left(1 \pm 2\sqrt{2/N}\right)^{-1/2} \simeq s_\mu\left(1 \pm \frac{1}{2} \times 2\sqrt{2/N}\right) = s_\mu \pm s_\mu\sqrt{\frac{2}{N}}$$

- It can be shown that these accuracy calculations are fairly accurate even when the posterior distribution (from which we have the MCMC sample) is not particularly normal

Example 4.4

- Data: $X_i|\alpha, \lambda \sim Ga(\alpha, \lambda)$, $i = 1, 2, \ldots, n$ (independent), where the index α and scale parameter λ are unknown
- Prior: $\alpha \sim Ga(a, b)$ and $\lambda \sim Ga(c, d)$, independent
- Determine the posterior density for $(\alpha, \lambda)^T$ and hence the posterior conditional densities for $\alpha|\lambda$ and $\lambda|\alpha$

Solution

...

Problem

- Although the FCD for λ is a standard distribution and easy to simulate from, the FCD for α is NOT!
- Therefore we can't use a Gibbs sampler for this analysis
- Fortunately there are other methods we can use ...

4.5 Metropolis–Hastings sampling

- The Gibbs sampler is a very powerful tool
- Only useful if the full conditional distributions (FCDs) are standard distributions (which are easy to simulate from)
- Fortunately there is a class of methods which can be used when the FCDs are non-standard
- These methods are known as Metropolis-Hastings schemes

- Want to simulate realisations from the posterior density $\pi(\boldsymbol{\theta}|\boldsymbol{x})$
- All of the FCDs are non-standard
- Choose a proposal distribution with density $q(\boldsymbol{\theta}^*|\boldsymbol{\theta})$, which is easy to simulate from
- This distribution gives us a way of proposing new values $\boldsymbol{\theta}^*$ from the current value $\boldsymbol{\theta}$

Metropolis–Hastings algorithm

1. Initialise the iteration counter to $j = 1$, and initialise the chain to $\boldsymbol{\theta}^{(0)}$
2. Generate a proposed value $\boldsymbol{\theta}^*$ using the proposal distribution $q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(j-1)})$
3. Evaluate the acceptance probability $\alpha(\boldsymbol{\theta}^{(j-1)}, \boldsymbol{\theta}^*)$ of the proposed move, where

$$\alpha(\boldsymbol{\theta}, \boldsymbol{\theta}^*) = \min\left\{1, \frac{\pi(\boldsymbol{\theta}^*|\boldsymbol{x})\, q(\boldsymbol{\theta}|\boldsymbol{\theta}^*)}{\pi(\boldsymbol{\theta}|\boldsymbol{x})\, q(\boldsymbol{\theta}^*|\boldsymbol{\theta})}\right\}$$

4. Set $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^*$ with probability $\alpha(\boldsymbol{\theta}^{(j-1)}, \boldsymbol{\theta}^*)$, and set $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^{(j-1)}$ otherwise
5. Change the counter from j to $j + 1$ and return to step 2

Metropolis–Hastings algorithm

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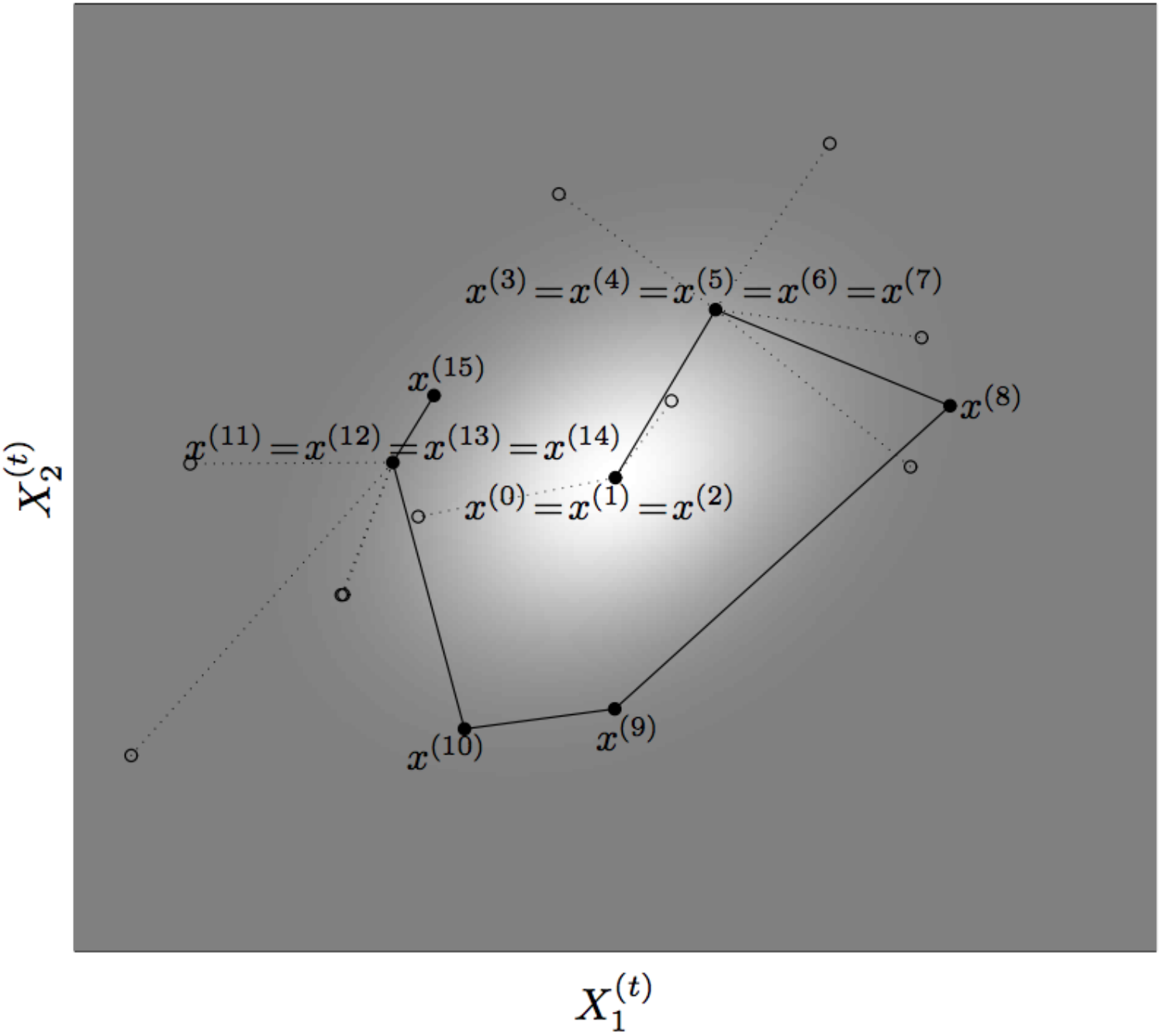
$x^{(3)} = x^{(4)} = x^{(5)} = x^{(6)} = x^{(7)}$
$x^{(8)}$
$x^{(15)}$
$x^{(11)} = x^{(12)} = x^{(13)} = x^{(14)}$
$x^{(0)} = x^{(1)} = x^{(2)}$
$x^{(10)}$
$x^{(9)}$
$X_2^{(t)}$
$X_1^{(t)}$

Comments

- At each stage, a new value is generated from the proposal distribution
- This value is either accepted, in which case the chain moves, or rejected, in which case the chain stays where it is
- Whether or not the move is accepted or rejected depends on an acceptance probability which itself depends on the relationship between the density of interest and the proposal distribution
- The posterior density $\pi(\boldsymbol{\theta}|\boldsymbol{x})$ only enters into the acceptance probability as a ratio, and so the method can be used when the posterior density is only known up to a scaling constant, that is,

$$\alpha(\boldsymbol{\theta}, \boldsymbol{\theta}^*) = \min\left\{1, \frac{\pi(\boldsymbol{\theta}^*)\, f(\boldsymbol{x}|\boldsymbol{\theta}^*)\, q(\boldsymbol{\theta}|\boldsymbol{\theta}^*)}{\pi(\boldsymbol{\theta})\, f(\boldsymbol{x}|\boldsymbol{\theta})\, q(\boldsymbol{\theta}^*|\boldsymbol{\theta})}\right\}$$

- This algorithm defines a Markov chain with $\pi(\boldsymbol{\theta}|\boldsymbol{x})$ as its stationary distribution
- It holds for all possible proposal distributions (subject to them generating realisations from the full parameter space)

Possible proposal distributions

- Are some choices of proposal distribution better than others?
- We now discuss some commonly used proposal distributions

4.5.1 Symmetric chains (Metropolis method)

- Use a symmetric proposal distribution: $q(\boldsymbol{\theta}^*|\boldsymbol{\theta}) = q(\boldsymbol{\theta}|\boldsymbol{\theta}^*), \forall\, \boldsymbol{\theta}, \boldsymbol{\theta}^*$
- The acceptance probability simplifies to

$$\alpha(\boldsymbol{\theta}, \boldsymbol{\theta}^*) = \min\left\{1, \frac{\pi(\boldsymbol{\theta}^*|\boldsymbol{x})}{\pi(\boldsymbol{\theta}|\boldsymbol{x})}\right\}$$

  and hence does not involve the proposal density at all
- Proposed moves which will take the chain to a region of higher posterior density are always accepted
- Moves which take the chain to a region of lower posterior density are accepted with probability proportional to the ratio of the two densities
- Moves which will take the chain to a region of very low density will be accepted with very low probability

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Random walk proposals

- Consider the random walk proposal in which the proposed value $\boldsymbol{\theta}^*$ at stage j is

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}^{(j-1)} + \boldsymbol{w}_j$$

  where the $\boldsymbol{w}_j$ are independent and identically distributed random $p \times 1$ vectors (completely independent of the state of the chain)
- Suppose that the $\boldsymbol{w}_j$ have density $f(\cdot)$, which is easy to simulate from, has mean $\mathbf{0}$ and is symmetric about its mean
- We can then simulate an innovation $\boldsymbol{w}_j$, and set the proposal value to $\boldsymbol{\theta}^* = \boldsymbol{\theta}^{(j-1)} + \boldsymbol{w}_j$
- What distribution should we use for $f(\cdot)$?

Choice of innovation distribution

- A distribution which is simple and easy to simulate from is always a good idea; for example, the uniform or normal $\cdots\cdots$
  Normal is generally better, but is a bit more expensive to simulate
- What variance should we choose for the innovation distribution?
- This choice will affect the acceptance probability, and hence the overall proportion of accepted moves
- If the variance of the innovation is too low, then most proposed values will be accepted, but the chain will move very slowly around the space — the chain is said to be too "cold"
- If the variance of the innovation is too large, very few proposed values will be accepted, but when they are, they will often correspond to quite large moves — the chain is said to be too "hot"
- Theoretically it has been shown that the optimal acceptance rate is around 0.234 — this is an asymptotic result (for large samples of data) — but experience suggests that an acceptance rate of around 20–30% is okay
- Thus, the variance of the innovation distribution should be "tuned" to get an acceptance rate of around this level

Example 4.5

- Suppose the posterior distribution is a standard normal distribution, with density $\phi(\cdot)$
- Construct a Metropolis–Hastings algorithm which samples this posterior distribution by using a uniform random walk proposal
- Examine how the acceptance rate for this algorithm depends on the width of the uniform distribution

Solution

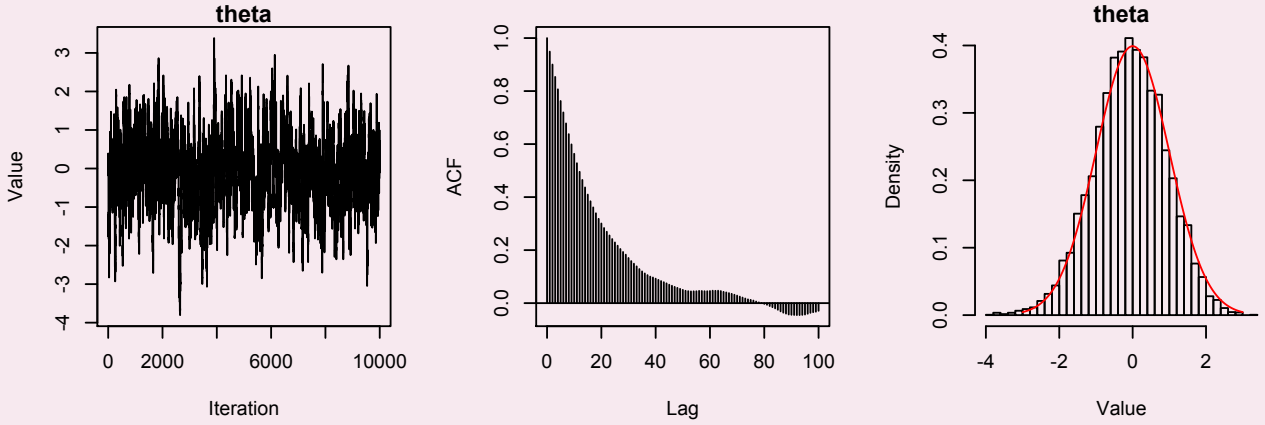
...

R commands

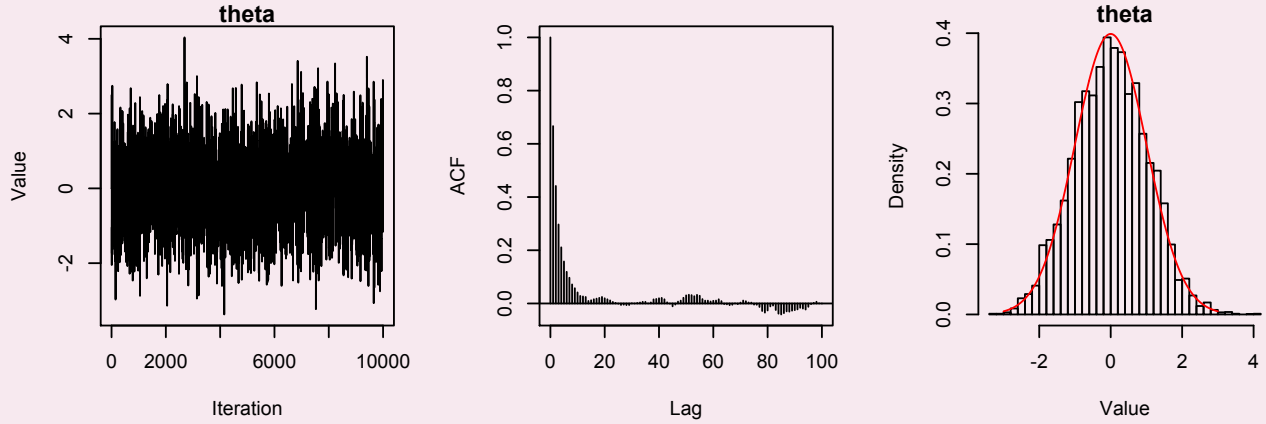
```
posterior=metropolis(N=10000,initial=0,a=1)
mcmcAnalysis(posterior,rows=1,show=F)
```

Sampling from a standard normal using Metropolis-Hastings

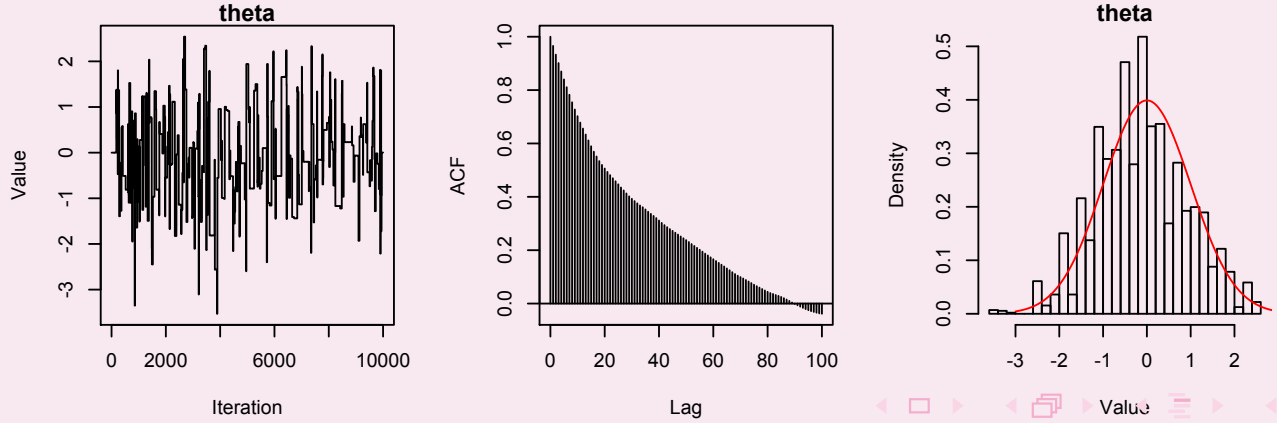
$a = 0.6$



$a = 6$



$a = 60$

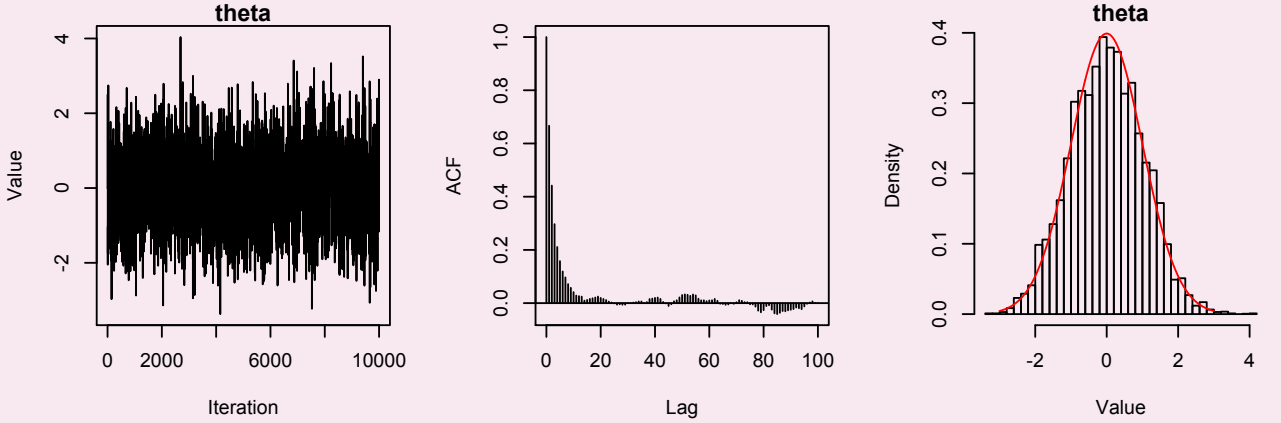


Comments

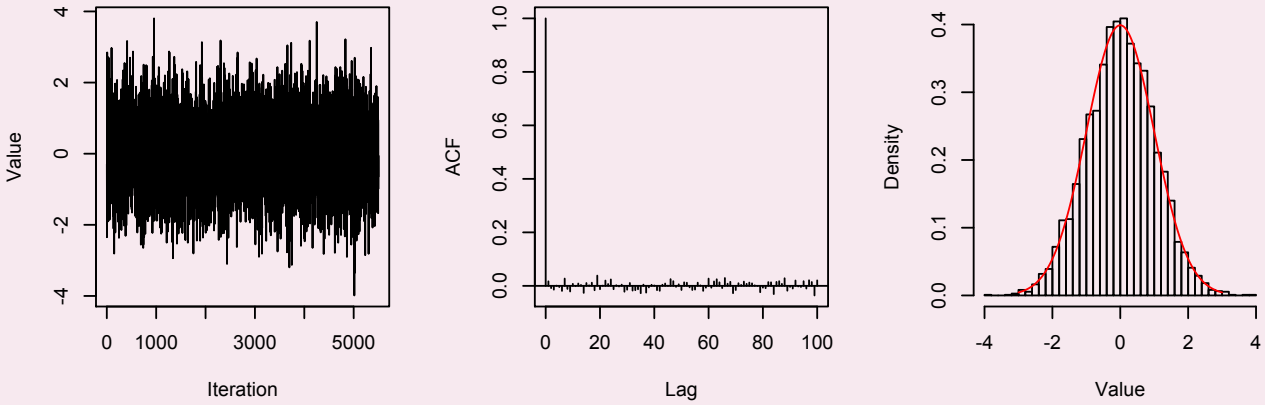
- $a = 0.6$ – this chain is too "cold"
  - The innovations are too small and are generally accepted
  - The acceptance rate for this chain was 0.911
  - The autocorrelations are too high and this chain would have to be thinned
- $a = 6$
  - The autocorrelations are much lower
  - The acceptance rate was 0.392 (nearer the asymptotic 0.234 M–H acceptance rate)
- $a = 60$ – this chain is too "hot"
  - Few proposed values are accepted (acceptance rate 0.039)
  - When they are, it results in a fairly large move to the chain
  - This gives fairly high autocorrelations and this chain would have to be thinned

Sampling from a standard normal using Metropolis-Hastings

$a = 6$



thinned



Normal random walk proposals

- Suppose we decide to use a normal random walk with $f(\cdot) = N_p(\mathbf{0}, \Sigma)$
- The proposal distribution is

$$q(\boldsymbol{\theta}^*|\boldsymbol{\theta}) = N_p(\boldsymbol{\theta}, \Sigma)$$

- Tuning this random walk requires us to choose Σ
  How can we do this?
- If the posterior distribution is approximately normally distributed (as it is with large data samples) then researchers have shown that the optimal choice is

$$\Sigma = \frac{2.38^2}{p} Var(\boldsymbol{\theta}|\boldsymbol{x})$$

- In practice, we don't know the posterior variance $Var(\boldsymbol{\theta}|\boldsymbol{x})$

- However, we could first run the MCMC algorithm substituting in the (generally much larger) prior variance $Var(\boldsymbol{\theta})$, that is, take

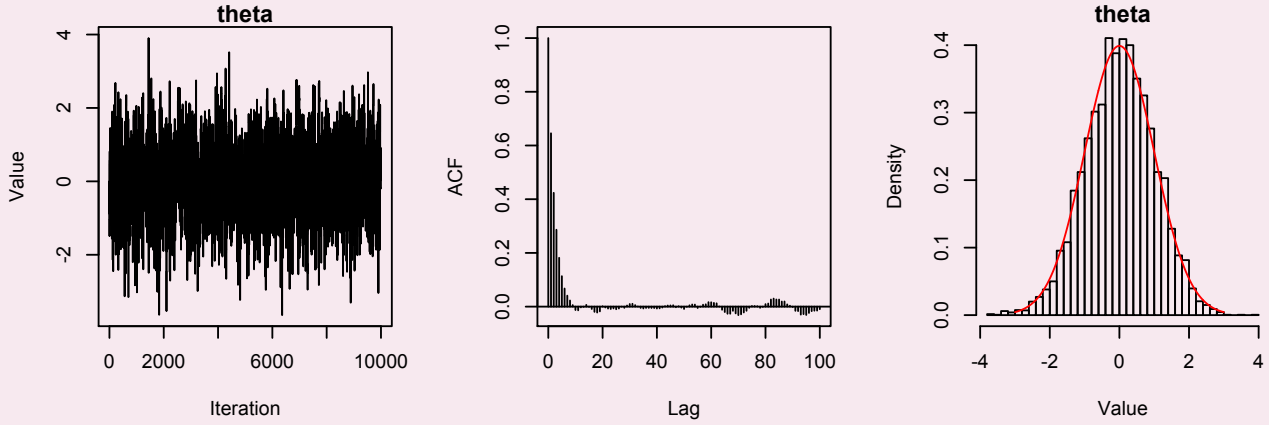
$$\Sigma = \frac{2.38^2}{p} Var(\boldsymbol{\theta})$$

- If this chain doesn't converge quickly then we can use the output of this MCMC run to get a better idea of $Var(\boldsymbol{\theta}|\boldsymbol{x})$ and run the MCMC code again – this will have more appropriate values for the parameter variances and correlations
- It has been shown from experience that it is not vital to get an extremely accurate value for Σ
- Often just getting the correct order of magnitude for its elements will be sufficient, that is, using say 0.1 rather than 0.01 or 1

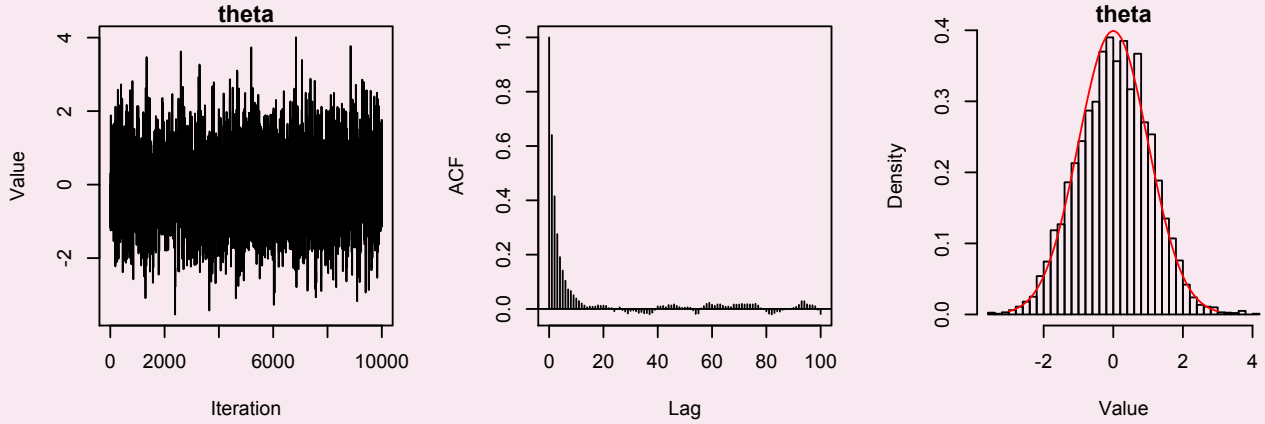
- Example: Assume the posterior distribution is a standard normal distribution. Then the optimal $\Sigma = 5.7$.

Sampling from a standard normal using normal random walk

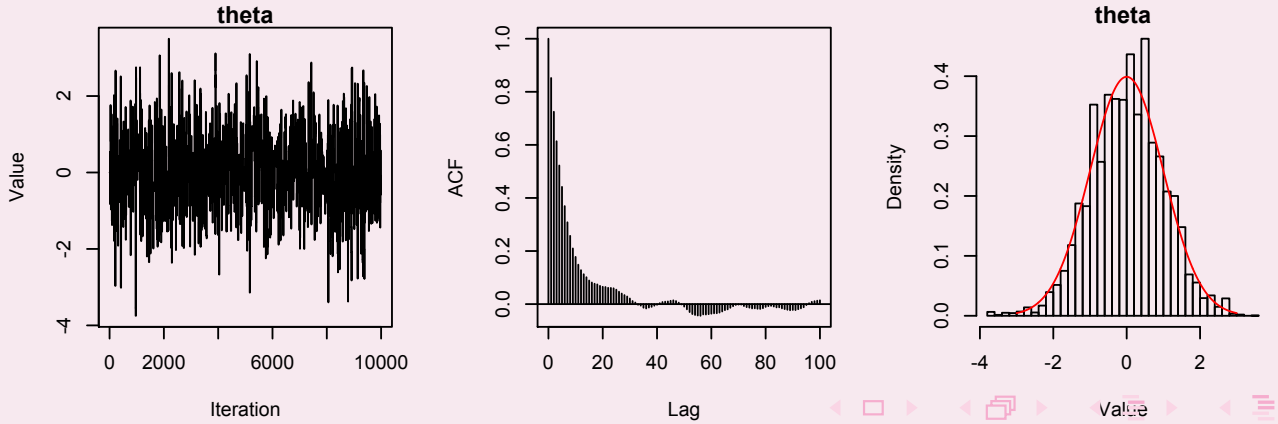
$\Sigma = 11$



$\Sigma = 5.7$



$\Sigma = 100$



4.5.2 Independence chains

- The proposal is formed independently of the position of the chain, and so $q(\boldsymbol{\theta}^*|\boldsymbol{\theta}) = f(\boldsymbol{\theta}^*)$ for some density $f(\cdot)$
- The acceptance probability is

$$\alpha(\boldsymbol{\theta}, \boldsymbol{\theta}^*) = \min\left\{1, \frac{\pi(\boldsymbol{\theta}^*|\boldsymbol{x})}{\pi(\boldsymbol{\theta}|\boldsymbol{x})} \Big/ \frac{f(\boldsymbol{\theta}^*)}{f(\boldsymbol{\theta})}\right\}$$

- A nice thing is that, when $f(\cdot)$ is close to $\pi(\cdot|\boldsymbol{x})$, the acceptance probability can be close to 1.
- Principle of choosing $f(\cdot)$: Simulation from $f(\cdot)$ can easily cover the support of posterior density.
- Don't use uniform density for $f(\cdot)$, because it takes values in a bounded region and some values of θ will never be sampled.
- Similarly, don't use underdispersed density for $f(\cdot)$, e.g. $N(0, \Sigma)$ with very small Σ.
- Therefore, use overdispersed density for $f(\cdot)$, and tune it so that the higher the acceptance probability, the better.

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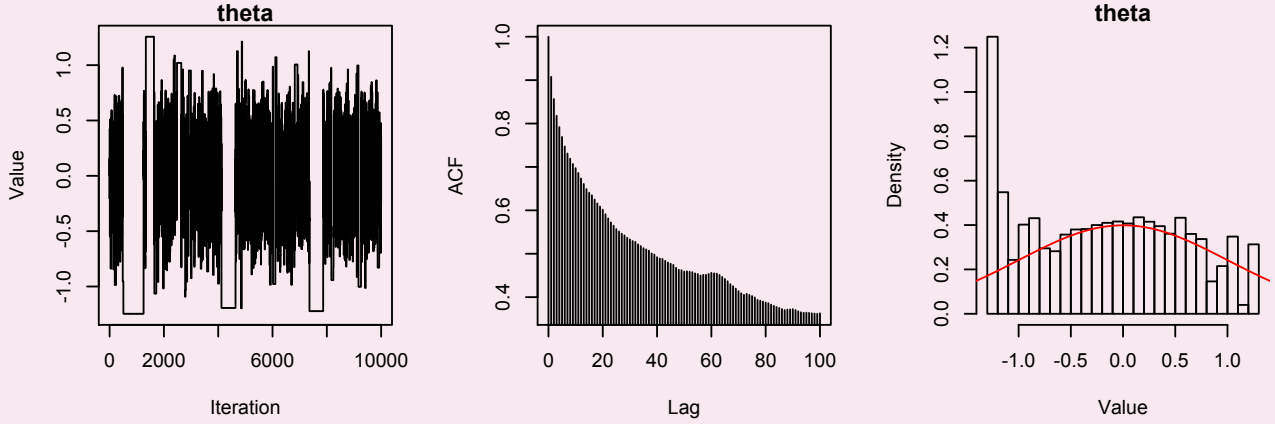
- Therefore, use overdispersed density for $f(\cdot)$, and tune it so that the higher the acceptance probability, the better.

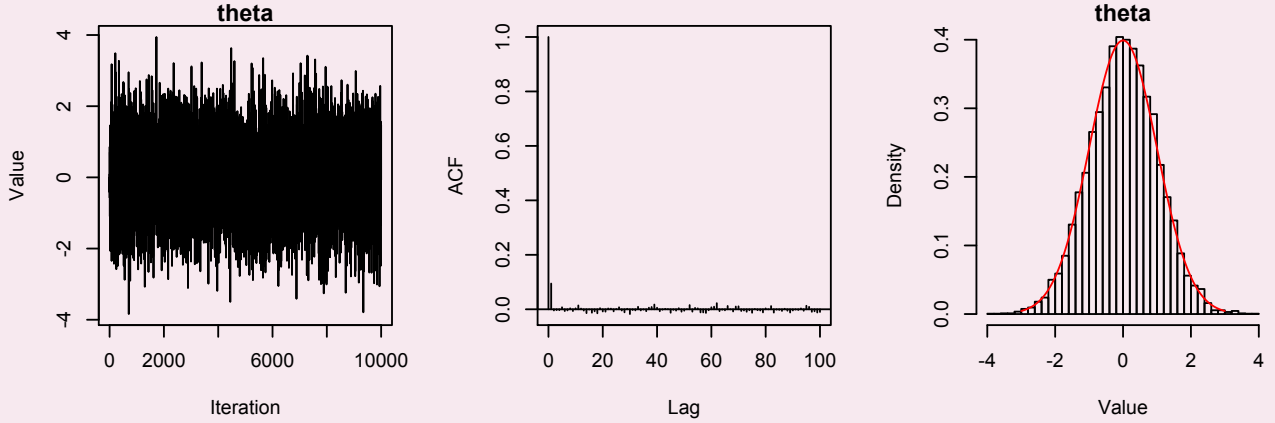
Sampling from a standard normal using normal independent chain

- Example: Consider the posterior is standard normal. Construct a Metropolis-Hastings algorithm using an independence chain with $f(\theta) = N(0, \Sigma)$.

  When $\Sigma = 0.1^2$, acceptance rate is 0.4.

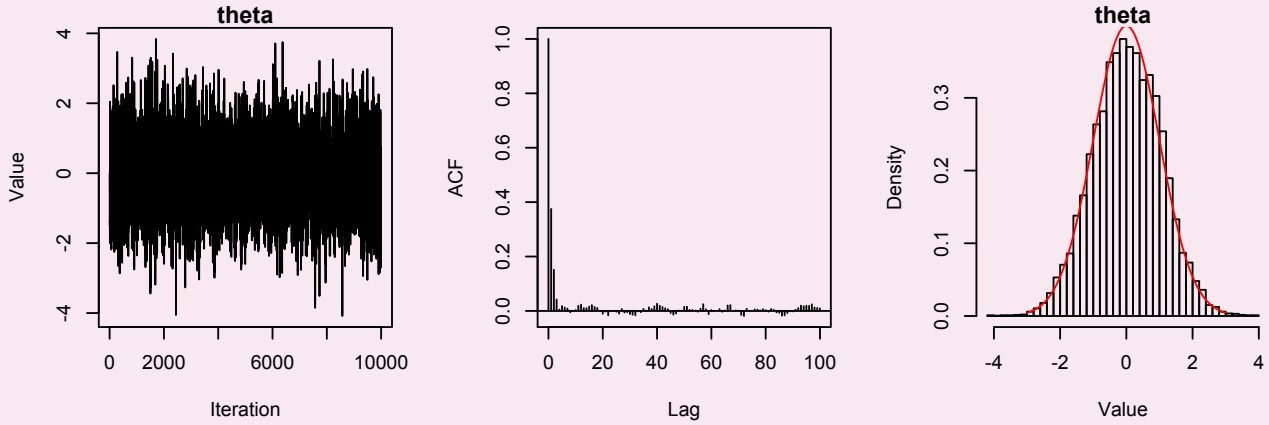


  $\Sigma = 1.6^2$, acceptance rate is 0.85.

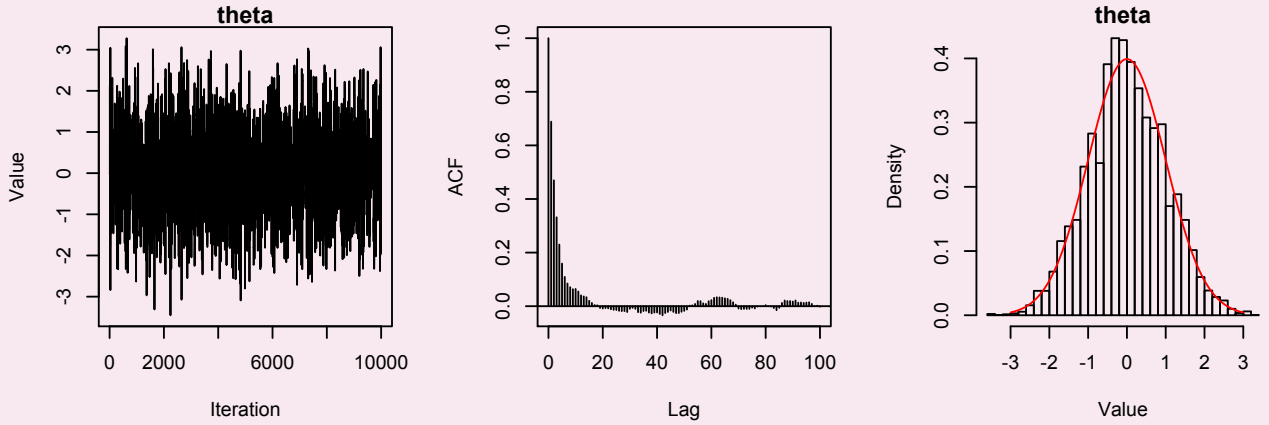


Sampling from a standard normal using normal independent chain

When $\Sigma = 6^2$, acceptance rate is 0.51.



$\Sigma = 30^2$, acceptance rate is 0.24.



- Choose $\Sigma = 1.6^2$ since the covered region is wide enough and the acceptance probability is the highest.
- Don't use underdispersed distribution, regardless its acceptance

Bayes Theorem via independence chains

- One possible choice for the proposal density is the prior density
- The acceptance probability is then

$$\alpha(\boldsymbol{\theta}, \boldsymbol{\theta}^*) = \min\left\{1, \frac{f(\boldsymbol{x}|\boldsymbol{\theta}^*)}{f(\boldsymbol{x}|\boldsymbol{\theta})}\right\},$$

  and hence depends only on the likelihood ratio of the proposal and the current value.
- It will not be underdispersed.

4.6 Hybrid methods

- The Metropolis-Hastings method in last section samples $\boldsymbol{\theta}$ in a single block, i.e. all parameters are updated at the same time.
- When the number of parameter is large, it is difficult to choose the proposal distribution. For example, when there are 5 parameters, the proposal distribution $N(0, \Sigma)$ has $5 \times 5 = 25$ tuning parameters in Σ.
- Recall the Gibbs sampler for how the componentwise update works.

4.6.1 Componentwise transitions

- Given a posterior distribution with FCDs that are awkward to sample from directly, we can define a Metropolis-Hastings scheme for each full conditional distribution, and apply them to each component in turn for each iteration
- This is like the Gibbs sampler, but each component update is a Metropolis-Hastings update, rather than a direct simulation from the FCD
- Each of these steps will require its own proposal distribution

Example

Componentwise Metropolist-Hasting algorithm in two-dimension.

Solution

...

The algorithm

1. Initialise the iteration counter to $j = 1$
   Initialise the state of the chain to $\boldsymbol{\theta}^{(0)} = (\theta_1^{(0)}, \ldots, \theta_p^{(0)})^T$
2. Let $\boldsymbol{\theta}_{-i}^{(j)} = \left(\theta_1^{(j)}, \ldots, \theta_{i-1}^{(j)}, \theta_{i+1}^{(j-1)}, \ldots, \theta_p^{(j-1)}\right)^T$, $i = 1, 2, \ldots, p$
   Obtain a new value $\boldsymbol{\theta}^{(j)}$ from $\boldsymbol{\theta}^{(j-1)}$ by successive generation of values
   - $\theta_1^{(j)} \sim \pi(\theta_1 | \boldsymbol{\theta}_{-1}^{(j)}, \boldsymbol{x})$ using a Metropolis–Hastings step with proposal distribution $q_1(\theta_1 | \theta_1^{(j-1)}, \boldsymbol{\theta}_{-1}^{(j)})$
   - $\theta_2^{(j)} \sim \pi(\theta_2 | \boldsymbol{\theta}_{-2}^{(j)}, \boldsymbol{x})$ using a Metropolis–Hastings step with proposal distribution $q_2(\theta_2 | \theta_2^{(j-1)}, \boldsymbol{\theta}_{-2}^{(j)})$

     $\vdots$
   - $\theta_p^{(j)} \sim \pi(\theta_p | \boldsymbol{\theta}_{-p}^{(j)}, \boldsymbol{x})$ using a Metropolis–Hastings step with proposal distribution $q_p(\theta_p | \theta_p^{(j-1)}, \boldsymbol{\theta}_{-p}^{(j)})$
3. Change counter j to $j + 1$, and return to step 2

The distributions $\pi(\theta_i | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})$ are just the FCDs

- Suppose we decide to use normal random walks for these M–H steps, that is, take $q_i(\theta_i^*|\theta_i, \boldsymbol{\theta}_{-i}^{(j)}) = N(\theta_i, \Sigma_{ij})$
- What is the appropriate value for Σ_{ij}?
- As the proposal in step j is targeting the conditional posterior density $\pi(\theta_i|\boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})$, the optimal choice of Σ_{ij} is

$$\Sigma_{ij} = \frac{2.38^2}{1} \, Var(\theta_i|\boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x}) = 2.38^2 \, Var(\theta_i|\boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})$$

- As these (conditional) posterior variances are not known before running the MCMC code, a sensible strategy might be to replace it with the (probably much larger) prior conditional variance or even the prior marginal variance, that is, use

$$\Sigma_{ij} = 2.38^2 \, Var(\theta_i|\boldsymbol{\theta}_{-i}^{(j)}) \qquad \text{or} \qquad \Sigma_{ij} = 2.38^2 \, Var(\theta_i)$$

- Again, recall that these values are to be used as a guide, generally to get the order of magnitude for the innovation variance

Hybrid methods

- The Gibbs sampler can be used to sample from multivariate posterior distributions provided that we can simulate from the full conditional distributions (FCDs). The acceptance probability is 1.
- The Metropolis-Hastings method can be used to sample from awkward FCDs. The acceptance probability is less than 1.
- We can combine these, when some FCDs can be simulated from directly and some can not, to increase the acceptance probability.

4.6.2 Metropolis within Gibbs

- Given a posterior distribution with full conditional distributions,
  - some of which may be simulated from directly,
  - and others of which have Metropolis-Hastings updating schemes,

  the Metropolis within Gibbs algorithm goes through each in turn, and simulates directly from the full conditional, or carries out a Metropolis-Hastings update as necessary
- This algorithm is, in fact, just the above algorithm but uses the full conditional distributions as the proposal distributions when they are easy to simulate from
- To see this, suppose that we can simulate from the FCD $\pi(\theta_i|\boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})$ and use this as the proposal distribution, that is, take $\theta_i^* \sim \pi(\theta_i|\boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})$

- Then the acceptance probability for this step is

$$
\begin{aligned}
\alpha(\theta_i, \theta_i^*) &= \min\left\{1, \frac{\pi(\theta_i^* | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})}{\pi(\theta_i | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})} \frac{q(\theta_i | \theta_i^*, \boldsymbol{\theta}_{-i}^{(j)})}{q(\theta_i^* | \theta_i, \boldsymbol{\theta}_{-i}^{(j)})}\right\} \\
&= \min\left\{1, \frac{\pi(\theta_i^* | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})}{\pi(\theta_i | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})} \frac{\pi(\theta_i | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})}{\pi(\theta_i^* | \boldsymbol{\theta}_{-i}^{(j)}, \boldsymbol{x})}\right\} \\
&= \min\{1, 1\} \\
&= 1,
\end{aligned}
$$

that is, we always accept the proposal from the FCD

Example 4.6

- Construct an MCMC scheme for the problem in Example 4.4 where we had a random sample of size n from a gamma $Ga(\alpha, \lambda)$ distribution and independent gamma $Ga(a, b)$ and $Ga(c, d)$ prior distributions for α and λ respectively
- Recall that the FCDs were

$$\pi(\alpha|\lambda, \boldsymbol{x}) \propto \frac{\alpha^{a-1} e^{(-b+n\log\bar{x}_g+n\log\lambda)\alpha}}{\Gamma(\alpha)^n}, \quad \alpha > 0$$

and

$$\pi(\lambda|\alpha, \boldsymbol{x}) \propto \lambda^{c+n\alpha-1}\, e^{-(d+n\bar{x})\lambda}, \quad \lambda > 0$$

Solution

...

R code

- Use the function `mwgGamma` in the `nclbayes` library
- Data: $n = 50$, $\bar{x} = 0.62$, $\bar{x}_g = 0.46$ and $s = 0.4$
- Prior: $a = 2$, $b = 1$, $c = 3$, $d = 1$
- Use a normal random walk proposal with variance $\Sigma_\alpha = 0.9^2$
- This gives a reasonable acceptance probability of 0.237

```
library(nclbayes)
posterior=mwgGamma(N=20000,initial=(xbar/s)^2,innov=0.9,
    priorparam=c(2,1,3,1),n=50,xbar=0.62,xgbar=0.46,show=TRUE)
mcmcAnalysis(posterior,rows=2,show=F)
posterior2=mcmcProcess(input=posterior,burnin=10,thin=20)
mcmcAnalysis(posterior2,rows=2)
```

- Using `burnin` $= 10$, `thin` $= 20$ produces (almost) un-autocorrelated posterior output

Analysis of MCMC output (all realisations)

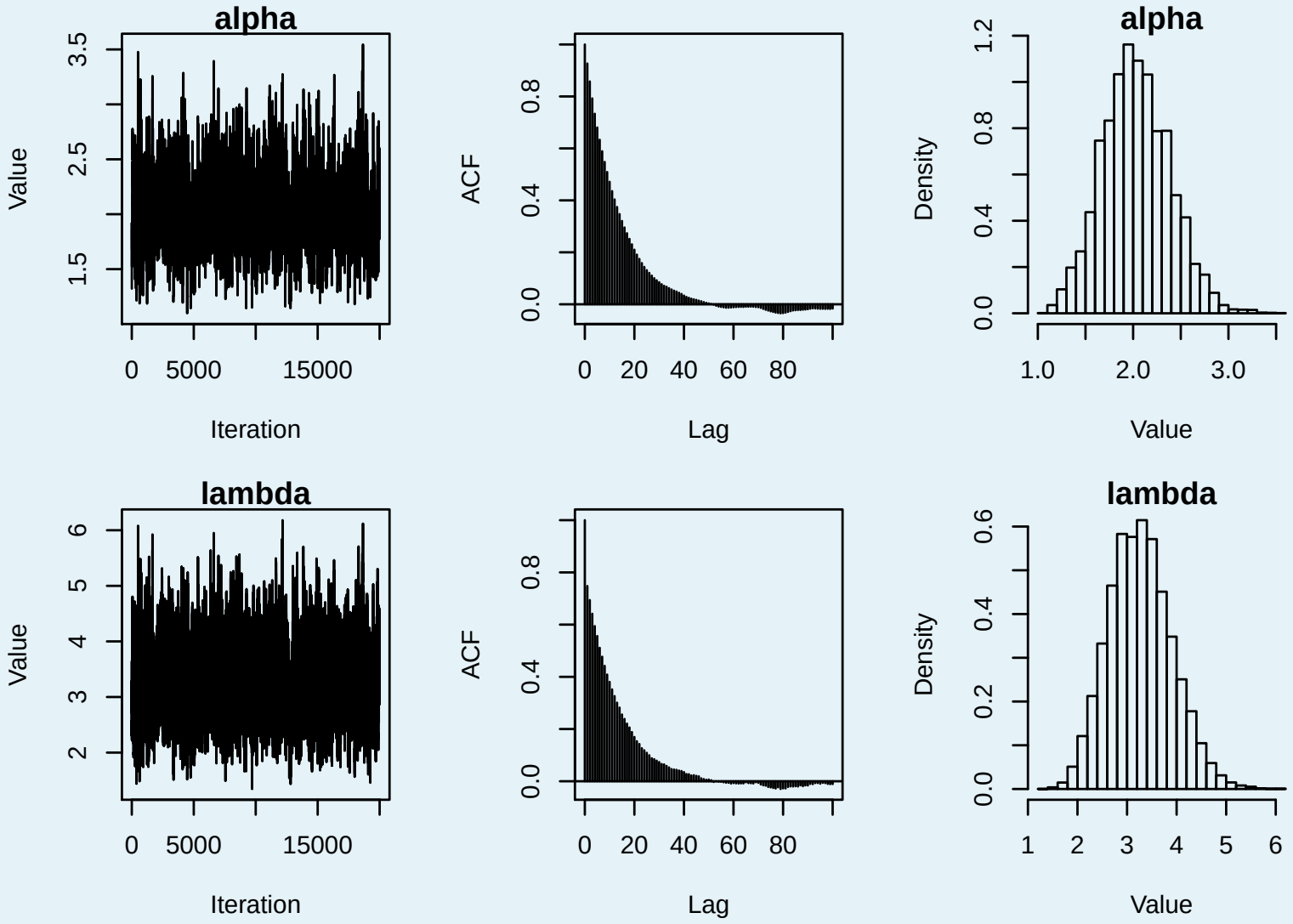


Figure: Trace plots, autocorrelation plots and histograms of the Metropolis within Gibbs sampler output

Analysis of MCMC output (with burnin = 10, thin = 20)

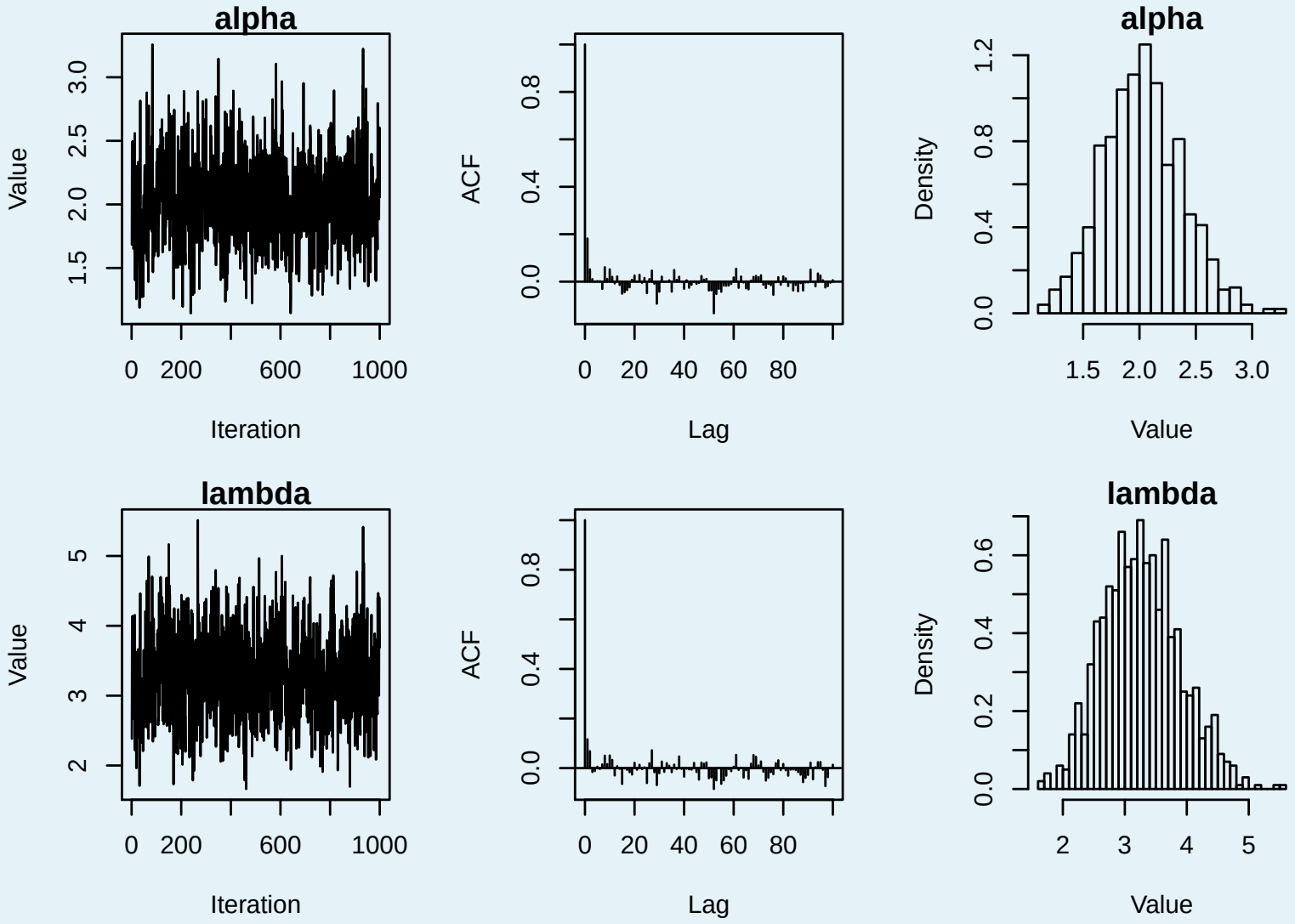


Figure: Trace plots, autocorrelation plots and histograms of the Metropolis within Gibbs sampler output

4.7 Summary

(i) Bayesian inference can be complicated when not using a conjugate prior distribution

(ii) One solution is to use Markov chain Monte Carlo (MCMC) methods

(iii) These work by producing realisations from the posterior distribution by constructing a Markov chain which has the posterior distribution as its stationary distribution

(iv) The MCMC methods we have studied are the Gibbs sampler, Metropolis within Gibbs algorithm and the Metropolis–Hastings algorithm

(v) When obtaining output from these algorithms, we need to assess whether there needs to be a burn-in and whether the output needs to be thinned (by looking at traceplots and autocorrelation plots) using `mcmcAnalysis` and `mcmcProcess`

(vi) The (converged and thinned) MCMC output are realisations from the posterior distribution. It can be used to

- obtain the posterior distribution for any (joint) functions of the parameters (such as $\sigma = 1/\sqrt{\tau}$ or $(\theta_1 = \mu - \tau, \theta_2 = e^{\mu+\tau/2})^T$)
- look at bivariate posterior distributions via scatter plots
- look at univariate marginal posterior distributions via histograms or boxplots
- obtain numerical summaries such as the mean, standard deviation and confidence intervals for single variables and correlations between variables

(vii) Equi-tailed posterior confidence intervals can be determined from the MCMC output using `mcmcCi`

4.8 Learning objectives

By the end of this chapter, you should be able to:

1. explain why not using a conjugate prior generally causes problems in determining the posterior distribution
2. describe the Gibbs sampler, explain why it is a Markov chain and give an outline as to why its stationary distribution is the posterior distribution
3. describe the issues of processing MCMC output (burn-in, autocorrelation, thinning etc.) and interpret numerical/graphical output
4. derive the full conditional densities for any posterior distribution and name these distributions if they are "standard" distributions given in the notes or on the exam paper

5. describe a Metropolis-Hastings algorithm in general terms and when using symmetric random walk proposals or independence proposals or general proposals
6. describe the hybrid methods: *componentwise transitions* and *Metropolis within Gibbs*
7. provide a detailed description of **any** of the MCMC algorithms as they apply to generating realisations from **any** posterior distribution