Linear Modeling, MSc Cognitive Systems

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These lecture notes cover the basic theory of linear models. My notes are heavily dependent on the MSc lecture notes in Statistics taught at the University of Sheffield, UK, and on the textbooks mentioned in these notes.

We begin by considering some facts about random variables. Then we look at how expectation and variance etc. are computed. Several typical probability distributions and their properties are discussed. The main topic of interest is maximum likelihood estimation. Then we cover the basic theory of linear models, generalized linear models, and linear mixed models. We close with a tutorial on Bayesian linear modeling.

Contents

1 Discrete random variables

A random variable X is a function $X : S \to \mathbb{R}$ that associates to each outcome $\omega \in S$ exactly one number $X(\omega) = x$.

S_X is all the x's (all the possible values of X, the support of X). I.e., $x \in S_X$.

Good example: number of coin tosses till H

- $X : \omega \to x$
- ω: H, TH, TTH,... (infinite)
- $x = 0, 1, 2, \ldots; x \in S_X$

Every discrete random variable X has associated with it a **probability mass/distribution function (PDF)**, also called **distribution function**.

$$p_X : S_X \to [0, 1] \tag{1}$$

defined by

$$p_X(x) = P(X(\omega) = x), x \in S_X \tag{2}$$

[**Note**: Books sometimes abuse notation by overloading the meaning of X. They usually have: $p_X(x) = P(X = x), x \in S_X$]

The **cumulative distribution function** is

$$F(a) = \sum_{\text{all } x \leq a} p(x) \tag{3}$$

1.1 Example: The Binomial random variable

Suppose that n independent trials are performed, there are two possible outcomes, success and failure, each with probability θ and $(1 - \theta)$ respectively.

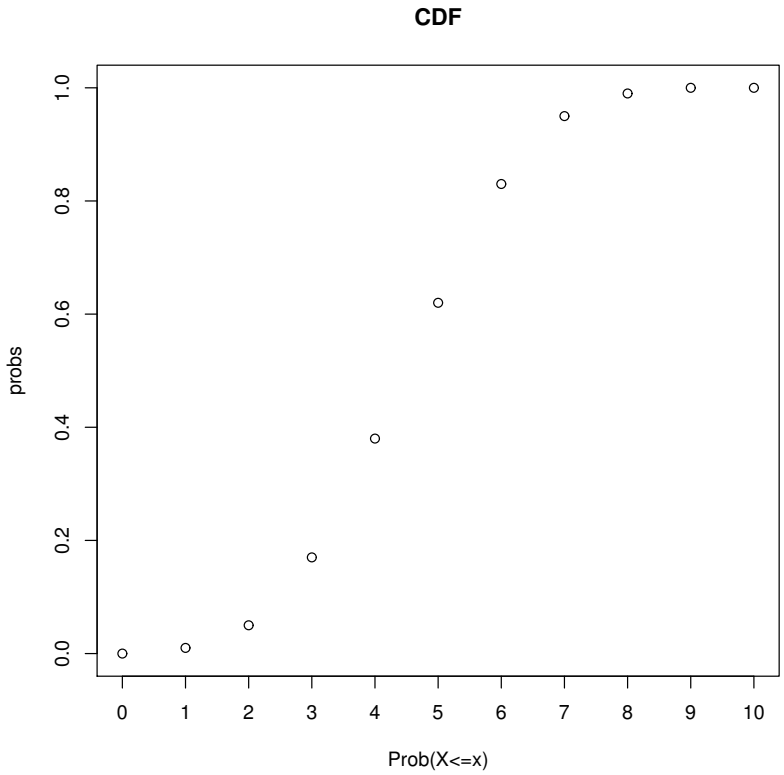
Then, the probability of x successes out of n is:

$$P(X = x) = \binom{n}{x} \theta^x (1 - \theta)^{n-x} \tag{4}$$

Example: n=10 coin tosses. What's the prob. of 1 or fewer successes? 2 or fewer? Let's just compute the probability of getting x or fewer successes where x=0 to 10. For this, we use the built in CDF function `pbinom`.

```r
## sample size
n<-10
## prob of success
p<-0.5
probs<-rep(NA,11)
for(x in 0:10){
  ## Cumulative Distribution Function:
probs[x+1]<-round(pbinom(x,size=n,prob=p),digits=2)
}
```

```r
## Plot the CDF:
plot(1:11,probs,xaxt="n",xlab="Prob(X<=x)",main="CDF")
axis(1,at=1:11,labels=0:10)
```

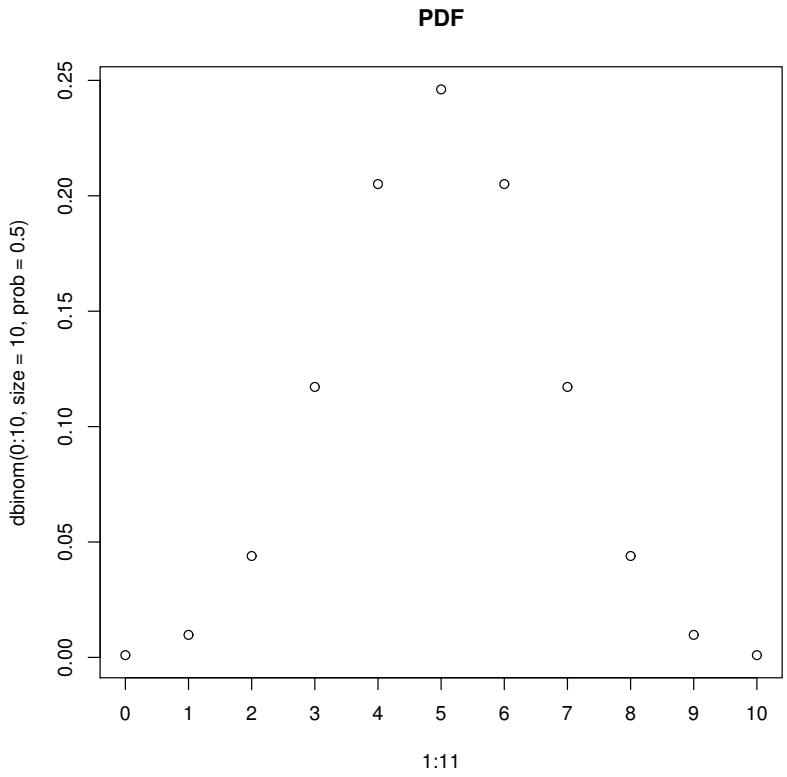


The probability of getting exactly 1 success: P(X=1).

```r
pbinom(1,size=10,prob=0.5)-pbinom(0,size=10,prob=0.5)

## [1] 0.009765625

choose(10,1) * 0.5 * (1-0.5)^9

## [1] 0.009765625
```

What about the PDF? The built-in function in R is `dbinom`:

```
## P(X=0)
dbinom(0,size=10,prob=0.5)

## [1] 0.0009765625

## Plot the pdf:
plot(1:11,dbinom(0:10,size=10,prob=0.5),main="PDF",
     xaxt="n")
axis(1,at=1:11,labels=0:10)
```



To summarize, a discrete random variable X will be defined by

1. the function $X : S \to \mathbb{R}$, where S is the set of outcomes (i.e., outcomes are $\omega in S$).
2. $X(\omega) = x$, and S_X is the **support** of X (i.e., $x \in S_X$).
3. A PDF is defined for X:

$$p_X : S_X \to [0, 1]$$

4. A CDF is defined for X:

$$F(a) = \sum_{\text{all } x \leq a} p(x)$$

2 *Continuous random variables*

As mentioned above in the discrete case, a random variable X is a function $X : S \to \mathbb{R}$ that associates to each outcome $\omega \in S$ exactly one number $X(\omega) = x$. S_X is all the x's (all the possible values of X, the support of X). I.e., $x \in S_X$.

X is a continuous random variable if there is a non-negative function f defined for all real $x \in (-\infty, \infty)$ having the property that for any set B of real numbers,

$$P\{X \in B\} = \int_B f(x)\, dx \tag{5}$$

Kerns has the following to add about the above:

> Continuous random variables have supports that look like
>
> $$S_X = [a, b] \text{ or } (a, b), \tag{6}$$
>
> or unions of intervals of the above form. Examples of random variables that are often taken to be continuous are:
>
> - the height or weight of an individual,
> - other physical measurements such as the length or size of an object, and
> - durations of time (usually).
>
> Every continuous random variable X has a probability density function (PDF) denoted f_X associated with it that satisfies three basic properties:
>
> 1. $f_X(x) > 0$ for $x \in S_X$,
> 2. $\int_{x \in S_X} f_X(x)\, \mathrm{d}x = 1$, and
> 3. $P(X \in A) = \int_{x \in A} f_X(x)\, \mathrm{d}x$, for an event $A \subset S_X$.
>
> We can say the following about continuous random variables:
>
> - Usually, the set A in condition 3 above takes the form of an interval, for example, $A = [c, d]$, in which case
>
> $$\mathbb{P}(X \in A) = \int_c^d f_X(x)\, \mathrm{d}x. \tag{7}$$
>
> - It follows that the probability that X falls in a given interval is simply the area under the curve of f_X over the interval.
> - Since the area of a line $x = c$ in the plane is zero, $\mathbb{P}(X = c) = 0$ for any value c. In other words, the chance that X equals a particular value c is zero, and this is true for any number c. Moreover, when $a < b$ all of the following probabilities are the same:
>
> $$\mathbb{P}(a \leq X \leq b) = \mathbb{P}(a < X \leq b) = \mathbb{P}(a \leq X < b) = \mathbb{P}(a < X < b). \tag{8}$$

- The PDF f_X can sometimes be greater than 1. This is in contrast to the discrete case; every nonzero value of a PMF is a probability which is restricted to lie in the interval $[0, 1]$.

$f(x)$ is the probability density function of the random variable X. Since X must assume some value, f must satisfy

$$1 = P\{X \in (-\infty, \infty)\} = \int_{-\infty}^{\infty} f(x)\, dx \tag{9}$$

If $B = [a, b]$, then

$$P\{a \leq X \leq b\} = \int_a^b f(x)\, dx \tag{10}$$

If $a = b$, we get

$$P\{X = a\} = \int_a^a f(x)\, dx = 0 \tag{11}$$

Hence, for any continuous random variable,

$$P\{X < a\} = P\{X \leq a\} = F(a) = \int_{-\infty}^{a} f(x)\, dx \tag{12}$$

F is the **cumulative distribution function**. Differentiating both sides in the above equation:

$$\frac{dF(a)}{da} = f(a) \tag{13}$$

The density (PDF) is the derivative of the CDF. In the discrete case [1] (p. 128):

$$f_X(x) = F_X(x) - \lim_{t \to x^-} F_X(t) \tag{14}$$

Ross[2] suggests that it is more intuitive to think about it as follows:

$$P\{a - \frac{\epsilon}{2} \leq X \leq a + \frac{\epsilon}{2}\} = \int_{a-\epsilon/2}^{a+\epsilon/2} f(x)\, dx \approx \epsilon f(a) \tag{15}$$

when ϵ is small and when $f(\cdot)$ is continuous. I.e., $\epsilon f(a)$ is the approximate probability that X will be contained in an interval of length ϵ around the point a.

[1] G. Jay Kerns. *Introduction to Probability and Statistics Using R*. 2010

[2] Sheldon Ross. *A first course in probability*. Pearson Education, 2002

2.1 *Example 1: Normal random variable*

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}, \quad -\infty < x < \infty. \tag{16}$$

We write $X \sim \texttt{norm}(\texttt{mean} = \mu, \texttt{sd} = \sigma)$, and the associated R function for the PDF is `dnorm(x, mean = 0, sd = 1)`, and the one for CDF is `pnorm`.

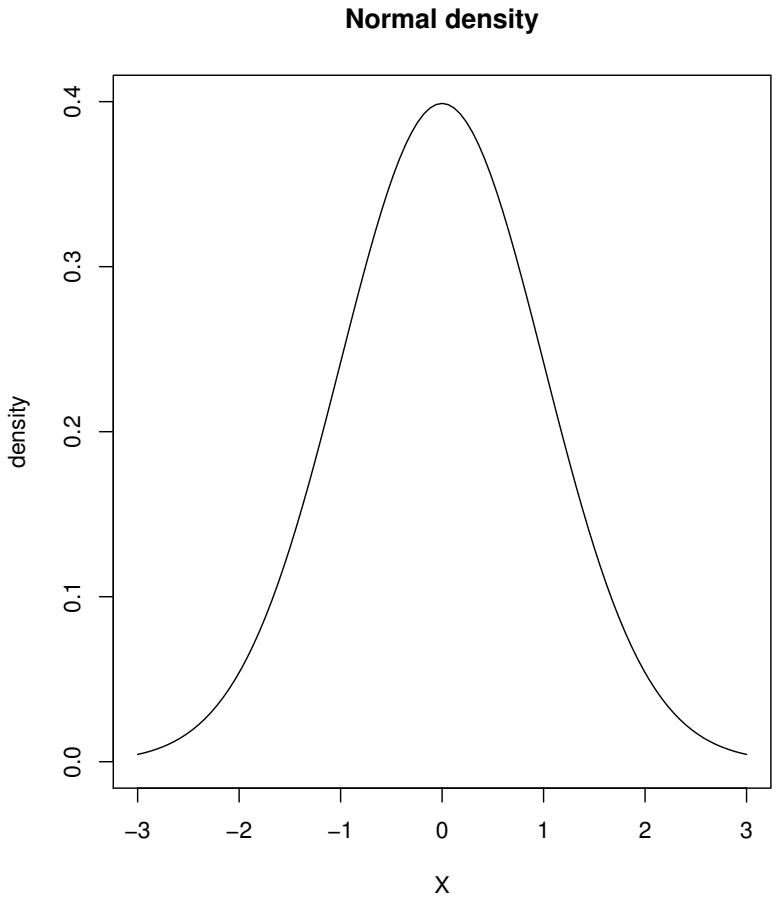


Figure 1: Normal distribution.

Note the default values for μ and σ as 0 and 1 respectively. Note also that R defines the PDF in terms of μ and σ, not μ and σ^2.

Computing probabilities using the CDF:

```
pnorm(Inf)-pnorm(-Inf)

## [1] 1

pnorm(2)-pnorm(-2)

## [1] 0.9544997

pnorm(1)-pnorm(-1)

## [1] 0.6826895
```

Standard or unit normal random variable If X is normally distributed with parameters μ and σ^2, then $Z = (X - \mu)/\sigma$ is normally distributed with parameters $\mu = 0, \sigma^2 = 1$.

We conventionally write $\Phi(x)$ for the CDF:

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{\frac{-y^2}{2}} dy \quad \text{where } y = (x - \mu)/\sigma \tag{17}$$

For example: $\Phi(2)$:

```
pnorm(2)

## [1] 0.9772499
```

For negative x we do:

$$\Phi(-x) = 1 - \Phi(x), \quad -\infty < x < \infty \tag{18}$$

In R:

```
1-pnorm(2)

## [1] 0.02275013

## alternatively:
pnorm(2,lower.tail=F)

## [1] 0.02275013
```

If Z is a standard normal random variable (SNRV) then

$$p\{Z \leq -x\} = P\{Z > x\}, \quad -\infty < x < \infty \tag{19}$$

Since $Z = ((X - \mu)/\sigma)$ is an SNRV whenever X is normally distributed with parameters μ and σ^2, then the CDF of X can be expressed as:

$$F_X(a) = P\{X \leq a\} = P\left(\frac{X - \mu}{\sigma} \leq \frac{a - \mu}{\sigma}\right) = \Phi\left(\frac{a - \mu}{\sigma}\right) \tag{20}$$

The standardized version of a normal random variable X is used to compute specific probabilities relating to X (it's also easier to compute probabilities from different CDFs so that the two computations are comparable).

3 *Expectations and Variances*

3.1 *Expectations and variances of discrete RVs*

The expectation can be seen as the long-run average value.

```r
x<-0:10
## expectation in our binomial example:
sum(x*dbinom(x,size=10,prob=0.5))

## [1] 5
```

$$E[X] = \sum_{i=1}^{n} x_i p(x_i) \tag{21}$$

In the binomial case, $E[X] = np$.
(Proof: see https://proofwiki.org/wiki/Expectation_of_Binomial_Distribution)

$$Var(X) = E[(X - \mu)^2] \tag{22}$$

In the binomial case, $Var(X) = np(1-p)$.
(Proof: see https://proofwiki.org/wiki/Variance_of_Binomial_Distribution)

3.2 *Expectations and variances of continuous RVs*

$$E[X] = \int_{-\infty}^{\infty} x f(x)\, dx \tag{23}$$

$$Var[X] = E[(X - \mu)^2] = E[X^2] - (E[X])^2 \tag{24}$$

3.3 *Example: The expectation and variance of the standard normal RV*

Expectation

$$E[Z] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x e^{-x^2/2}\, dx$$

Let $u = -x^2/2$.
Then, $du/dx = -2x/2 = -x$. I.e., $du = -x\, dx$ or $-du = x\, dx$.
We can rewrite the integral as:

$$E[Z] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^u x\, dx$$

Replacing $x\, dx$ with $-du$ we get:

$$-\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^u\, du$$

which yields:

$$-\frac{1}{\sqrt{2\pi}} [e^u]_{-\infty}^{\infty}$$

Replacing u with $-x^2/2$ we get:

$$-\frac{1}{\sqrt{2\pi}} [e^{-x^2/2}]_{-\infty}^{\infty} = 0$$

Variance We know that

$$\mathrm{Var}(Z) = E[Z^2] - (E[Z])^2$$

Since $(E[Z])^2 = 0$ (see immediately above), we have

$$\mathrm{Var}(Z) = E[Z^2] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underset{\text{This is } Z^2.}{\overset{\uparrow}{x^2}} e^{-x^2/2}\, dx$$

Write x^2 as $x \times x$ and use integration by parts:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underset{u}{\overset{\uparrow}{x}} \underset{dv/dx}{\overset{\uparrow}{x e^{-x^2/2}}}\, dx = \frac{1}{\sqrt{2\pi}} \underset{u}{\overset{\uparrow}{x}} \underset{v}{\overset{\uparrow}{-e^{-x^2/2}}} - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underset{v}{\overset{\uparrow}{-e^{-x^2/2}}} \underset{du/dx}{\overset{\uparrow}{1}}\, dx = 1$$

[Explained in p. 274 of Grinstead and Snell[3]: "The first summand above can be shown to equal 0, since as $x \to \pm\infty$, $e^{-x^2/2}$ gets small more quickly than x gets large. The second summand is just the standard normal density integrated over its domain, so the value of this summand is 1. Therefore, the variance of the standard normal density equals 1."

[3] C.M. Grinstead and J.L. Snell. *Introduction to probability*. American Mathematical Society, 1997

4 *Some useful continuous distributions*

4.1 *Exponential random variables*

For some $\lambda > 0$,

$$f(x) = \begin{cases} \lambda e^{-\lambda x} & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases}$$

A continuous random variable with the above PDF is an exponential random variable (or is said to be exponentially distributed).

The CDF:

$$\begin{aligned} F(a) =& P(X \leq a) \\ =& \int_0^a \lambda e^{-\lambda x}\, dx \\ =& \left[-e^{-\lambda x}\right]_0^a \\ =& 1 - e^{-\lambda a} \quad a \geq 0 \end{aligned}$$

[Note: the integration requires the u-substitution: $u = -\lambda x$, and then $du/dx = -\lambda$, and then use $-du = \lambda dx$ to solve.]

Expectation and variance of an exponential random variable For some $\lambda > 0$ (called the rate), if we are given the PDF of a random variable X:

$$f(x) = \begin{cases} \lambda e^{-\lambda x} & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases}$$

Find E[X].

[This proof seems very strange and arbitrary—one starts really generally and then scales down, so to speak. The standard method can equally well be used, but this is more general, it allows for easy calculation of the second moment, for example. Also, it's an example of how reduction formulae are used in integration.]

$$E[X^n] = \int_0^\infty x^n \lambda e^{-\lambda x}\, dx$$

Use integration by parts:

Let $u = x^n$, which gives $du/dx = nx^{n-1}$. Let $dv/dx = \lambda e^{-\lambda x}$, which gives $v = -e^{-\lambda x}$. Therefore:

$$\begin{aligned} E[X^n] &= \int_0^\infty x^n \lambda e^{-\lambda x}\, dx \\ &= \left[-x^n e^{-\lambda x}\right]_0^\infty + \int_0^\infty e^{\lambda x} n x^{n-1}\, dx \\ &= 0 + \frac{n}{\lambda} \int_0^\infty \lambda e^{-\lambda x} n^{n-1}\, dx \end{aligned}$$

Thus,

$$E[X^n] = \frac{n}{\lambda} E[X^{n-1}]$$

If we let $n = 1$, we get $E[X]$:

$$E[X] = \frac{1}{\lambda}$$

Note that when $n = 2$, we have

$$E[X^2] = \frac{2}{\lambda} E[X] = \frac{2}{\lambda^2}$$

Variance is, as usual,

$$var(X) = E[X^2] - (E[X])^2 = \frac{2}{\lambda^2} - (\frac{1}{\lambda})^2 = \frac{1}{\lambda^2}$$

4.2 *Weibull distribution*

$$f(x \mid \alpha, \beta) = \alpha\beta(\beta x)^{\alpha-1} \exp(-(\beta x)^\alpha) \tag{25}$$

When $\alpha = 1$, we have the exponential distribution.

4.3 Gamma distribution

[The text is an amalgam of Kerns[4] and RossRossProb. I don't put it in double-quotes as a citation because it would look ugly.]

[4] G. Jay Kerns. *Introduction to Probability and Statistics Using R*. 2010

This is a generalization of the exponential distribution. We say that X has a gamma distribution and write $X \sim \texttt{gamma}(\texttt{shape} = \alpha, \texttt{rate} = \lambda)$, where $\alpha > 0$ (called shape) and $\lambda > 0$ (called rate). It has PDF

$$f(x) = \begin{cases} \frac{\lambda e^{-\lambda x}(\lambda x)^{\alpha-1}}{\Gamma(\alpha)} & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases}$$

$\Gamma(\alpha)$ is called the gamma function:

$$\Gamma(\alpha) = \int_0^\infty e^{-y} y^{\alpha-1}\, dy \underset{\text{integration by parts}}{=} (\alpha-1)\Gamma(\alpha-1)$$

Note that for integral values of n, $\Gamma(n) = (n-1)!$ (follows from above equation).

The associated R functions are `gamma(x, shape, rate = 1)`, `pgamma`, `qgamma`, and `rgamma`, which give the PDF, CDF, quantile function, and simulate random variates, respectively. If $\alpha = 1$ then $X \sim \texttt{exp}(\texttt{rate} = \lambda)$. The mean is $\mu = \alpha/\lambda$ and the variance is $\sigma^2 = \alpha/\lambda^2$.

To motivate the gamma distribution recall that if X measures the length of time until the first event occurs in a Poisson process with rate λ then $X \sim \texttt{exp}(\texttt{rate} = \lambda)$. If we let Y measure the length of time until the α^{th} event occurs then $Y \sim \texttt{gamma}(\texttt{shape} = \alpha, \texttt{rate} = \lambda)$. When α is an integer this distribution is also known as the **Erlang** distribution.

The Chi-squared distribution is the gamma distribution with $\lambda = 1/2$ and $\alpha = n/2$, where n is an integer:

Mean and variance of gamma distribution Let X be a gamma random variable with parameters α and λ.

$$\begin{aligned} E[X] &= \frac{1}{\Gamma(\alpha)} \int_0^\infty x\lambda e^{-\lambda x}(\lambda x)^{\alpha-1}\, dx \\ &= \frac{1}{\lambda\Gamma(\alpha)} \int_0^\infty e^{-\lambda x}(\lambda x)^{\alpha}\, dx \\ &= \frac{\Gamma(\alpha+1)}{\lambda\Gamma(\alpha)} \\ &= \frac{\alpha}{\lambda} \end{aligned}$$

(See derivation of $\Gamma(\alpha)$, p. 215 of [5].)

[5] Sheldon Ross. *A first course in probability*. Pearson Education, 2002

It is easy to show (exercise) that

$$Var(X) = \frac{\alpha}{\lambda^2}$$

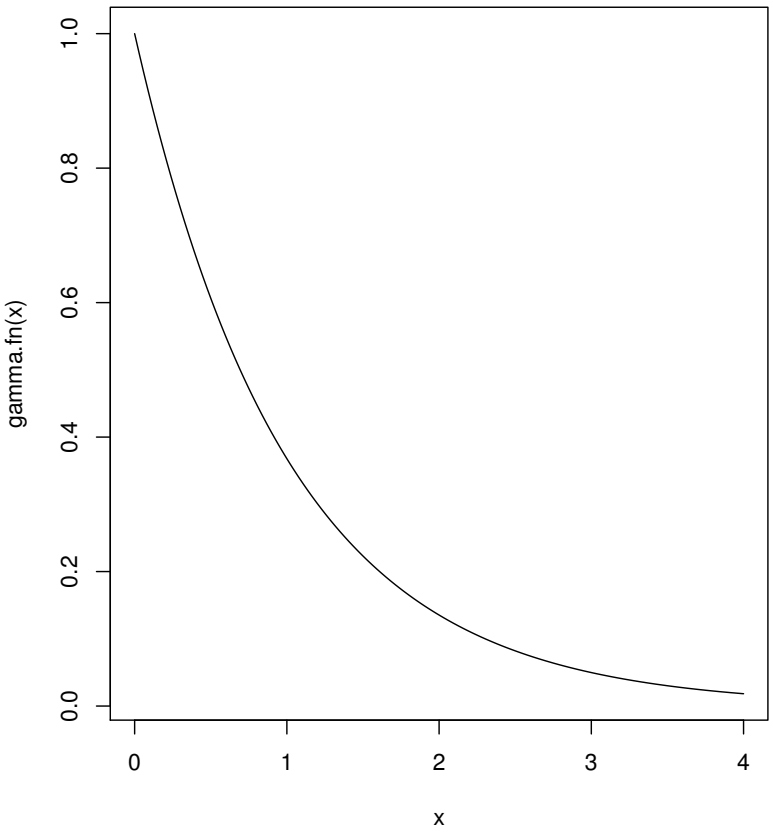


Figure 2: The gamma distribution.

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4.4 *Uniform random variable*

A random variable (X) with the continuous uniform distribution on the interval (α, β) has PDF

$$f_X(x) = \begin{cases} \frac{1}{\beta-\alpha}, & \alpha < x < \beta, \\ 0, & \text{otherwise} \end{cases} \tag{26}$$

The associated R function is $\mathsf{dunif}(\mathtt{min} = a, \mathtt{max} = b)$. We write $X \sim \mathsf{unif}(\mathtt{min} = a, \mathtt{max} = b)$. Due to the particularly simple form of this PDF we can also write down explicitly a formula for the CDF F_X:

$$F_X(a) = \begin{cases} 0, & a < 0, \\ \frac{a-\alpha}{\beta-\alpha}, & \alpha \leq t < \beta, \\ 1, & a \geq \beta. \end{cases} \tag{27}$$

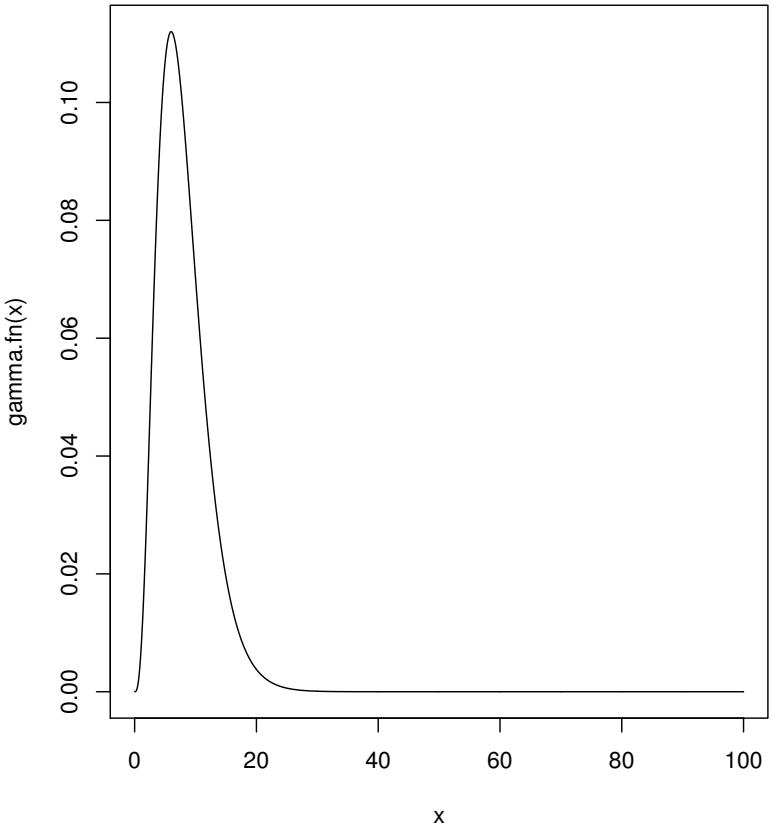


Figure 3: The chi-squared distribution.

$$E[X] = \frac{\beta + \alpha}{2} \tag{28}$$

$$Var(X) = \frac{(\beta - \alpha)^2}{12} \tag{29}$$

4.5 Beta distribution

This is a generalization of the continuous uniform distribution.

$$f(x) = \begin{cases} \frac{1}{B(a,b)} x^{a-1}(1-x)^{b-1} & \text{if } 0 < x < 1 \\ 0 & \text{otherwise} \end{cases}$$

where

$$B(a,b) = \int_0^1 x^{a-1}(1-x)^{b-1}\, dx$$

There is a connection between the beta and the gamma:

$$B(a,b) = \int_0^1 x^{a-1}(1-x)^{b-1}\,dx = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

which allows us to rewrite the beta PDF as

$$f(x) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\,x^{a-1}(1-x)^{b-1}, \quad 0 < x < 1. \tag{30}$$

The mean and variance are

$$E[X] = \frac{a}{a+b} \text{ and } Var(X) = \frac{ab}{(a+b)^2\,(a+b+1)}. \tag{31}$$

5 *Jointly distributed random variables*

5.1 *Discrete case*

[This section is an extract from Kerns. I omit quotes as that would make the text harder to read.]

Consider two discrete random variables X and Y with PMFs f_X and f_Y that are supported on the sample spaces S_X and S_Y, respectively. Let $S_{X,Y}$ denote the set of all possible observed **pairs** (x, y), called the **joint support set** of X and Y. Then the **joint probability mass function** of X and Y is the function $f_{X,Y}$ defined by

$$f_{X,Y}(x,y) = \mathbb{P}(X = x,\, Y = y), \quad \text{for } (x,y) \in S_{X,Y}. \tag{32}$$

Every joint PMF satisfies

$$f_{X,Y}(x,y) > 0 \text{ for all } (x,y) \in S_{X,Y}, \tag{33}$$

and

$$\sum_{(x,y)\in S_{X,Y}} f_{X,Y}(x,y) = 1. \tag{34}$$

It is customary to extend the function $f_{X,Y}$ to be defined on all of $\mathbb{R}^2$ by setting $f_{X,Y}(x,y) = 0$ for $(x,y) \notin S_{X,Y}$.

In the context of this chapter, the PMFs f_X and f_Y are called the **marginal PMFs** of X and Y, respectively. If we are given only the joint PMF then we may recover each of the marginal PMFs by using the Theorem of Total Probability:

$$\begin{aligned} f_X(x) &= \mathbb{P}(X = x), && (35)\\ &= \sum_{y\in S_Y} \mathbb{P}(X = x,\, Y = y), && (36)\\ &= \sum_{y\in S_Y} f_{X,Y}(x,y). && (37) \end{aligned}$$

By interchanging the roles of X and Y it is clear that

$$f_Y(y) = \sum_{x \in S_X} f_{X,Y}(x, y). \tag{38}$$

Given the joint PMF we may recover the marginal PMFs, but the converse is not true. Even if we have **both** marginal distributions they are not sufficient to determine the joint PMF; more information is needed.

Associated with the joint PMF is the **joint cumulative distribution function** $F_{X,Y}$ defined by

$$F_{X,Y}(x, y) = \mathbb{P}(X \leq x,\, Y \leq y), \quad \text{for } (x, y) \in \mathbb{R}^2.$$

The bivariate joint CDF is not quite as tractable as the univariate CDFs, but in principle we could calculate it by adding up quantities of the form in Equation 32. The joint CDF is typically not used in practice due to its inconvenient form; one can usually get by with the joint PMF alone.

Example: Discrete bivariate case Roll a fair die twice. Let X be the face shown on the first roll, and let Y be the face shown on the second roll. For this example, it suffices to define

$$f_{X,Y}(x, y) = \frac{1}{36}, \quad x = 1, \ldots, 6,\ y = 1, \ldots, 6.$$

The marginal PMFs are given by $f_X(x) = 1/6$, $x = 1, 2, \ldots, 6$, and $f_Y(y) = 1/6$, $y = 1, 2, \ldots, 6$, since

$$f_X(x) = \sum_{y=1}^{6} \frac{1}{36} = \frac{1}{6}, \quad x = 1, \ldots, 6,$$

and the same computation with the letters switched works for Y.

Here, and in many other ones, the joint support can be written as a product set of the support of X "times" the support of Y, that is, it may be represented as a cartesian product set, or rectangle, $S_{X,Y} = S_X \times S_Y$, where $S_X \times S_Y = \{(x, y) :\ x \in S_X,\, y \in S_Y\}$. This form is a necessary condition for X and Y to be **independent** (or alternatively **exchangeable** when $S_X = S_Y$). But please note that in general it is not required for $S_{X,Y}$ to be of rectangle form.

5.2 *Continuous case*

For random variables X and y, the **joint cumulative pdf** is

$$F(a, b) = P(X \leq a, Y \leq b) \quad -\infty < a, b < \infty \tag{39}$$

The **marginal distributions** of F_X and F_Y are the CDFs of each of the associated RVs:

1. The CDF of X:

$$F_X(a) = P(X \leq a) = F_X(a, \infty) \tag{40}$$

2. The CDF of Y:

$$F_Y(a) = P(Y \leq b) = F_Y(\infty, b) \tag{41}$$

Definition 1 ***Jointly continuous****: Two RVs X and Y are jointly continuous if there exists a function $f(x, y)$ defined for all real x and y, such that for every set C:*

$$P((X, Y) \in C) = \iint\limits_{(x,y)\in C} f(x, y)\, dx\, dy \tag{42}$$

*$f(x, y)$ is the **joint PDF** of X and Y.*
Every joint PDF satisfies

$$f(x, y) \geq 0 \text{ for all } (x, y) \in S_{X,Y}, \tag{43}$$

and

$$\iint\limits_{S_{X,Y}} f(x, y)\, \mathrm{d}x\, \mathrm{d}y = 1. \tag{44}$$

For any sets of real numbers A and B, and if $C = \{(x, y) : x \in A, y \in B\}$, it follows from equation 42 that

$$P((X \in A, Y \in B) \in C) = \int_B \int_A f(x, y)\, dx\, dy \tag{45}$$

Note that

$$F(a, b) = P(X \in (-\infty, a]), Y \in (-\infty, b])) = \int_{-\infty}^{b} \int_{-\infty}^{a} f(x, y)\, dx\, dy \tag{46}$$

Differentiating, we get the joint pdf:

$$f(a, b) = \frac{\partial^2}{\partial a \partial b} F(a, b) \tag{47}$$

One way to understand the joint PDF:

$$P(a < X < a + da, b < Y < b + db) = \int_b^{d+db} \int_a^{a+da} f(x, y)\, dx\, dy \approx f(a, b) dadb \tag{48}$$

Hence, $f(x, y)$ is a measure of how probable it is that the random vector (X, Y) will be near (a, b).

5.3 Marginal probability distribution functions

If X and Y are jointly continuous, they are individually continuous, and their PDFs are:

$$\begin{aligned} P(X \in A) =& P(X \in A, Y \in (-\infty, \infty)) \\ =& \int_A \int_{-\infty}^{\infty} f(x,y)\, dy\, dx \\ =& \int_A f_X(x)\, dx \end{aligned} \tag{49}$$

where

$$f_X(x) = \int_{-\infty}^{\infty} f(x,y)\, dy \tag{50}$$

Similarly:

$$f_Y(y) = \int_{-\infty}^{\infty} f(x,y)\, dx \tag{51}$$

5.4 Independent random variables

Random variables X and Y are independent iff, for any two sets of real numbers A and B:

$$P(X \in A, Y \in B) = P(X \in A)P(Y \in B) \tag{52}$$

In the jointly continuous case:

$$f(x,y) = f_X(x) f_Y(y) \quad \text{for all } x, y \tag{53}$$

A necessary and sufficient condition for the random variables X and Y to be independent is for their joint probability density function (or joint probability mass function in the discrete case) $f(x,y)$ to factor into two terms, one depending only on x and the other depending only on y.

Easy-to-understand example from Kerns Let the joint PDF of (X,Y) be given by

$$f_{X,Y}(x,y) = \frac{6}{5}\left(x + y^2\right), \quad 0 < x < 1,\ 0 < y < 1.$$

The marginal PDF of X is

$$\begin{aligned} f_X(x) &= \int_0^1 \frac{6}{5}\left(x+y^2\right)\,\mathrm{d}y, \\ &= \frac{6}{5}\left(xy+\frac{y^3}{3}\right)\Big|_{y=0}^{1}, \\ &= \frac{6}{5}\left(x+\frac{1}{3}\right), \end{aligned}$$

for $0 < x < 1$, and the marginal PDF of Y is

$$\begin{aligned} f_Y(y) &= \int_0^1 \frac{6}{5}\left(x+y^2\right)\,\mathrm{d}x, \\ &= \frac{6}{5}\left(\frac{x^2}{2}+xy^2\right)\Big|_{x=0}^{1}, \\ &= \frac{6}{5}\left(\frac{1}{2}+y^2\right), \end{aligned}$$

for $0 < y < 1$.

In this example the joint support set was a rectangle $[0,1] \times [0,1]$, but it turns out that X and Y are not independent. This is because $\frac{6}{5}\left(x+y^2\right)$ cannot be stated as a product of two terms ($f_X(x)f_Y(y)$).

5.5 Sums of independent random variables

[This is taken nearly verbatim from Ross.]

Suppose that X and Y are independent, continuous random variables having probability density functions f_X and f_Y. The cumulative distribution function of $X+Y$ is obtained as follows:

$$\begin{aligned} F_{X+Y}(a) =& P(X+Y \le a) \\ &= \iint\limits_{x+y\le a} f_{XY}(x,y)\,dx\,dy \\ &= \iint\limits_{x+y\le a} f_X(x)f_Y(y)\,dx\,dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{a-y} f_X(x)f_Y(y)\,dx\,dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{a-y} f_X(x)\,dx f_Y(y)\,dy \\ &= \int_{-\infty}^{\infty} F_X(a-y)f_Y(y)\,dy \end{aligned} \tag{54}$$

The CDF F_{X+Y} is the **convolution** of the distributions F_X and F_Y.

If we differentiate the above equation, we get the pdf f_{X+Y}:

$$\begin{aligned} f_{X+Y} =& \frac{d}{dx}\int_{-\infty}^{\infty} F_X(a-y)f_Y(y)\,dy \\ =& \int_{-\infty}^{\infty} \frac{d}{dx}F_X(a-y)f_Y(y)\,dy \\ =& \int_{-\infty}^{\infty} f_X(a-y)f_Y(y)\,dy \end{aligned} \tag{55}$$

5.6 Conditional distributions

Discrete case Recall that the conditional probability of B given A, denoted $\mathbb{P}(B \mid A)$, is defined by

$$\mathbb{P}(B \mid A) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(A)}, \quad \text{if } \mathbb{P}(A) > 0. \tag{56}$$

If X and Y are discrete random variables, then we can define the conditional PMF of X given that $Y = y$ as follows:

$$\begin{aligned} p_{X|Y}(x \mid y) =& P(X = x \mid Y = y) \\ =& \frac{P(X = x, Y = y)}{P(Y = y)} \\ =& \frac{p(x,y)}{p_Y(y)} \end{aligned} \tag{57}$$

for all values of y where $p_Y(y) = P(Y = y) > 0$.

The **conditional cumulative distribution function** of X given $Y = y$ is defined, for all y such that $p_Y(y) > 0$, as follows:

$$\begin{aligned} F_{X|Y} =& P(X \leq x \mid Y = y) \\ =& \sum_{a \leq x} p_{X|Y}(a \mid y) \end{aligned} \tag{58}$$

If X and Y are independent then

$$p_{X|Y}(x \mid y) = P(X = x) = p_X(x) \tag{59}$$

See the examples starting p. 264 of Ross.

Continuous case [Taken almost verbatim from Ross.]

If X and Y have a joint probability density function $f(x,y)$, then the conditional probability density function of X given that $Y = y$ is defined, for all values of y such that $f_Y(y) > 0$,by

$$f_{X|Y}(x \mid y) = \frac{f(x,y)}{f_Y(y)} \tag{60}$$

We can understand this definition by considering what $f_{X|Y}(x \mid y)\,dx$ amounts to:

$$\begin{aligned} f_{X|Y}(x \mid y)\,dx &= \frac{f(x,y)}{f_Y(y)}\frac{dxdy}{dy} \\ &= \frac{f(x,y)dxdy}{f_Y(y)dy} \\ &= \frac{P(x < X < d + dx, y < Y < y + dy)}{y < P < y + dy} \end{aligned} \tag{61}$$

5.7 Joint and marginal expectation

[Taken nearly verbatim from Kerns.]

Given a function g with arguments (x, y) we would like to know the long-run average behavior of $g(X, Y)$ and how to mathematically calculate it. Expectation in this context is computed by integrating (summing) with respect to the joint probability density (mass) function.

Discrete case

$$\mathbb{E}\, g(X,Y) = \sum_{(x,y)\in S_{X,Y}}\sum g(x,y)\, f_{X,Y}(x,y). \tag{62}$$

Continuous case

$$\mathbb{E}\, g(X,Y) = \iint_{S_{X,Y}} g(x,y)\, f_{X,Y}(x,y)\,\mathrm{d}x\,\mathrm{d}y, \tag{63}$$

5.8 Covariance and correlation

There are two very special cases of joint expectation: the **covariance** and the **correlation**. These are measures which help us quantify the dependence between X and Y.

Definition 2 *The **covariance** of X and Y is*

$$Cov(X,Y) = \mathbb{E}(X - \mathbb{E}X)(Y - \mathbb{E}Y). \tag{64}$$

Shortcut formula for covariance:

$$\mathrm{Cov}(X,Y) = \mathbb{E}(XY) - (\mathbb{E}X)(\mathbb{E}Y). \tag{65}$$

The **Pearson product moment correlation** between X and Y is the covariance between X and Y rescaled to fall in the interval $[-1, 1]$. It is formally defined by

$$\mathrm{Corr}(X,Y) = \frac{\mathrm{Cov}(X,Y)}{\sigma_X \sigma_Y}. \tag{66}$$

The correlation is usually denoted by $\rho_{X,Y}$ or simply ρ if the random variables are clear from context. There are some important facts about the correlation coefficient:

1. The range of correlation is $-1 \leq \rho_{X,Y} \leq 1$.
2. Equality holds above ($\rho_{X,Y} = \pm 1$) if and only if Y is a linear function of X with probability one.

Continuous example (from Kerns) Let us find the covariance of the variables (X, Y) from an example numbered 7.2 in Kerns. The expected value of X is

$$\mathbb{E}X = \int_0^1 x \cdot \frac{6}{5}\left(x + \frac{1}{3}\right) \mathrm{d}x = \frac{2}{5}x^3 + \frac{1}{5}x^2\Big|_{x=0}^1 = \frac{3}{5},$$

and the expected value of Y is

$$\mathbb{E}Y = \int_0^1 y \cdot \frac{6}{5}\left(\frac{1}{2} + y^2\right) \mathrm{d}x = \frac{3}{10}y^2 + \frac{3}{20}y^4\Big|_{y=0}^1 = \frac{9}{20}.$$

Finally, the expected value of XY is

$$\begin{aligned}
\mathbb{E}XY &= \int_0^1 \int_0^1 xy \frac{6}{5}\left(x + y^2\right) \mathrm{d}x \, \mathrm{d}y, \\
&= \int_0^1 \left(\frac{2}{5}x^3 y + \frac{3}{10}xy^4\right)\Big|_{x=0}^1 \mathrm{d}y, \\
&= \int_0^1 \left(\frac{2}{5}y + \frac{3}{10}y^4\right) \mathrm{d}y, \\
&= \frac{1}{5} + \frac{3}{50},
\end{aligned}$$

which is 13/50. Therefore the covariance of (X, Y) is

$$\mathrm{Cov}(X, Y) = \frac{13}{50} - \left(\frac{3}{5}\right)\left(\frac{9}{20}\right) = -\frac{1}{100}.$$

5.9 *Conditional expectation*

Recall that

$$f_{X|Y}(x \mid y) = P(X = x \mid Y = y) = \frac{p_{X,Y}(x, y)}{p_Y(y)} \tag{67}$$

for all y such that $P(Y = y) > 0$.

It follows that

$$\begin{aligned}
E[X \mid Y = y] =& \sum_x x P(X = x \mid Y = y) \\
=& \sum_x x p_{X|Y}(x \mid y)
\end{aligned} \tag{68}$$

$E[X \mid Y]$ is that **function** of the random variable Y whose value at $Y = y$ is $E[X \mid Y = y]$. $E[X \mid Y]$ is a random variable.

Relationship to 'regular' expectation Conditional expectation given that $Y = y$ can be thought of as being an ordinary expectation on a reduced sample space consisting only of outcomes for which $Y = y$. All properties of expectations hold. Two examples (to-do: spell out the other equations):

Example 1

$$E[g(X) \mid Y = y] = \begin{cases} \sum_x g(x) p_{X|Y}(x, y) & \text{in the discrete case} \\ \int_{-\infty}^{\infty} g(x) f_{X|Y}(x \mid y)\, dx & \text{in the continuous case} \end{cases}$$

Example 2

$$E\left[\sum_{i=1}^{n} X_i \mid Y = y\right] = \sum_{i=1}^{n} E[X_i \mid Y = y] \tag{69}$$

Proposition 1 ***Expectation of the conditional expectation***

$$E[X] = E[E[X \mid Y]] \tag{70}$$

If Y is a discrete random variable, then the above proposition states that

$$E[X] = \sum_y E[X \mid Y = y] P(Y = y) \tag{71}$$

6 Maximum Likelihood Estimation

Suppose we toss a fair coin 10 times, and count the number of heads each time; we repeat this experiment 5 times in all. The observed sample values are $x_1, x_2, \ldots, x_5$.

```
(x<-rbinom(5,size=10,prob=0.5))

## [1] 6 7 9 8 3
```

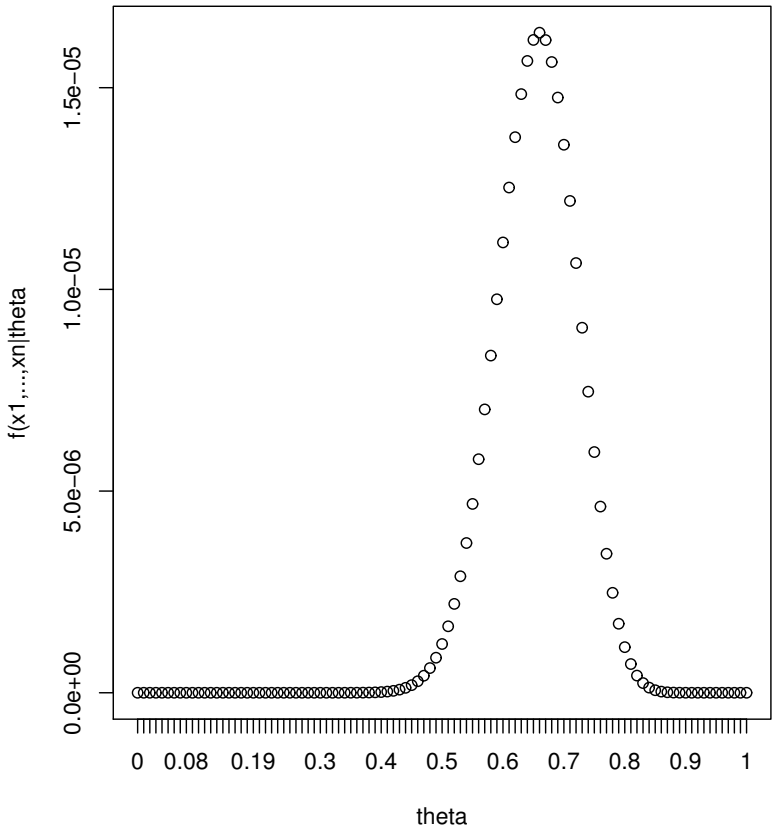
The joint probability of getting all these values (assuming independence) depends on the parameter we set for the probability θ:

$$P(X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n) = f(X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n; \theta) \tag{72}$$

So, the above probability is a function of θ. When this quantity is expressed as a function of θ, we call it the likelihood function.

The value of θ for which this function has the maximum value is the maximum likelihood estimate.

```
## probability parameter fixed at 0.5
theta<-0.5
prod(dbinom(x,size=10,prob=theta))

## [1] 1.208633e-06

## probability parameter fixed at 0.1
theta<-0.1
prod(dbinom(x,size=10,prob=theta))

## [1] 2.269431e-25

## probability parameter fixed at 0.9
theta<-0.9
prod(dbinom(x,size=10,prob=theta))

## [1] 4.205301e-10

## let's compute the product for
## a range of probabilities:
theta<-seq(0,1,by=0.01)
store<-rep(NA,length(theta))
for(i in 1:length(theta)){
store[i]<-prod(dbinom(x,size=10,prob=theta[i]))
}

plot(1:length(store),store,xaxt="n",xlab="theta",
     ylab="f(x1,...,xn|theta")
axis(1,at=1:length(theta),labels=theta)
```

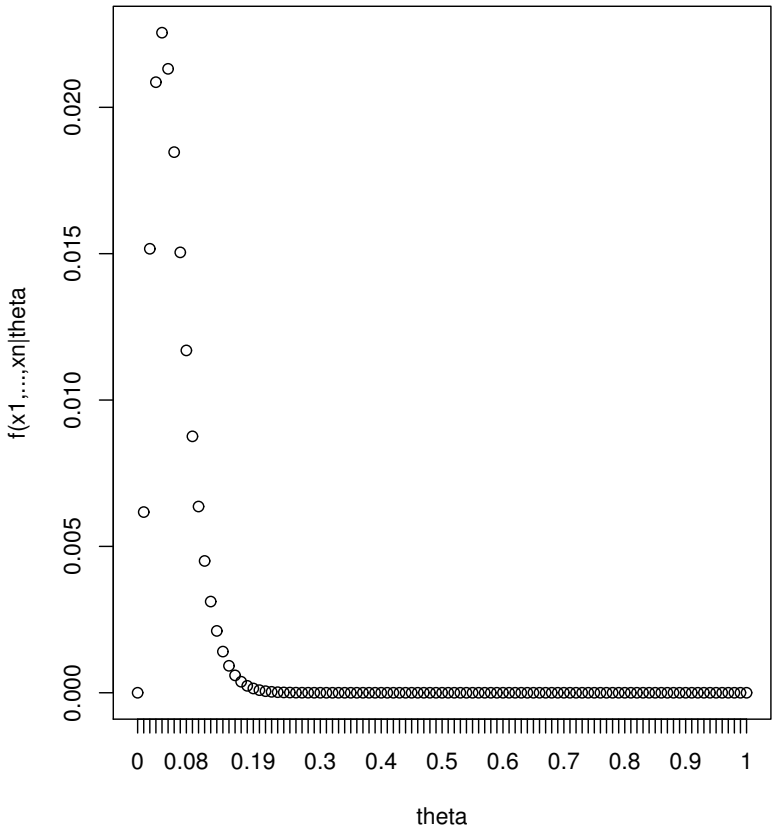


As another example, if the data had been generated by a binomial process with a different θ value than the one chosen above (0.5):

```
(x<-rbinom(5,size=10,prob=0.1))

## [1] 1 0 0 0 1
```

our likelihood function would look like this:

```
theta<-seq(0,1,by=0.01)
store<-rep(NA,length(theta))
for(i in 1:length(theta)){
store[i]<-prod(dbinom(x,size=10,prob=theta[i]))
}

plot(1:length(store),store,xlab="theta",
     ylab="f(x1,...,xn|theta",xaxt="n")
axis(1,at=1:length(theta),labels=theta)
```



Thus, the function f is the value of the joint probability **distribution** of the random variables $X_1, \ldots, X_n$ at $X_1 = x_1, \ldots, X_n = x_n$. Since the sample values have been observed and are fixed, $f(x_1, \ldots, x_n; \theta)$ is a function of θ. The function f is called a **likelihood function**.

Continuous case

Here, f is the joint probability **density**, the rest is the same as above.

Definition 3 *If $x_1, x_2, \ldots, x_n$ are the values of a random sample from a population with parameter θ, the **likelihood function** of the sample is given by*

$$L(\theta) = f(x_1, x_2, \ldots, x_n; \theta) \tag{73}$$

for values of θ within a given domain. Here, $f(X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n; \theta)$ is the joint probability distribution or density of the random variables $X_1, \ldots, X_n$ at $X_1 = x_1, \ldots, X_n = x_n$.

So, the method of maximum likelihood consists of maximizing the likelihood function with respect to θ. The value of θ that maximizes

the likelihood function is the **MLE** (maximum likelihood estimate) of θ.

6.1 Example 1: MLE of the Binomial distribution

$$L(\theta) = \binom{n}{x}\theta^x(1-\theta)^{n-x} \tag{74}$$

Taking logs gives us the log likelihood. It is usually easier to work with the log likelihood because all products become sums and those are easier to deal with:

$$\ell(\theta) = \log\binom{n}{x} + x\log\theta + (n-x)\log(1-\theta) \tag{75}$$

Differentiating and equating to zero to get the maximum:

$$\ell'(\theta) = \frac{x}{\theta} - \frac{n-x}{1-\theta} = 0 \tag{76}$$

How to get the second term: let $u = 1-\theta$.

Then, $du/d\theta = -1$. Now, $y = (n-x)\log(1-\theta)$ can be rewritten in terms of u: $y = (n-x)\log(u)$. So, $dy/du = \frac{n-x}{u}$.

Now, by the chain rule, $dy/d\theta = dy/du \times du/d\theta = \frac{n-x}{u} \times (-1) = -\frac{n-x}{1-\theta}$.

Rearranging terms, we get:

$\frac{x}{\theta} - \frac{n-x}{1-\theta} = 0 \Leftrightarrow \frac{x}{\theta} = \frac{n-x}{1-\theta} \Leftrightarrow \hat{\theta} = \frac{x}{n}$

6.2 Example 2: MLE of the Normal distribution

Let $X_1, \ldots, X_n$ constitute a random variable of size n from a normal population with mean μ and variance σ^2, find joint maximum likelihood estimates of these two parameters.

$$\begin{aligned} L(\mu;\sigma^2) = & \quad \prod N(x_i;\mu,\sigma) && (77)\\ = & \quad (\tfrac{1}{\sigma\sqrt{2\pi}})^n \exp(-\tfrac{1}{2\sigma^2}\textstyle\sum_{i=1}^n (x_i-\mu)^2) && (78)\\ & && (79)\end{aligned}$$

Taking logs and differentiating with respect to μ and σ, we get:

$$\hat{\mu} = \frac{1}{n}\sum x_i = \bar{x} \tag{80}$$

and

$$\hat{\sigma}^2 = \frac{1}{n}\sum (x_i - \bar{x})^2 \tag{81}$$

Note that the above MLE for the variance is biased, and the unbiased estimate is:

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum(x_i - \bar{x})^2 \tag{82}$$

For large n, the difference is negligible.

6.3 *Example 3: MLE of the Exponential distribution*

$$f(x;\lambda) = \lambda \exp(-\lambda x) \tag{83}$$

Log likelihood:

$$\ell = n \log \lambda - \sum \lambda x_i \tag{84}$$

Differentiating and equating to zero:

$$\ell'(\lambda) = \frac{n}{\lambda} - \sum x_i = 0 \tag{85}$$

$$\frac{n}{\lambda} = \sum x_i \tag{86}$$

I.e.,

$$\frac{1}{\hat{\lambda}} = \frac{\sum x_i}{n} \tag{87}$$

6.4 *Practical implications*

Whenever we obtain some data, we make an assumption about the generative process; we have to define the random variable X that we believe generated the data. A common assumption made is that

$X \sim Normal(\mu, \sigma^2)$

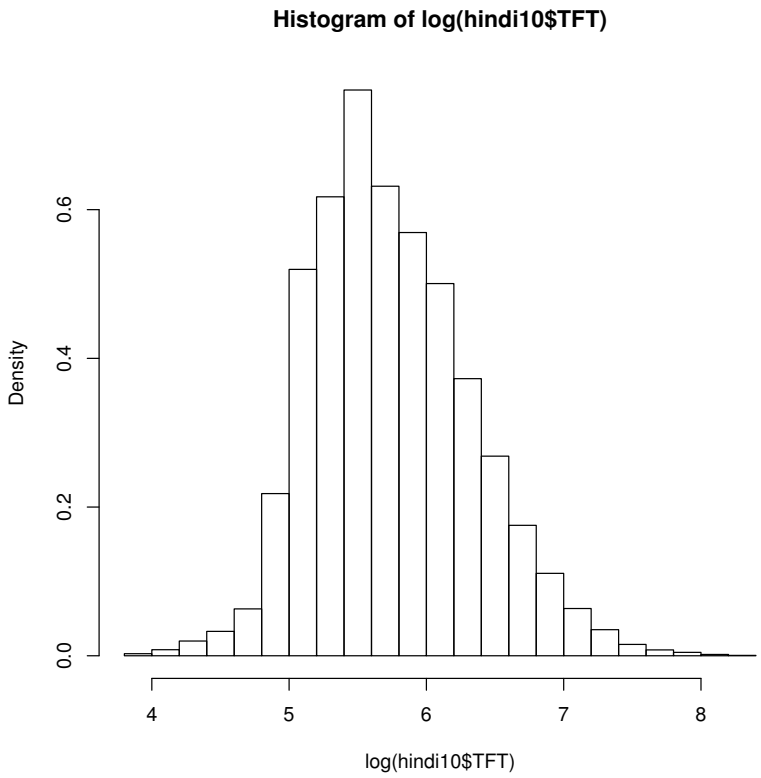
Once we've made this assumption, an obvious question arises: what should the values of μ and σ be? MLE is intended to answer that question.

As an example, consider the eyetracking data I released earlier. For now we will remove 0 ms reading times as missing data.

```
hindi10<-read.table("datacode/hindi10.txt",header=T)
summary(hindi10$TFT)

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##     0.0     0.0   226.0   273.5   380.0  3888.0

hindi10<-subset(hindi10,TFT>0)
summary(hindi10$TFT)

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##    50.0   208.0   294.0   376.4   454.0  3888.0
```

A histogram reveals the following distribution of reading times on the log scale. It's a slight stretch, but we start with the guess that this is roughly a normal distribution:

```
hist(log(hindi10$TFT),freq=FALSE)
```



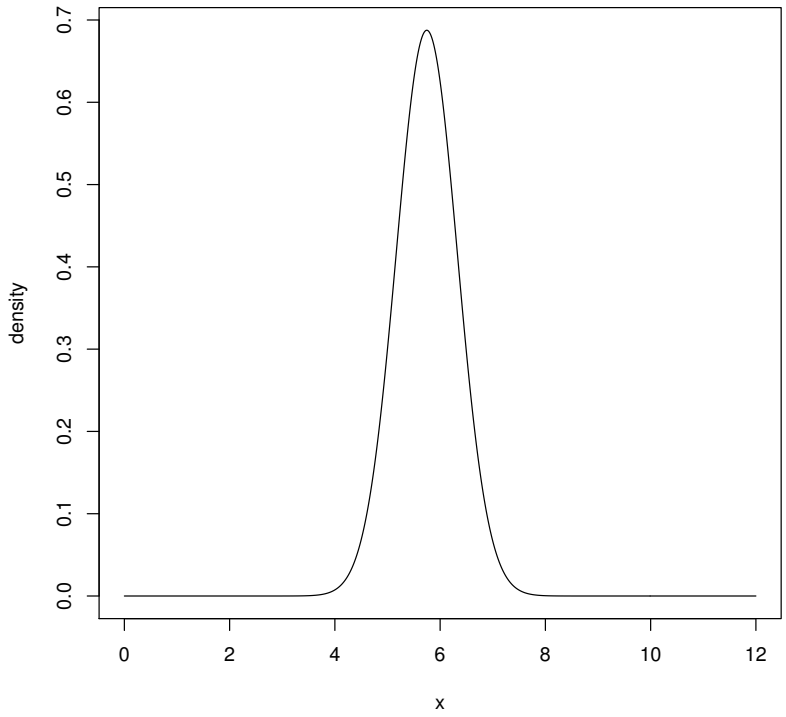
We take the mean and the (bias-corrected) variance estimates as the parameters of the underlying generative distribution. **This is where MLE becomes relevant**.

```
(xbar<-mean(log(hindi10$TFT)))

## [1] 5.746552

(xvar<-var(log(hindi10$TFT)))

## [1] 0.336665
```

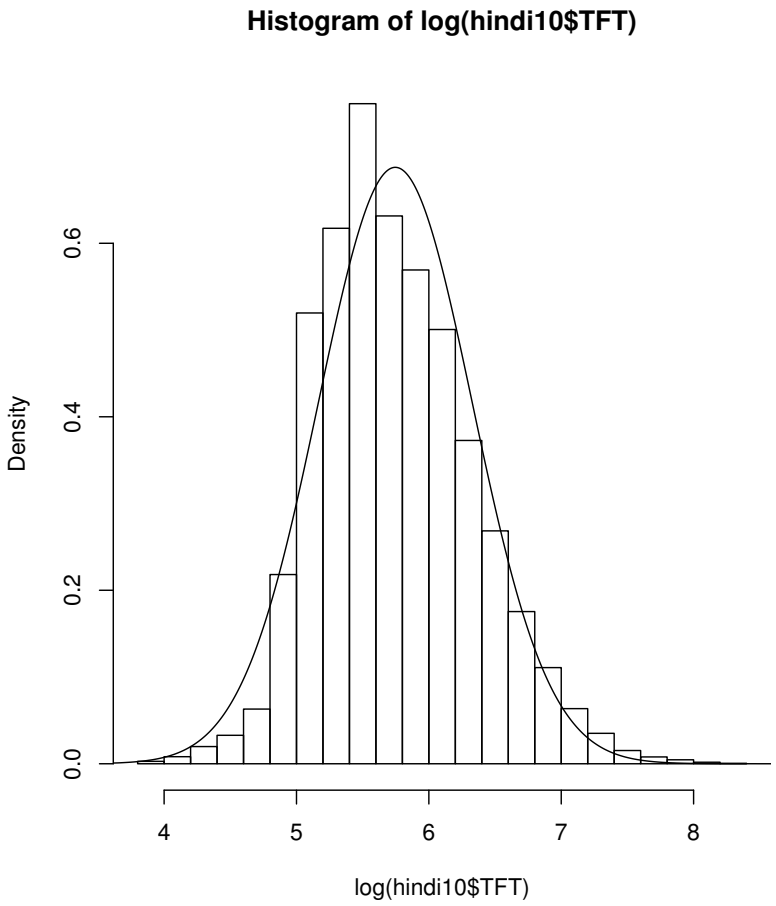
The MLEs imply that the underlying generative distribution is the following one:

```
xvals<-seq(0,12,by=0.01)
plot(xvals,dnorm(xvals,
```

```
                  mean=xbar,
                 sd=sqrt(xvar)),
     type="l",ylab="density",xlab="x")
```




```
## The empirical distribution and
## our theoretical distribution:
hist(log(hindi10$TFT),freq=FALSE)
xvals<-seq(0,4000,by=0.01)
lines(xvals,dnorm(xvals,
                  mean=xbar,sd=sqrt(xvar)))
```



Exercise: using the raw reading times in ms, compute the mean $\hat{\mu}$ and variance $\hat{\sigma}^2$, and then plot the sample distribution (the histogram) and the theoretical normal distribution on top of it using these estimates, as done in the example above. Comment on the differences between the sample distribution and the theoretical distribution we assume here.

Computing the MLE using an optimizer Note that you can use the function `optim` to compute the maximum likelihood estimates, once you define some log-likelihood function whose parameters need to be estimated.

```
## define negative log lik:
nllh.normal<-function(theta,data){
  ## mean and sd
  m<-theta[1]
  s<-theta[2]
  x <- data
```

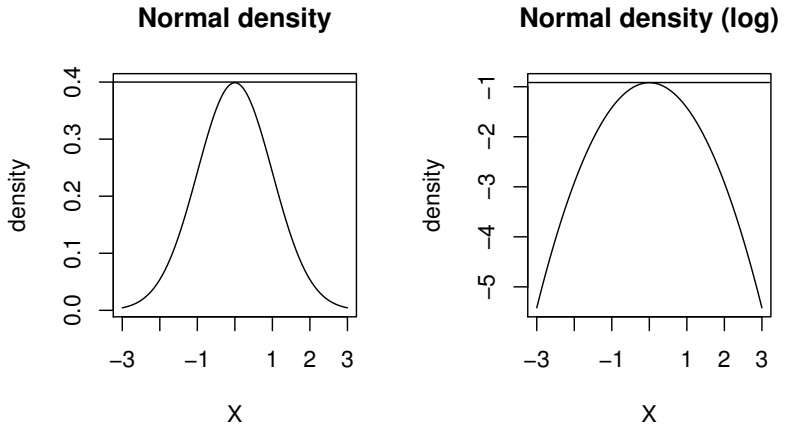
```
  n<-length(x)
  logl<- sum(dnorm(x,mean=m,sd=s,log=TRUE))
  ## return negative log likelihood:
  -logl
  }

## example output:
nllh.normal(theta=c(40,4),log(hindi10$TFT))

## [1] 766646

## find the MLEs using optim:
## need to specify some starting values:
opt.vals.default<-optim(theta<-c(500,50),
                        nllh.normal,
      data=log(hindi10$TFT),
      hessian=TRUE)

## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced
## Warning in dnorm(x, mean = m, sd = s, log = TRUE): NaNs produced

## result of optimization:
(estimates.default<-opt.vals.default$par)

## [1] 5.7462876 0.5801042

## compare with MLE:
xbar

## [1] 5.746552

## bias corrected sd:
sqrt(xvar)

## [1] 0.5802284
```

7 *Asymptotic properties of MLEs*

In the previous section we introduced maximum likelihood estimation. Recall the case of the normal distribution. For simplicity, consider

the case where $X \sim N(\mu = 0, \sigma^2 = 1)$. Given some data $x_1, \ldots, x_n$, what does its likelihood function look like? It is easy to visualize the likelihood function, both on the original scale and the log scale (Figure 4).

Figure 4: The likelihood and log likelihood.



Maximizing this (log) likelihood amounts to finding that maximum point at the center of the distribution. It's easy to do it visually, of course. What we learnt in the last chapter was how to do it analytically; we also saw how to use `optim` to find the maximum using an optimization function.

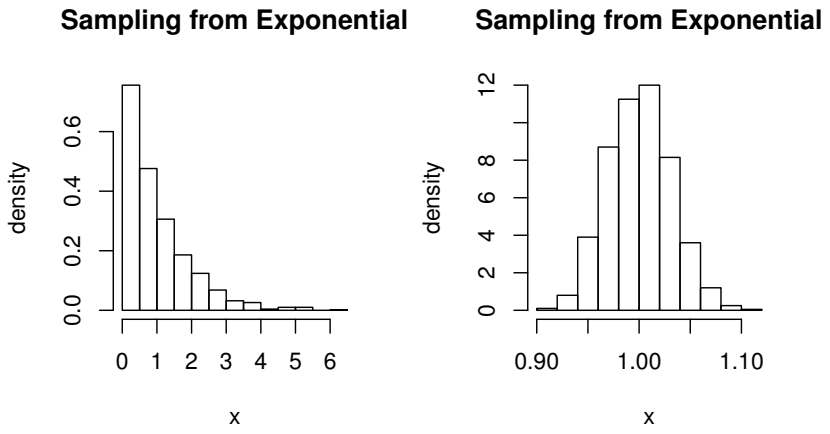
So, we can generally work out the MLE for the expectation and variance of a random variable by deriving a closed form expression, or we can compute it by using some optimization technique.

MLEs have the important property that they are asymptotically normally distributed. This means that if we repeatedly takes samples of data, and record the distribution of the sample mean, it will be normal if sample size is large enough, regardless of whether the underlying

distribution we are sampling from is normal or not (this is assuming that the underlying distribution has a mean and variance defined for it—the Cauchy distribution does not, for example).

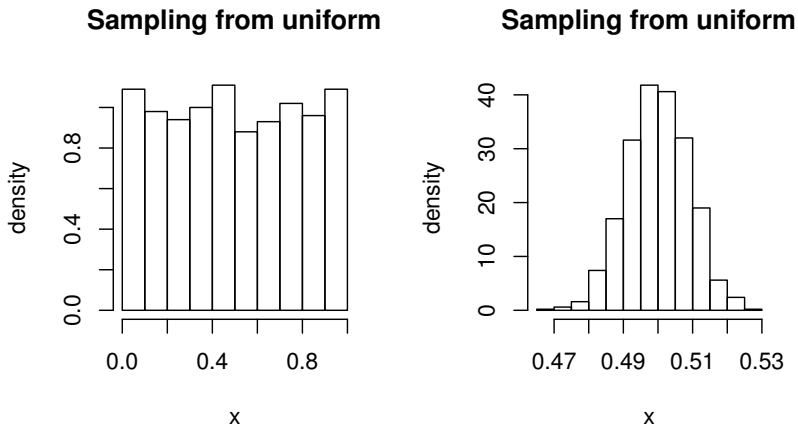
To get an intuition about this, consider the situation where we repeatedly sample from an exponential distribution. Even though the underlying distribution is not normal, the distribution of the mean under repeated sampling is.

```
n_rep<-1000
samp_distrn_mean<-rep(NA,n_rep)
for(i in 1:n_rep){
x<-rexp(1000)
samp_distrn_mean[i]<-mean(x)
}

op<-par(mfrow=c(1,2),pty="s")
hist(x,xlab="x",ylab="density",freq=FALSE,main="Sampling from Exponential")
hist(samp_distrn_mean,xlab="x",ylab="density",freq=FALSE,
     main="Sampling from Exponential")
```



Let's take some other even wilder distribution, say the uniform:

```
n_rep<-1000
samp_distrn_mean<-rep(NA,n_rep)
for(i in 1:n_rep){
x<-runif(1000)
samp_distrn_mean[i]<-mean(x)
}

op<-par(mfrow=c(1,2),pty="s")
hist(x,xlab="x",ylab="density",freq=FALSE,main ="Sampling from uniform")
hist(samp_distrn_mean,xlab="x",ylab="density",freq=FALSE,
     main="Sampling from uniform")
```



We will now look at this asymptotic property of the distribution of the sample means analytically.

7.1 The binomial distribution

Suppose that we have found the maximum likelihood estimate, say of p in the binomial distribution. Recall that we do this by taking the first derivative $\ell'(p)$ and then equating it to zero, and then solving for p.

It turns out that the second derivative of the log likelihood gives you an estimate of the variance of the sampling distribution of the sample mean (SDSM) that I just discussed above. The square root of this variance is called standard error (SE).

Here is an informal explanation for why the second derivative does this. The second derivative is telling us the rate at which the rate of change is happening in the slope, i.e., the rate of curvature of the curve (take a look at Figure 5). When the variance of the SDSM is small, then we have a fast rate of change in slope (high value for second derivative), and so if we take the inverse of the second derivative, we

get a small value, an estimate of the small variance (small SE^2). And when the variance is high, we have a slow rate of change in slope (low value for second derivative). I summarize this in Table 1 and a visualization is shown in Figure 5.

Variance of SDSM	Rate of slope change	2nd derivative
small	Fast change in slope	large
large	Slow change in slope	small

Table 1: Variance of the SDSM and the relationship with the second derivative.

So if we invert the second derivative, we get a large value, which is an estimate of the large variance (large SE^2).

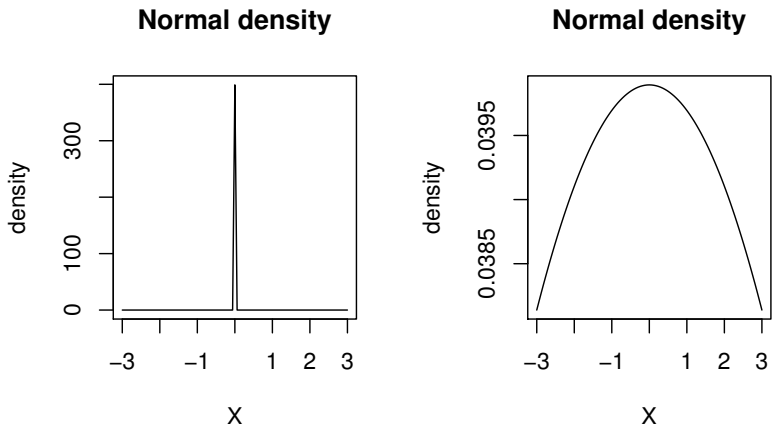


Figure 5: How variance relates to the second derivative.

Notice that all these second derivatives would be negative, because we are approaching a maximum as we reach the peak of the curve. So when we take an inverse to estimate the variances, we get negative values. It follows that if we were to take a negative of the inverse, we'd get a positive value.

This is the reasoning that leads to the following steps for computing the variance of the SDSM:

1. Take the second partial derivative of the log-likelihood.
2. Compute the negative of the expectation of the second partial derivative. This is called the Information Matrix $I(\theta)$.
3. Invert this matrix to obtain estimates of the variances and covariances. To get standard errors take the square root of the diagonal elements in the matrix.

It's better to see this through an example. Let's look at the binomial distribution, which has parameter p.

$$L(p) = \binom{n}{x} p^x (1-p)^{n-x} \tag{88}$$

The Log likelihood is:

$$\ell(p) = \log \binom{n}{x} + x \log p + (n-x) \log(1-p) \tag{89}$$

Taking the first derivative:

$$\ell'(p) = \frac{x}{p} - \frac{n-x}{1-p} \tag{90}$$

Taking the second partial derivative with respect to p:

$$\ell''(p) = -\frac{x}{p^2} - \frac{n-x}{(1-p)^2} \tag{91}$$

The quantity $-\ell''(p)$ is called **observed Fisher information**.
Taking expectations:

$$E(\ell''(p)) = E(-\frac{x}{p^2} - \frac{n-x}{(1-p)^2}) \tag{92}$$

Exploiting that fact the $E(x/n) = p$ and so $E(x) = E(n \times x/n) = np$, we get

$$E(\ell''(p)) = E(-\frac{x}{p^2} - \frac{n-x}{(1-p)^2}) = -\frac{np}{p^2} - \frac{n-np}{(1-p)^2} \underset{exercise}{=} -\frac{n}{p(1-p)} \tag{93}$$

Next, we negate and invert the expectation:

$$-\frac{1}{E(\ell''(\theta))} = \frac{p(1-p)}{n} \tag{94}$$

Evaluating this at $\hat{p}$, the estimated value of the parameter, we get:

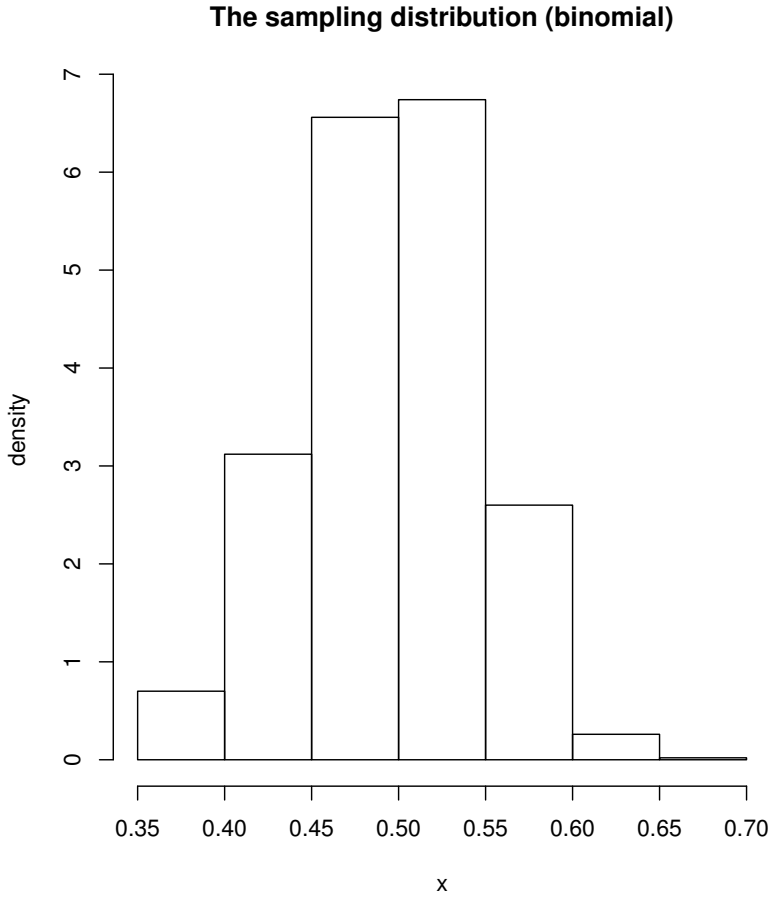
$$-\frac{1}{E(\ell''(\theta))} = \frac{\hat{p}(1-\hat{p})}{n} = \frac{1}{I(p)} \tag{95}$$

$I(p)$ is called **expected Fisher Information**. Note that is a 1×1 matrix, so we can call it the Information Matrix. If we take the square root of the inverse Information Matrix

$$\sqrt{\frac{1}{I(p)}} = \sqrt{\frac{\hat{p}(1-\hat{p})}{n}} \tag{96}$$

we have the **estimated standard error**. This is the standard deviation of the sampling distribution of the sample means. Maybe a little simulation will make this clear.

```
## analytic calculation of SE from a single expt:
## number of heads in 100 coin tosses:
n<-100
p<-0.5
(x<-rbinom(1,n=n,prob=p))

##   [1] 1 0 1 1 0 1 1 0 1 0 0 0 0 1 1 0 1 0 1 0 0 0 1 0 0 0 1 1 0 1 1 0 1 0 1
##  [36] 0 1 1 0 1 0 1 1 1 1 1 0 0 0 0 0 0 1 0 1 1 1 1 0 0 0 0 1 1 0 1 1 0 0 1
##  [71] 0 1 1 1 1 1 0 1 0 1 0 1 0 1 1 0 0 0 0 1 1 0 0 1 1 0 1 1 0 0

hat_p <- sum(x)/n
(SE_2<-(hat_p*(1-hat_p))/n)

## [1] 0.002499

(SE<-sqrt(SE_2))

## [1] 0.04999

## by repeated sampling:
samp_distrn_means<-rep(NA,1000)
for(i in 1:1000){
  x<-rbinom(1,n=n,prob=p)
  samp_distrn_means[i]<-sum(x)/n
}
hist(samp_distrn_means,xlab="x",ylab="density",
     freq=F,main="The sampling distribution (binomial)")
## this is the SE of the SDSM:
sd(samp_distrn_means)

## [1] 0.05079151
```



Here is another example of how we get the standard error, in the normal distribution.

7.2 *The normal distribution*

This example is partly based on Khuri[6] (p. 309). Let $X_1, \ldots, X_n$ be a sample of size n from $N(\mu, \sigma^2)$, both parameters of the normal, and both unknown. Let our parameters be defined as $\theta = (\mu, \sigma)$.

[6] André I Khuri. *Advanced calculus with applications in statistics*, volume 486. Wiley, 2003

$$L(x \mid \mu, \sigma) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp[-\frac{1}{2\sigma^2} \sum (x_i - \mu)^2] \tag{97}$$

The log likelihood is:

$$\ell = -\frac{n}{2} \log \frac{1}{(2\pi\sigma^2)} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (x_i - \mu)^2 \tag{98}$$

Taking partial derivatives with respect to μ and σ we have:

$$\frac{\partial \ell}{\partial \mu} = \frac{1}{2\sigma^2} \sum_{i=1}^{n} (x_i - \mu) \tag{99}$$

$$\frac{\partial \ell}{\partial \sigma} = \frac{n}{\sigma} + \frac{\sum (x_i - \mu)^2}{\sigma^3} \tag{100}$$

Equating these to zero gives us the estimates of μ and σ^2: $\hat{\mu} = \bar{x}$ and $\hat{\sigma} = \sqrt{\frac{1}{n}\sum (x_i - \bar{x})^2}$, given the particular data $x_1, \ldots, x_n$.

We can verify that $\hat{\mu}$ and $\hat{\sigma}^2$ are the values of μ and σ that maximize $L(x \mid \mu, \sigma)$. This can be done by taking the second order partial derivatives, and finding out whether we are at a maximum or not.

Note that there are four second order partial derivative now. It is convenient to write the four partial derivatives in the above example as a matrix, and this matrix is called a **Hessian matrix**.

If this matrix is positive definite (i.e., if the determinant[7] of the matrix is greater than 0), we are at a maximum.

The Hessian is also going to lead us to the information matrix as in the previous binomial example: we just take the negative of the expectation of the Hessian, and invert it to get the variance covariance matrix. (This is just like in the binomial example above, except that we have two parameters to worry about rather than one.)[8]

Consider the Hessian matrix H of the second partial derivatives of the log likelihood ℓ.

$$H = \begin{pmatrix} \frac{\partial^2 \ell}{\partial \mu^2} & \frac{\partial^2 \ell}{\partial \mu \partial \sigma} \\ \frac{\partial^2 \ell}{\partial \mu \partial \sigma} & \frac{\partial^2 \ell}{\partial \sigma^2} \end{pmatrix} \tag{101}$$

Now, if we compute the second-order partial derivatives, we will get:

$$\frac{\partial^2 \ell}{\partial \mu^2} = -\frac{n}{\sigma^2} \tag{102}$$

$$\frac{\partial^2 \ell}{\partial \mu \partial \sigma} = -\frac{3}{2\sigma^2} \sum (x_i - \mu) = 0 \tag{103}$$

This is zero because the sum of the deviation of x_i about μ are always going to be 0.

$$\frac{\partial^2 \ell}{\partial \sigma^2} = -\frac{n}{\sigma^2} - \frac{3\sum_{i=1}^{n} (x_i - \mu)^2}{\sigma^4} \tag{104}$$

Note that we can simplify the last term:

$$-\frac{3\sum_{i=1}^{n} (x_i - \mu)^2}{\sigma^4} = -3\frac{n}{\sigma^2} \tag{105}$$

That's because we can rewrite as

$$-3n\frac{(x_i - \mu)^2}{n\sigma^4} = -\frac{3n\sigma^2}{\sigma^4} = -\frac{3n}{\sigma^2} \tag{106}$$

So, the Hessian is

[7] Suppose a a matrix represents a system of linear equations, as happens in linear modeling. A determinant of a matrix tells us whether there is a unique solution to this system of equations; when the determinant is non-zero, there is a unique solution. Given a matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

the determinant is $ad - bc$. In this course, we don't need to know much about the determinant. This is the only place in this course that this term turns up.

[8] Please review the Foundations of Mathematics notes if you have forgotten how to invert a matrix.

$$H = \begin{pmatrix} \frac{\partial^2 \ell}{\partial \mu^2} & \frac{\partial^2 \ell}{\partial \mu \partial \sigma} \\ \frac{\partial^2 \ell}{\partial \mu \partial \sigma} & \frac{\partial^2 \ell}{\partial \sigma^2} \end{pmatrix} = \begin{pmatrix} -\frac{n}{\sigma^2} & 0 \\ 0 & -\frac{n}{\sigma^2} - \frac{3n}{\sigma^2} \end{pmatrix} \tag{107}$$

The determinant of the Hessian is

$$-\frac{n}{\sigma^2}(-\frac{4n}{\sigma^2}) = \frac{4n^2}{\sigma^4} > 0 \tag{108}$$

Hence, (μ, σ^2) is a point of local maximum of ℓ. Since it's the only maximum (we established that when we took the first derivative), it must also be the absolute maximum.

As mentioned above, if we take the negation of the expectation of the Hessian, we get the Information Matrix, and if we invert the Information Matrix, we get the variance-covariance matrix.

Once we take the negation of the expectation, we get ($\theta = (\mu, \sigma)$):

$$I(\theta) = \begin{pmatrix} \frac{n}{\sigma^2} & 0 \\ 0 & \frac{4n}{\sigma^2} \end{pmatrix} \tag{109}$$

Next, if we take the inverse and evaluate it at the MLEs, we will get:

$$I(\theta)^{-1} = \frac{1}{\frac{4n^2}{\sigma^4}} \begin{pmatrix} \frac{4n}{\sigma^2} & 0 \\ 0 & \frac{n}{\sigma^2} \end{pmatrix} = \begin{pmatrix} \frac{\sigma^2}{n} & 0 \\ 0 & \frac{\sigma^2}{4n} \end{pmatrix} \tag{110}$$

And finally, if we take the square root of each element in the matrix, we get the standard error of μ to be $\frac{\sigma}{\sqrt{n}}$, and the standard error of the σ to be $\frac{\sigma}{2\sqrt{n}}$.[9] The estimated standard error of the sample mean should look familiar!

[9] Please check I got this right. There may be a mistake here, need to check this.

So, the conclusion is that asymptotically,

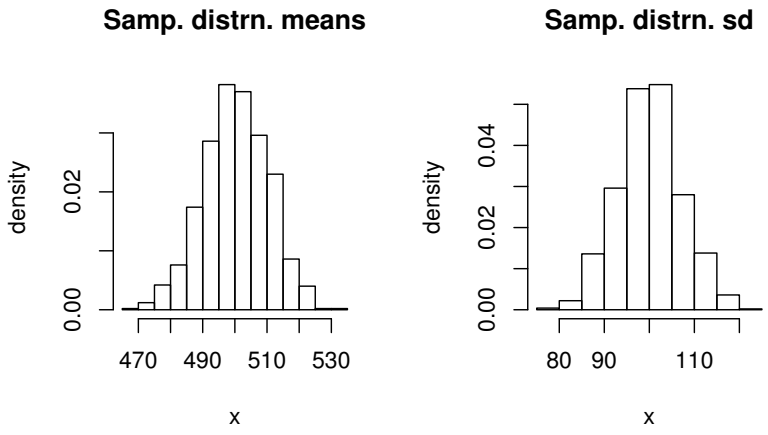
$$\begin{pmatrix} \hat{\mu} \\ \hat{\sigma} \end{pmatrix} \xrightarrow{d} N\left(\begin{pmatrix} \mu \\ \sigma \end{pmatrix}, \begin{pmatrix} \frac{\sigma^2}{n} & 0 \\ 0 & \frac{\sigma^2}{4n} \end{pmatrix} \right) \tag{111}$$

To summarize, when we have a single sample, we compute the sample mean and standard deviation, $\hat{\mu}$ and $\hat{\sigma}$, and then compute the standard error of the sampling distribution of $\hat{\mu}$ (generally, we don't pay attention to the sampling distribution of $\hat{\sigma}^2$.

We can quickly simulate the sampling distribution of the mean to get a feel for what this means:

```
nsim<-1000
n<-100
mu<-500
sigma<-100
samp_distrn_means<-rep(NA,nsim)
samp_distrn_sd<-rep(NA,nsim)
for(i in 1:nsim){
```

```
  x<-rnorm(n,mean=mu,sd=sigma)
  samp_distrn_means[i]<-mean(x)
  samp_distrn_sd[i]<-sd(x)
}
op<-par(mfrow=c(1,2),pty="s")
hist(samp_distrn_means,main="Samp. distrn. means",
     freq=F,xlab="x",ylab="density")
hist(samp_distrn_sd,main="Samp. distrn. sd",
     freq=F,xlab="x",ylab="density")
## estimate from simulation:
sd(samp_distrn_means)

## [1] 10.09288

## estimate from a single sample of size n:
sigma/sqrt(n)

## [1] 10
```



Once we have found the asymptotic distribution of the MLE in this way, we can obtain a so-called 95% confidence interval:

$$\hat{\mu} \pm 2SE(\hat{\mu}) \tag{112}$$

So, for the mean, we have a 95% confidence interval as follows:

$$\hat{\mu} \pm 2\frac{\hat{\sigma}}{\sqrt{n}} \tag{113}$$

In our example:

```
## lower bound:
mu-(2*sigma/sqrt(n))

## [1] 480

## upper bound:
mu+(2*sigma/sqrt(n))

## [1] 520
```

This CI has an extremely confusing interpretation: if you were to (hypothetically) repeatedly sample, and compute the CI each time, the true mean μ would be contained in 95% of those intervals that we hypothetically calculated each time. The confusing thing is that the single CI that you plot based on a single sample does not give you what you would intuitively expect it to: the range over which you can be 95% sure that the true parameter value μ lies. This kind of interval can only be computed in the Bayesian setting; the CI does not have this interpretation because μ has no probability distribution defined over it, it is a point value.

The above simulation can be used to understand the idea of a 95% CI:

```
lower<-rep(NA,nsim)
upper<-rep(NA,nsim)
for(i in 1:nsim){
  x<-rnorm(n,mean=mu,sd=sigma)
  lower[i]<-mean(x) - 2 * sd(x)/sqrt(n)
  upper[i]<-mean(x) + 2 * sd(x)/sqrt(n)
}
## check how many CIs contain mu:
CIs<-ifelse(lower<mu & upper>mu,1,0)
table(CIs)

## CIs
##   0   1
```

```
##  37 963

## 95% CIs contain true mean:
table(CIs)[2]/sum(table(CIs))

##     1
## 0.963
```

The reason that we spent so much energy and time understanding the asymptotic properties of MLEs is that in the next chapter we will be looking maximum likelihood estimates of parameters of the linear model:

$$y = \beta_0 + \beta_1 x + \varepsilon \tag{114}$$

One of the issues of interest in linear models is an estimate of the uncertainty of the maximum likelihood estimates of β_0 and β_1. This estimate of uncertainty is the standard error, and this is what we will depend on for doing statistical inference (null hypothesis significance testing).

8 *Basic linear modeling theory*

[Note, in this section, context will determine whether β or x is a scalar or a matrix. Most of the time, we will be using matrix notation.]

Consider the deterministic function:

$$y = \phi(f(x), \beta) = \beta_0 + \beta_1 x \tag{115}$$

For example,

$$f(x) = (1 \; x) \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \tag{116}$$

Now consider a non-deterministic version:

$$y = \phi(f(x), \beta, \epsilon) = \beta_0 + \beta_1 x + \epsilon \tag{117}$$

The general linear model is a non-deterministic function like the one above:

$$Y = f(x)\beta + \epsilon \tag{118}$$

The matrix formulation will be written like this:

$$Y = X\beta + \epsilon \Leftrightarrow y_j = f(x_j)^T \beta + \epsilon_j, i = 1, \ldots, n \tag{119}$$

$E[Y] = X\beta$. Here, β is a $p \times 1$ matrix, and X, the **design matrix**, is $n \times p$.

8.1 *Least squares estimation: Geometric argument*

When we have a deterministic model $y = \phi(f(x), \beta) = \beta_0 + \beta_1 x = X\beta$, this implies a perfect fit to all data points. This is like solving the equation $Ax = b$ in linear algebra: we solve for β in $X\beta = y$ using, e.g., Gaussian elimination.

When we have a non-deterministic model $y = \phi(f(x), \beta, \epsilon) = \beta_0 + \beta_1 x + \epsilon$, there is no unique solution. Now, the equation Ax is an approximation to b in $Ax = b$. We try to get Ax as close to b as possible, i.e., $\mid b - Ax \mid$ is minimized. The problem now becomes finding $\hat{x}$ such that $A\hat{x} = \hat{b}$.

Now, notice that $(Y - X\hat{\beta})$ and $X\beta$ are perpendicular to each other. Because the dot product of two perpendicular (orthogonal) vectors is o, we get the result:

$$(Y - X\hat{\beta})^T X\beta = 0 \Leftrightarrow (Y - X\hat{\beta})^T X = 0 \tag{120}$$

Multiplying out the terms, we proceed as follows. One result that we use here is that $(AB)^T = B^T A^T$.

$$\begin{aligned} &(Y - X\hat{\beta})^T X = 0 \\ &(Y^T - \hat{\beta}^T X^T) X = 0 \\ \Leftrightarrow &Y^T X - \hat{\beta}^T X^T X = 0 \\ \Leftrightarrow &Y^T X = \hat{\beta}^T X^T X \\ \Leftrightarrow &(Y^T X)^T = (\hat{\beta}^T X^T X)^T \\ \Leftrightarrow &X^T Y = X^T X\hat{\beta} \end{aligned} \tag{121}$$

This gives us the important result:

$$\hat{\beta} = (X^T X)^{-1} X^T Y \tag{122}$$

X is of full rank, therefore $X^T X$ is invertible.

Rank is the number of linearly independent columns or rows. The row rank and column rank of an mxn matrix will be the same, so we can just talk of rank of a matrix. An mxn matrix X with rank(X)=min(m,n) is called full rank.

Example:

```
(X<-matrix(c(rep(1,8),rep(c(-1,1),each=4),
             rep(c(-1,1),each=2,2)),ncol=3))
```

```
##      [,1] [,2] [,3]
## [1,]    1   -1   -1
## [2,]    1   -1   -1
## [3,]    1   -1    1
## [4,]    1   -1    1
## [5,]    1    1   -1
## [6,]    1    1   -1
## [7,]    1    1    1
## [8,]    1    1    1
```

```
library(Matrix)
## full rank:
rankMatrix(X)

## [1] 3
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 1.776357e-15

## det non-zero:
det(t(X)%*%X)

## [1] 512
```

Notice that the inverted matrix is also symmetric. We will use this fact soon.

The matrix $V = X^T X$ is a symmetric matrix, which means that $V^T = V$. The symmetric matrix will be of great interest to us in this course.

8.2 *The expectation and variance of the parameters beta*

Our model is:

$$Y = X\beta + \epsilon \tag{123}$$

Let $\epsilon \sim N(0, \sigma^2)$. In other words, we are assuming that each value generated by the random variable ϵ is independent and it has the same distribution, i.e., it is identically distributed. This is sometimes shortened to the iid assumption. So we should technically be writing:

$$Y = X\beta + \epsilon \quad \epsilon \sim N(0, \sigma^2) \tag{124}$$

and add that Y are independent and identically distributed. Note that the independence assumption is grossly violated in our Hindi data—we have multiple measures from each subject, and multiple measures also from each item. So it is not legitimate to fit such a model to our data (this is HW4).

Some consequences of the above statements:

1. $E(\epsilon) = 0$
2. $Var(\epsilon) = \sigma^2 I_n$
3. $E[Y] = X\beta = \mu$

4. $Var(Y) = \sigma^2 I_n$

We can now derive the expectation and variance of the vector β. We need a fact about variances: $Var(aB)$, where a is a constant, is $a^2 Var(B)$. In the matrix setting, Var(AB), where A is a constant, is $AVar(B)A^T$.

$$E[\hat{\beta}] = (X^T X)^{-1} X^T Y = (X^T X)^{-1} X^T X \beta = \beta \tag{125}$$

Next, we compute the variance:

$$Var(\hat{\beta}) = Var([(X^T X)^{-1} X^T] Y) \tag{126}$$

Expanding the right hand side out:

$$Var([(X^T X)^{-1} X^T] Y) = [(X^T X)^{-1} X^T] Var(Y) [(X^T X)^{-1} X^T]^T \tag{127}$$

Replacing Var(Y) with its variance $\sigma^2 I$, and unpacking the transpose on the right-most expression $[(X^T X)^{-1} X^T]^T$:

$$Var(\beta) = [(X^T X)^{-1} X^T] \sigma^2 I X [(X^T X)^{-1}]^T \tag{128}$$

Since σ^2 is a scalar we can move it to the left, and any matrix multiplied by I is the matrix itself, so we ignore I, getting:

$$Var(\beta) = \sigma^2 [(X^T X)^{-1} X^T X [(X^T X)^{-1}]^T \tag{129}$$

Since $(X^T X)^{-1} X^T X = I$, we can simplify to

$$Var(\beta) = \sigma^2 [(X^T X)^{-1}]^T \tag{130}$$

Now, $(X^T X)^{-1}$ is symmetric, so $[(X^T X)^{-1}]^T = (X^T X)^{-1}$. This gives us:

$$Var(\beta) = \sigma^2 (X^T X)^{-1} \tag{131}$$

An example:

```
y<-as.matrix(hindi10$TFT)
x<-log(hindi10$word_len)
m0<-lm(y~x)

## design matrix:
X<-model.matrix(m0)
head(X,n=4)
```

```
##   (Intercept)         x
## 1           1 0.6931472
## 2           1 1.3862944
## 3           1 1.3862944
## 4           1 2.4849066

## (X^TX)^{-1}
invXTX<-solve(t(X)%*%X)
## estimated beta:
(beta<-invXTX%*%t(X)%*%y)

##                 [,1]
## (Intercept) 210.7777
## x           129.4064

## estimated variance of beta:
(hat_sigma<-summary(m0)$sigma)

## [1] 269.5443

(hat_var<-hat_sigma^2*invXTX)

##             (Intercept)         x
## (Intercept)    31.35647 -21.61119
## x             -21.61119  16.88379
```

What we have here is a bivariate normal distribution as an estimate of the β parameters:

$$\begin{pmatrix}\hat{\beta}_0\\ \hat{\beta}_1\end{pmatrix} \sim N(\begin{pmatrix}210.7777\\ 129.4064\end{pmatrix}, \begin{pmatrix}31.35647 & -21.61119\\ -21.61119 & 16.88379\end{pmatrix}) \tag{132}$$

The variance of a bivariate distribution has the variances along the diagonal, and the covariance between β_0 and β_1 on the off-diagonals. Covariance is defined as:

$$Cov(\beta_0, \beta_1) = \rho\sigma_{\beta_0}\sigma_{\beta_1} \tag{133}$$

where ρ is the correlation between β_0 and β_1.

So $\beta_0 \sim N(210.78, 31.36)$ and $\beta_0 \sim N(129.41, 16.88)$, and $Cov(\beta_0, \beta_1) = -21.61$. So the correlation between the β is

```
## hat rho:
-21.61/(sqrt(31.36)*sqrt(16.88))

## [1] -0.9392485
```

8.3 Statistical inference

In the model output we see:

```
round(summary(m0)$coefficients[,1:3],
             digits=3)

##             Estimate Std. Error t value
## (Intercept)  210.778      5.600  37.641
## x            129.406      4.109  31.493
```

We know what the first two columns are. The third column is based on the following quantity:

$$t^2 = \frac{(\hat{\beta}_0 - \beta_0)^2}{Var(\beta_0)} \tag{134}$$

This is called the Wald statistic, and the test, which is called a Wald test, says that the following quantity has a chi-squared distribution (with degrees of freedom p, the number of parameters). Consider β_0, i.e., p=1:

$$t^2 = \frac{(\hat{\beta}_0 - \beta_0)^2}{Var(\beta_0)} \sim \chi^2_1 \tag{135}$$

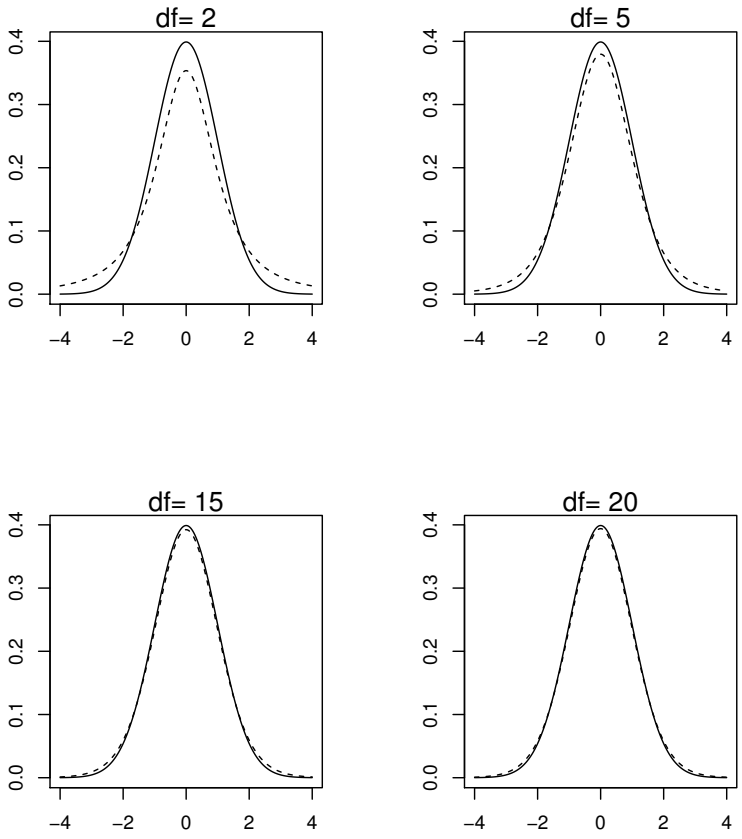
An alternative version of the test is:

$$\frac{\hat{\beta} - \beta}{\sqrt{Var(\beta)}} \sim Normal(0, 1) \tag{136}$$

The t-value refers to the fact that we are using an approximation of N(0,1), the t-distribution with $n - 1$ degrees of freedom. For small sample sizes (say $n < 18$), the use of the t-distribution rather than the normal has important consequences because the t-distribution for such small n has fatter tails than the normal—more probability mass is located in the tails of the t-distribution than in the normal. For larger sample sizes, the normal and t-distribution are essentially indistinguishable. We can visualize this difference between the t-distribution and normal distribution quite easily.

```
range <- seq(-4,4,.01)

op<-par(mfrow=c(2,2),pty="s")

 for(i in c(2,5,15,20)){
   plot(range,dnorm(range),type="l",lty=1,
        xlab="",ylab="",
        cex.axis=1)
```

```
  lines(range,dt(range,df=i),lty=2,lwd=1)
  mtext(paste("df=",i),cex=1.2)
}
```



8.4 *The notorious p-value, and Type S and M errors*

Note that R also prints out a "p-value":

```
summary(m0)$coef
```

```
##             Estimate Std. Error  t value      Pr(>|t|)
## (Intercept) 210.7777   5.599685 37.64100 1.800690e-299
## x           129.4064   4.108989 31.49348 1.968918e-212
```

This is the **conditional** probability of getting an estimate as extreme or more extreme than the absolute value $|\pm 210.78|$ for β_0, assuming that the true distribution is $N(0, Var(\hat{\beta}_0))$.

We can compute it by hand using the CDF of the normal or t-distribution (there are some rounding errors piling up here, so the numbers don't match the lm output exactly):

```
2*pnorm(210.78,mean=0,sd=sqrt(31.36),
        lower.tail=FALSE)

## [1] 0

2*pt(210.78/sqrt(31.36),df=length(y)-1,
   lower.tail=FALSE)

## [1] 1.910062e-299
```

So, this hypothesis test is rejecting the null hypothesis that $\beta_0 = 0$. Rejecting the null hypothesis implies that $\beta_0 \neq 0$. Note that Gelman and Hill go to some trouble to get rid of the t-value and p-value; this is because at least Gelman doesn't think much of this null hypothesis testing business, with good reason—the p-value has probably caused more harm to science, and probably killed a lot of people in medicine, than any other statistical construct.

The p-value is widely misunderstood, even by veteran scientists. Here are some things people **incorrectly** think is true of p-values:

1. Mistake: A lower p-value gives me more confidence in the specific alternative hypothesis I am interested in verifying.

   Reality: A lower p-value only gives me more confidence that the null is false. It doesn't tell me which of the infinity of possible μ is true.

2. Mistake: A p-value greater than 0.05 tells me that the null hypothesis is true.

   Reality: The p-value is a conditional probability: $P(X > |\bar{x}| \mid H_0)$. To conclude that the null is true when $p > 0.05$ is like concluding that, if the probability of the streets being wet given that it has just rained is higher than 0.05, then I can conclude that it has just rained: $P(\text{streets wet} \mid \text{rained}) \approx 1 \Rightarrow$ It has just rained. It is an embarrassing fact that a remarkable number of scientists in linguistics, psychology, and computer sciencts don't understand this point.

   The mistake is reminiscent of a misunderstanding about the meaning of a material implication in formal logic. The following inference is not logically valid:

   (a) $p \rightarrow q$

   (b) q

(c) Therefore p

If we had had $p \leftrightarrow q$, then we could draw this conclusion. Google for "affirming the consequent" for more.

3. Mistake: It is widely assumed that if $p < 0.05$, we have found out that the alternative is true, i.e., that there is a true effect.

   An example is an MIT "senior research scientist" at CSAIL (see the interview with this "professor", http://www.collective-evolution.com/2015/02/17/mit-professor-explains-the-vaccine-autism-connection/), who claims that vaccines are causing autism in children. This is based on a linear model fit, regressing number of autism case against amount of vaccination (or something like that, I forget the details).

   Reality: Two points here are that correlation does not imply causation, and there will be at least a 0.05 (but as high as 0.40 in some cases) probability of incorrectly rejecting the null. Most published significant results are in fact false. For recent attempts to get a handle on this, see: http://www.nature.com/news/first-results-from-psychology-s-largest-reproducibility-test-1.17433.

In frequentist statistics, we can also compute Type I and Type II error rates. Type I error is the probability of incorrectly rejecting the null (when it's actually true); this is typically set at 0.05 by the researcher and is called the α value. Type II error is defined as the probability of incorrectly "accepting" (more accurately, failing to reject) the null hypothesis when it's false. (1-Type II) error is called power, and is the probability of correctly rejecting the null.[10]

Another important point is that just computing the p-value is not particularly informative. If you have some way to determine an estimate of the true effect size for a particular phenomenon (say, through a meta-analsis or literature review or expert knowledge about the topic you are studying), then you can and should (I would say, must) also compute Type S and M errors; see the Gelman and Carlin article[11] for further discussion.

For example, if your true effect size is believed to be D=15, then we can compute (apart from statistical power) these error rates, which are defined as follows:

1. Type S error: the probability that the sign of the effect is incorrect, given that (a) the result is statistically significant, or (b) the result is statistically non-significant.

2. Type M error: the expectation of the ratio of the absolute magnitude of the effect to the hypothesized true effect size (conditional on whether the result is significant or not). Gelman and Carlin also

[10] Note that all our definitions here are with respect to the null hypothesis—it is a mistake to think that Type II error is the probability of failing to accept the alternative hypothesis when it's true. We can only ever reject or not reject the null; our hypothesis test is always with reference to the null.

[11] Andrew Gelman and John Carlin. Beyond power calculations assessing type s (sign) and type m (magnitude) errors. *Perspectives on Psychological Science*, 9(6):641–651, 2014

call this the exaggeration ratio, which is perhaps more descriptive than "Type M error".

Suppose a particular study has standard error 46, and sample size 37. And suppose that our estimated true D=15. Then, we proceed as follows:

```
## probable effect size derived from past studies:
D<-15
## SE from the study of interest:
se<-46
stddev<-se*sqrt(37)
nsim<-10000
drep<-rep(NA,nsim)
for(i in 1:nsim){
drep[i]<-mean(rnorm(37,mean=D,sd=stddev))
}

##power: a depressingly low 0.056
pow<-mean(ifelse(abs(drep/se)>2,1,0))

## which cells in drep are significant at alpha=0.05?
signif<-which(abs(drep/se)>2)

## Type S error rate | signif: 19%
types_sig<-mean(drep[signif]<0)
## Type S error rate | non-signif: 37%
types_nonsig<-mean(drep[-signif]<0)

## Type M error rate | signif: 7
typem_sig<-mean(abs(drep[signif])/D)
## Type M error rate | not-signif: 2.3
typem_nonsig<-mean(abs(drep[-signif])/D)
```

So, you can see that the Type S error and the exaggeration ratio, conditional on a result being significant, are pretty high. The practical implication of this is that if most studies in psycholinguistics are low powered, then it doesn't matter much whether you got a significant result or not. You could be (and probably are) barking up the wrong tree. The main take-away point here is: run high powered studies, and replicate the results. There's really no statistical test out there that can match consistent replication.

8.5 Hypothesis tests and the sampling distribution of the mean

An important detail about the above Wald test or statistic is that it that the null hypothesis is expressed not over the data $X_1, X_2, \ldots, X_n$ generated by a random variable X, but over the **sampling distribution of the mean** of such data under repeated sampling. We discussed the sampling distribution in section 7, but I present the same idea in a different way below.

Suppose I gather independent and identically distributed data $x_1, \ldots, x_n$, each of which is generated by a random variable X.

For each sample, suppose I compute the mean $\bar{x}$. Now, $\bar{X}$ is also a random variable; it is just a linear combination of values generated by instances of the random variable X, which, we will assume, has some mean (expectation) μ and some variance σ^2:

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X = \frac{1}{n}X_1 + \cdots + \frac{1}{n}X_n \tag{137}$$

So, its expectation is

$$\begin{aligned} E[\bar{X}] =& E[\frac{1}{n}X_1 + \cdots + \frac{1}{n}X_n] \\ =& \frac{1}{n}(E[X] + \cdots + E[X]) \\ =& \frac{1}{n}(\mu + \cdots + \mu) \\ =& \frac{1}{n}n\mu \\ =& \mu \end{aligned} \tag{138}$$

And its variance is

$$\begin{aligned} Var(\bar{X}) =& Var(\frac{1}{n}X_1 + \cdots + \frac{1}{n}X_n) \\ =& \frac{1}{n^2}Var(X_1 + \cdots + X_n) \end{aligned} \tag{139}$$

Now, $X_1, \ldots, X_n$ are independent. We will use the fact that the variance of the sum of independent RVs is the sum of their variances. (If they were not independent, then the variance of the sum would have to take covariance between the X's into account; more on this later). This gives us:

$$\begin{aligned}\frac{1}{n^2}Var(X_1 + \cdots + X_n) &= \frac{1}{n^2}(Var(X) + \cdots + Var(X)) \\ &= \frac{1}{n^2} n Var(X) \\ &= \frac{1}{n} Var(X) \\ &= \frac{\sigma^2}{n}\end{aligned} \tag{140}$$

We have derived the very important result that the mean and variance of the sampling distribution of the sample means is

$$E[\bar{X}] = \mu \quad Var(\bar{X}) = \frac{\sigma^2}{n} \tag{141}$$

The practical implication of this result is huge. From a *single* sample $x_1, \ldots, x_n$, we can derive the distribution of hypothetical sample means under repeated sampling. That is, we can say something about what the plausible and implausible values of the sample mean are. This is the basis for all hypothesis testing and statistical inference in the frequentist framework we are studying.

Note that I was careful above to not stipulate that X is normally distributed. As discussed in section 7, one amazing fact is that, as long as X has a mean and variance defined for it, the sampling distribution of the sample mean $\bar{X}$ will have a normal distribution if sample size n is large enough. There statement is called the Central Limit Theorem, which I will write compactly as:

$$\bar{X} \sim N(\mu, \sigma^2/n) \quad X \sim f(X), E[X] = \mu, Var(X) = \sigma^2 \quad n \text{ large} \tag{142}$$

In our linear model example above, the variance estimate of β is an estimate of σ^2/n. This is the square of the standard error ($\sigma/\sqrt{n}$). Make sure you distinguish it from the standard deviation σ; note that $\sigma/\sqrt{n}$ is also a standard deviation, but it's the standard deviation of the sampling distribution of the sample mean.

8.6 Hypothesis testing using the likelihood ratio

Suppose now that we have some data $x_1, \ldots, x_n$ from a random variable X whose distribution depends on the parameter θ. Suppose also that we want to test a hypothesis H_0 against H_1.

Define the **likelihood ratio test statistic** as

$$\lambda = 2\{\ell(\theta_1) - \ell(\theta_0)\} \tag{143}$$

where θ_1 and θ_0 are the estimates of θ under the alternative and null hypotheses, respectively. The likelihood ratio test rejects H_0 if λ is sufficiently large. As the sample size approaches infinity,

$$\lambda = \chi^2_r \tag{144}$$

where r is called degrees of freedom and is the difference in the number of parameters estimated under H_1 and H_0. This is called Wilks' theorem.

Note that sometimes you will see the form:

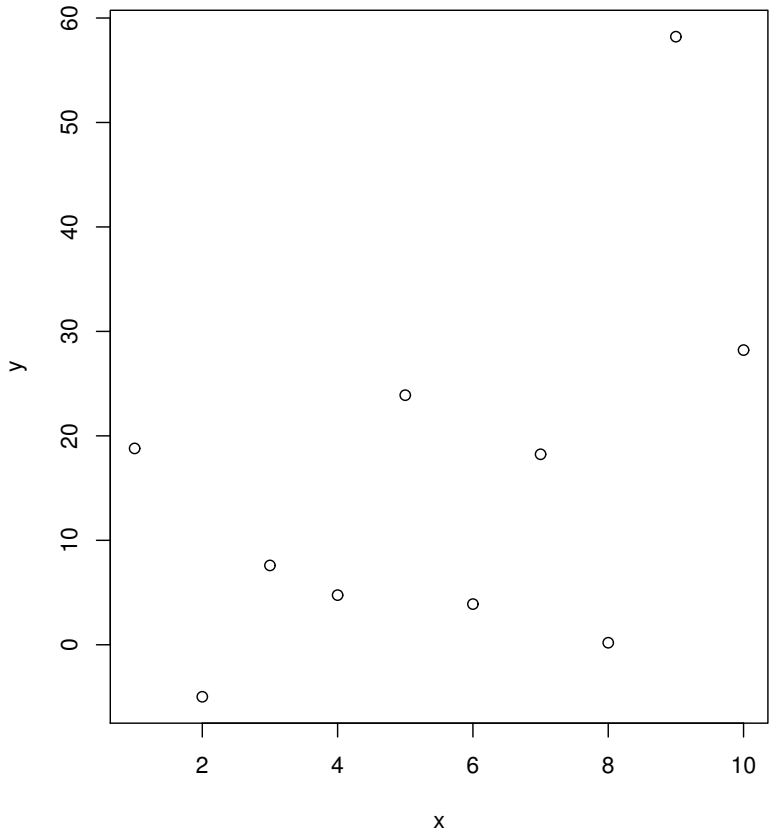
$$\lambda = -2\{\ell(\theta_0) - \ell(\theta_1)\} \tag{145}$$

I hope it is clear that both statements are saying the same thing; in the second case, we are just subtracting the alternative hypothesis log likelihood from the null hypothesis log likelihood.

A practical example will make the usage of this test clear. Let's just simulate a linear model:

```
x<-1:10
y<- 10 + 2*x+rnorm(10,sd=10)
```

```
plot(x,y)
```




```r
## null hypothesis model:
m0<-lm(y~1)
## alternative hypothesis model:
m1<-lm(y~x)
```

```r
lambda<- -2*(logLik(m0)-logLik(m1))
## observed value:
lambda[1]
```

```
## [1] 3.008948
```

```r
## critical value:
qchisq(0.95,df=1)
```

```
## [1] 3.841459
```

```r
# p-value:
pchisq(lambda[1],df=1,lower.tail=FALSE)
```

```
## [1] 0.08280602
```

Here, we fit the null hypothesis model which only has an intercept term β_0, and the alternative model that has β_1 as well. Finally, we compare the λ with the critical chi-squared value for degrees of freedom 1. We also computed the probability of getting a λ as extreme as we got assuming that the null is true:

Note that in the likelihood test above, we are comparing one nested model against another: the null hypothesis model is nested inside the alternative hypothesis model.

Another way to test hypotheses is to use analysis of variance, or ANOVA.

8.7 *Hypothesis testing using Analysis of variance (ANOVA)*

We can compare two models, one nested inside another, as follows:

```
anova(m0,m1)

## Analysis of Variance Table
##
## Model 1: y ~ 1
## Model 2: y ~ x
##   Res.Df    RSS Df Sum of Sq      F Pr(>F)
## 1      9 3039.3
## 2      8 2249.6  1    789.75 2.8085 0.1323
```

The F-score you get here is actually the square of the t-value you get in the linear model summary:

```
sqrt(anova(m0,m1)$F[2])

## [1] 1.675869

summary(m1)$coefficients[2,3]

## [1] 1.675869
```

This is because $t^2 = F$. The proof is discussed on page 9 of the Dobson and Barnett book.

The ANOVA works as follows. First define the residual as:

$$e = Y - X\hat{\beta} \tag{146}$$

The square of this is:

$$e^T e = (Y - X\hat{\beta})^T (Y - X\hat{\beta}) \tag{147}$$

Define the **deviance** as:

$$\begin{aligned} D =& \frac{1}{\sigma^2}(Y - X\hat{\beta})^T(Y - X\hat{\beta}) \\ =& \frac{1}{\sigma^2}(Y^T - \hat{\beta}^T X^T)(Y - X\hat{\beta}) \\ =& \frac{1}{\sigma^2}(Y^T Y - Y^T X\hat{\beta} - \hat{\beta}^T X^T Y + \beta^T X^T X\hat{\beta}) \\ =& \frac{1}{\sigma^2}(Y^T Y - \hat{\beta}^T X^T Y) \end{aligned} \tag{148}$$

Notice that $-Y^T X\hat{\beta} + \beta^T X^T X\hat{\beta} = 0$; they are scalar 1×1.

Assume that we have data of size n. Now suppose we have a null hypothesis $H_0 : \beta = \beta_0$ and an alternative hypothesis $H_1 : \beta = \beta_1$. Let the null hypothesis have q parameters, and the alternative p, where $q < p < n$. Let X_0 be the design matrix for H_0, and X_1 the design matrix for H_1. Compute the deviances D_0 and D_1 for each hypothesis, and compute ΔD:

$$\begin{aligned} \Delta D =& D_0 - D_1 = \frac{1}{\sigma^2}[(Y^T Y - \hat{\beta}_0 X_0^T Y) - (Y^T Y - \hat{\beta}_1 X_1^T Y)] \\ =& \frac{1}{\sigma^2}[\hat{\beta}_1 X_1^T Y - \hat{\beta}_0 X_0^T Y] \end{aligned} \tag{149}$$

It turns out that the F-statistic has the following distribution if the null hypothesis is true:

$$F = \frac{\Delta D/(p-q)}{D_1/(n-p)} \sim F(p-q, n-p) \tag{150}$$

So, an extreme value of F is inconsistent with the null and we reject it.

The F-statistic is:

$$\begin{aligned} F =& \frac{\Delta D/(p-q)}{D_1/(n-p)} \\ =& \frac{\hat{\beta}_1 X_1^T Y - \hat{\beta}_0^T X_0^T Y}{p-q} \Big/ \frac{Y^T Y - \hat{\beta}_1^T X_1^T Y}{n-p} \end{aligned} \tag{151}$$

Traditionally, the way the F-test is summarized is:

Source of variance	df	Sum of squares	Mean square
Model with β_0	q	$\beta_0^T X_0^T Y$	
Improvement due to β_1	p-q	$\hat{\beta}_1 X_1^T Y - \hat{\beta}_0^T X_0^T Y$	$\frac{\hat{\beta}_1 X_1^T Y - \hat{\beta}_0^T X_0^T Y}{p-q}$
Residual	n-p	$Y^T Y - \hat{\beta}_1^T X_1^T Y$	$\frac{Y^T Y - \hat{\beta}_1^T X_1^T Y}{n-p}$
Total	n	$y^T y$	

Table 2: default

There is much more to say here about ANOVA, but this is the basic idea.

8.8 Multiple regression

You are already familiar with multiple regression from the Gelman and Hill book, so I will not discuss this in much detail, except to note that in multiple regression an important issue is **multicollinearity**.

This occurs when multiple predictors are highly correlated. The consequence of this is that X^TX can be nearly singular and the estimation equation

$$X^TX\beta = X^TY \tag{152}$$

is ill-conditioned: small changes in the data can cause large changes in β (signs will flip for example). Also, some of the elements of $\sigma^2(X^TX)^{-1}$ will be large–standard errors can covariances can be large.

We can check for multicollinearity using the Variance Inflation Factor, VIF. Consider word length and syllable length as predictors in the Hindi data:

```
library(car)
vif(lm(TFT~syll_len+word_len,hindi10))

## syll_len word_len
## 3.425663 3.425663
```

Here is a somewhat worse situation:

```
m<-lm(TFT ~ word_complex + word_freq + type_freq+
         word_bifreq + type_freq+
         word_len + IC + SC,
       hindi10)
summary(m)

##
## Call:
## lm(formula = TFT ~ word_complex + word_freq + type_freq + word_bifreq +
##     type_freq + word_len + IC + SC, data = hindi10)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -524.8 -149.4  -66.2   74.8 3511.9
##
## Coefficients:
##                Estimate Std. Error t value Pr(>|t|)
## (Intercept)   2.315e+02  8.047e+00  28.763  < 2e-16
## word_complex -3.235e+01  4.452e+00  -7.268 3.84e-13
## word_freq    -9.432e-04  9.789e-04  -0.964   0.3353
```

```
## type_freq    -9.898e-04  5.185e-04  -1.909   0.0563
## word_bifreq  -1.043e-02  5.575e-03  -1.871   0.0613
## word_len      3.540e+01  1.764e+00  20.061  < 2e-16
## IC            1.055e-01  5.042e-01   0.209   0.8342
## SC            1.920e+01  3.896e+00   4.927 8.45e-07
##
## Residual standard error: 248.6 on 14884 degrees of freedom
##   (4775 observations deleted due to missingness)
## Multiple R-squared:  0.05745,Adjusted R-squared:  0.057
## F-statistic: 129.6 on 7 and 14884 DF,  p-value: < 2.2e-16

round(vif(m),digits=3)

## word_complex    word_freq    type_freq  word_bifreq     word_len
##        1.874        4.425        4.455        1.089        2.437
##           IC           SC
##        1.202        1.238
```

If the predictors are uncorrelated, VIF will be near 1 in each case. Dobson et al mention that VIF of greater than 5 is cause for worry.

The definition of VIF_j for a predictor j is:

$$VIF_j = \frac{1}{1 - R_j^2} \tag{153}$$

where R_j^2 is called the coefficient of determination, and quantifies goodness of fit of the model. We define this next.

Recall that the residual sum of squares is

$$e^T e = (Y - X\hat{\beta})^T (Y - X\hat{\beta}) = \hat{S} \tag{154}$$

We can compare this sum of squares with the minimal model, which has $E[Y] = \mu$. In this model, the design matrix is an $n \times 1$ design matrix, so $X^T X = n$:

```
X<-matrix(rep(1,10),ncol=1)
##
t(X)%*%X

##      [,1]
## [1,]   10
```

and $X^T Y = \sum y_i$. And $\hat{\beta} = \hat{\mu} = \bar{y}$. So, for this simple model, the sum of squares $\hat{S}_0$ is:

$$\hat{S}_0 = Y^T Y - n\bar{y}^2 \tag{155}$$

R^2 is defined as follows:

$$R^2 = \frac{\hat{S}_0 - \hat{S}}{\hat{S}_0} = \frac{\hat{\beta} X^T Y - n\bar{y}^2}{Y^T Y - n\bar{y}^2} \tag{156}$$

The interpretation of R^2 is the proportion of variance explained by the model. Note that R^2 always increases if predictors are added, so an adjustment is made, called adjusted R^2:

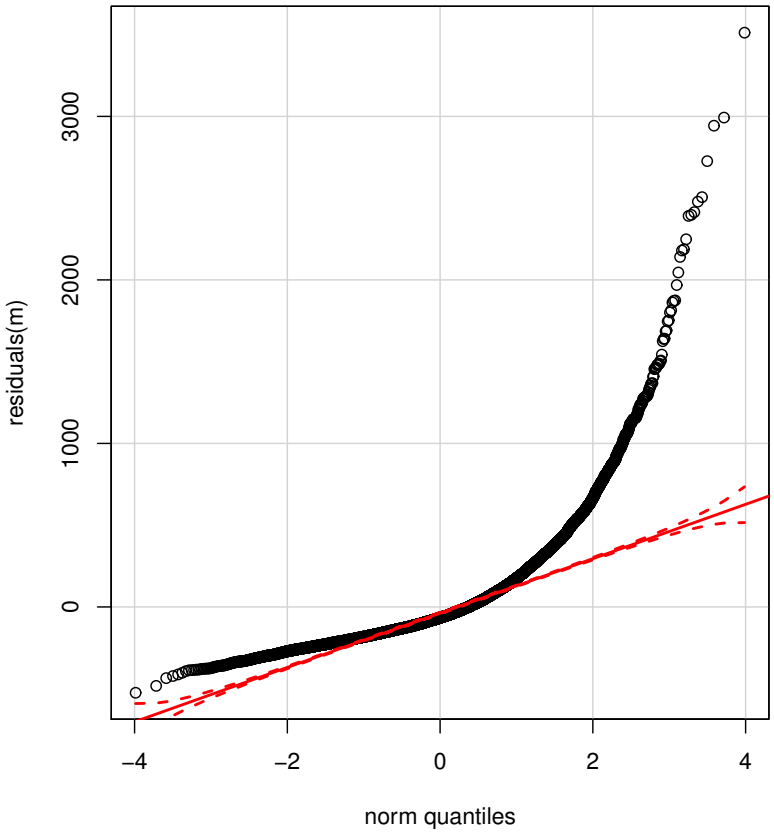
$$R^2_{Adj} = 1 - \frac{((Y - X\hat{\beta})^T (Y - X\hat{\beta}))/(n-p)}{(Y^T Y - n\bar{y}^2)/(n-1)} \tag{157}$$

I will discuss orthogonality of the design matrix later in the course in the context of design of experiments.

8.9 Checking model assumptions

In practical terms, the first thing you need to check is whether the residuals are normally distributed. This can be done by plotting the residuals against the quantiles of the normal distribution:

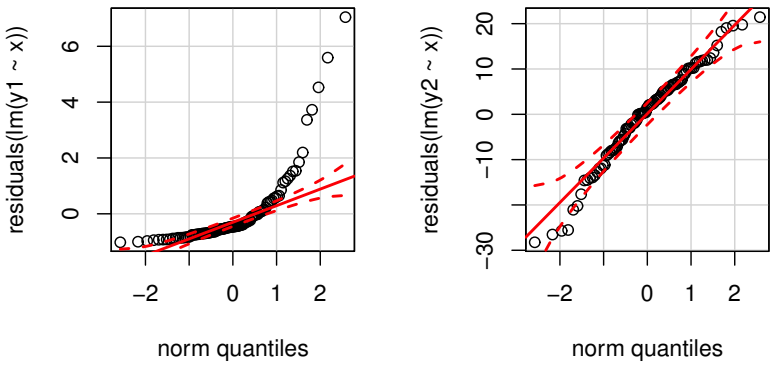
```
library(car)
qqPlot(residuals(m))
```



I have heard people say that there is no need to check for normality of residuals; indeed, Gelman and Hill state that it is the least important assumption in linear models. **However, this is a highly misleading statement and should be disregarded when the goal is null hypothesis testing**.

The normality assumption is necessary for hypothesis testing, but one other consequence of a violation of normality in linguistics is that it can reduce statistical power. We can test this with a simulation. Let's simulate data with non-normal residuals:

```
op<-par(mfrow=c(1,2),pty="s")
x<-1:100
y1<- 10 + 2*x+rchisq(100,df=1)
qqPlot(residuals(lm(y1~x)))
y2<- 10 + 2*x+rnorm(100,sd=10)
qqPlot(residuals(lm(y2~x)))
```



We know that $H_0 : \beta_1 = 0$ is false: it's 0.01. So here is an example of how often the statistical test fails to detect this significant effect compared to the case when the residual is normal.

```
nsim<-1000
n<-100
x<-1:n
store_y1_results<-rep(NA,nsim)
store_y2_results<-rep(NA,nsim)
for(i in 1:nsim){
  e<-rchisq(n,df=1)
  e<-scale(e,scale=F)
  y1<- 10 + 0.01*x + e
  m1<-lm(y1~x)
  store_y1_results[i]<-summary(m1)$coefficients[2,4]
  y2<- 10 + 0.01*x + rnorm(n,sd=1.2)
  m2<-lm(y2~x)
  store_y2_results[i]<-summary(m2)$coefficients[2,4]
```

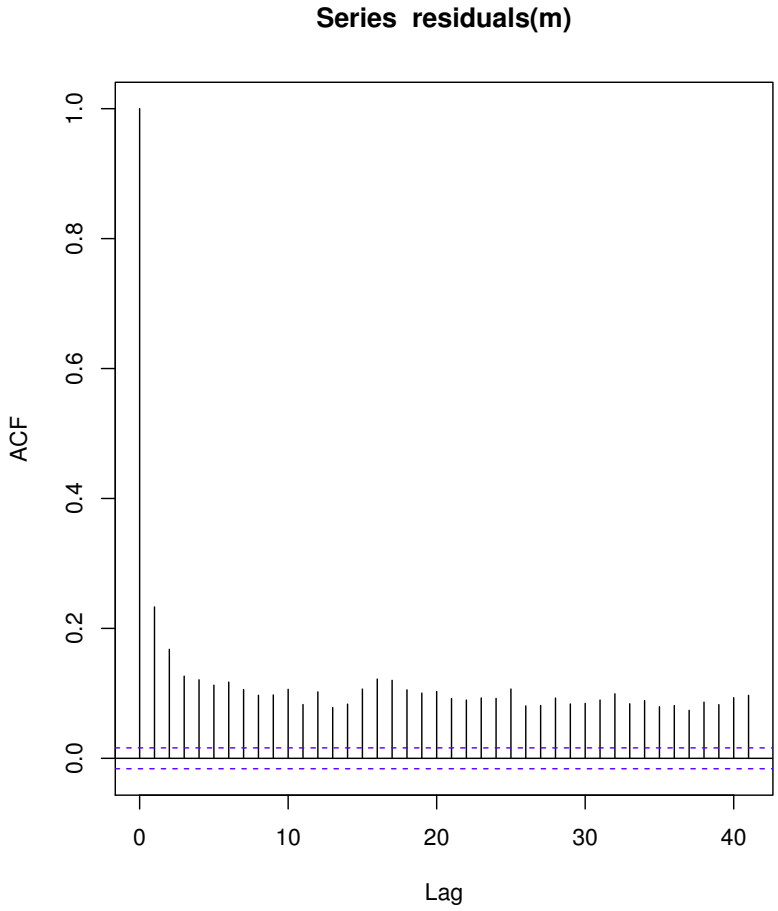
```
}

## power
y1_results<-table(store_y1_results<0.05)
y1_results[2]/sum(y1_results)

##  TRUE
## 0.529

y2_results<-table(store_y2_results<0.05)
y2_results[2]/sum(y2_results)

##  TRUE
## 0.654
```

The above simulation is just a crude demonstration and can be improved on considerably to reflect reality (exercise).

How to test for normality of residuals? Komogorov-Smirnov and Shapiro-Wilk are formal tests of normality and are only useful for large samples; they not very powerful and not much better than diagnostic plots. These tests may be useful as follow-ups if non-normality is suspected.

Apart from normality, we should also check the independence assumption (the errors are assumed to be independent). Index-plots plot residuals against observation number; note that they are not useful for small samples. An alternative is to compute the correlation between e_i, e_{i+1} pairs of residuals. The auto-correlation function is not normally used in linear modeling (it's used more in time-series analyses), but can be used to check for this correlation:

```
acf(residuals(m))
```

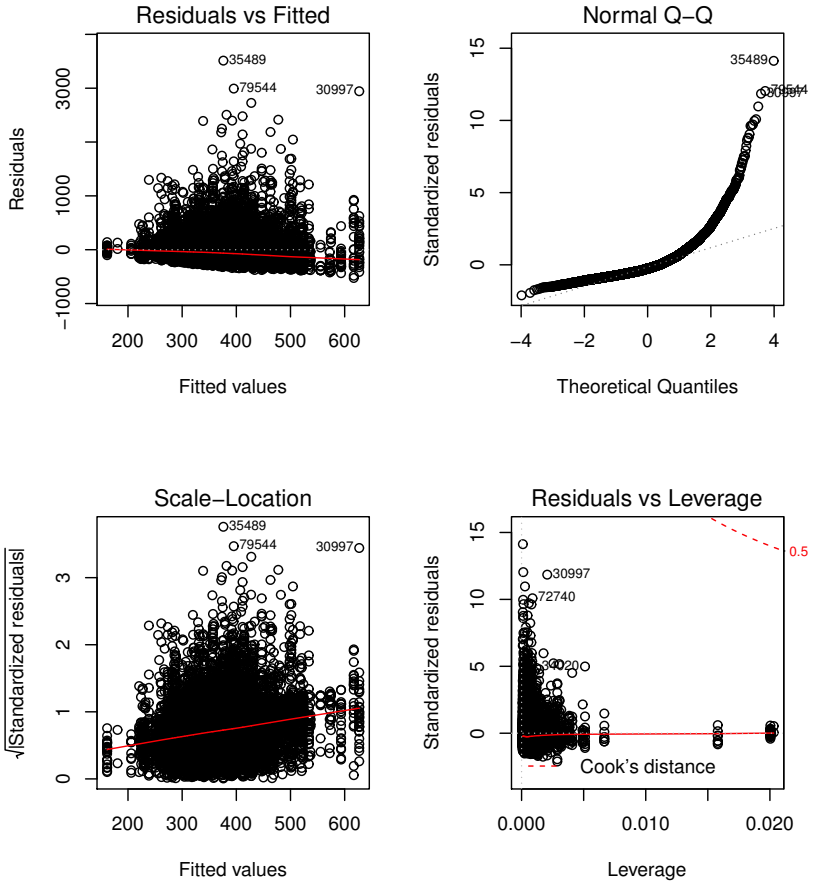


In our model (which is the multiple regression we did in connection with the collinearity issue), we have a serious violation of independence.

Finally, we should check for homoscedasticity (equality of variance). For checking this, plot residuals against fitted values. Fan out suggests violation. A quadratic trend in a plot of residuals against predictor x could suggest that a quadratic predictor term is needed; note that $X^T e = 0$, so we will never have a perfect straight line in such a plot.

R also provides a diagnostics plot, which is generated using the model fit:

```
op<-par(mfrow=c(2,2),pty="s")
plot(m)
```



I explain some relevant concepts next.

Standardized deletion residuals (`studres` in R) We can write

$$e = Y - X\hat{\beta} = Y - X(X^TX)^{-1}X^TY = My \tag{158}$$

where

$$M = I_n - X(X^TX)^{-1}X^T \tag{159}$$

M is symmetric, idempotent $n \times n$.
Define:

$$\hat{\beta}_{-i} = (X_{-i}^TX_{-i})^{-1}X_{-i}^TY_{-i} \tag{160}$$

where the $-i$ refers to removing data point i. Standardized deletion residuals are

$$s_{-i} = \frac{e_i}{\hat{\sigma}_{-i}\sqrt{m_{ii}}} \tag{161}$$

where m_{ii} is the i-th diagonal element of M. We can compute s_{-i} from s_i:

$$s_{-i} = \frac{s_i\sqrt{n-p-1}}{\sqrt{n-p-s_i^2}} \sim t_{n-p-1} \tag{162}$$

If n is large, $s_{-i} \approx s_i$.

Influence and leverage (See `lm.influence$hat` in R)

A point can influence the parameter estimates without being an exceptional outlier. Influence does not depend on "outlyingness". Potential to influence (e.g., by being an extreme x value) is called leverage; once the y value is also extreme, we have influence. I.e., it takes an extreme x and y value to be influential, and it takes only an extreme x value to have leverage.

Leverage more formally defined: recall that $M = I_n - X(X^TX)^{-1}X^T$. Define a hat matrix $H = I - M = X(X^TX)^{-1}X^T$. It's called a hat matrix because it puts a hat on y: $\hat{y} = X\hat{\beta} = Hy$. Since x_i^T is the i-th row of X, we have $h_{ii} = x_i^T(X^TX)^{-1}x_i$. The measure for leverage is:

$$h_{ii} = 1 - m_{ii} \tag{163}$$

Notice that h_{ii} is a scalar, so trace$(h_{ii}) = h_{ii}$. So (because for a square matrix A,B, tr(AB)= tr(BA)):

$$h_{ii} = tr(x_i^T(X^TX)^{-1}x_i) = tr(x_i^Tx_i(X^TX)^{-1}) \tag{164}$$

Since $X^TX = \sum_{i=1}^n x_ix_i^T$, h_{ii} represents the magnitude of $x_ix_i^T$ relative to the sum of the values for all observations. Note that h_{ii} only depends on X.

Also note that

$$\sum_{i=1}^{n} h_{ii} = tr(X^TX(X^TX)^{-1}) = tr(I_p) = p \quad mean(h_{ii}) = p/n \tag{165}$$

h_{ii} measures leverage because $Var(e_i) = \sigma^2 m_{ii} = \sigma^2(1-h_{ii})$ and $Var(\hat{y}_i) = \sigma^2 h_{ii}$. Therefore h_{ii} has to lie between 0 and 1. When it is close to one, the fitted value will be close to the actual value of y_i—signalling potential for leverage.

A cutoff one can use to identify high leverage points is $h_{ii} > 2p/n$ or $h_{ii} > 3p/n$.

The leverage of a data point is directly related to how far away it is from the mean:

$$h_{ii} = n^{-1} + \frac{(x_i - \bar{x})^2}{S_{xx}} \tag{166}$$

Cook's distance D: A measure of influence Let s_i be the i-th standardized residual, $\hat{\beta}_{-i}$ the estimate of the vector of parameters with the i-th row removed.

$$D_i = \frac{(\hat{\beta} - \hat{\beta}_{-i})^T (X^T X)^{-1} (\hat{\beta} - \hat{\beta}_{-i})}{p\hat{\sigma}^2} = \frac{s_i^2 h_{ii}}{p(1 - h_{ii})} \tag{167}$$

A data point is influential if it is outlying as well as high leverage. Cutoff for Cook's distance is $\frac{4}{n}$.

8.10 Correcting for multiple testing

This is relevant if you are doing null hypothesis significance testing.

Suppose we are performing n tests and in each test we specify the probability of making a type I error to be β (note: don't confuse this as type II error). Then, if the tests are independent, the probability of at least one false positive claim in the n tests is given by

$$1 - (1 - \beta)^n = \alpha \Leftrightarrow \beta = 1 - (1 - \alpha)^{1/n} \tag{168}$$

This is called the Šidák correction, and has a stronger bound than the Bonferroni correction and so has greater statistical power.

The Bonferroni just divides β with the number of statistical tests done. So 10 tests would give a corrected α of 0.05/10=0.005.

8.11 Transformations: Box-Cox procedure

If the normality assumption is not satisfied, what can we do? One option is to relax the assumption that the errors are normally distributed; we will see this in the Bayesian part of the course.

The more conventional thing to do is to find a transformation of the random variable Y such that the errors are normally distributed. Let's assume that there exists a transformation $f_\lambda(Y)$ such that

$$f_\lambda(y_i) = x_i^T \beta + \epsilon_i \quad \epsilon_i \sim N(0, \sigma^2) \tag{169}$$

The function f_λ is a family of transformations, so for any particular value of λ, we can define a transformation $z_\lambda = f_\lambda(y)$ on our dependent variable. An example is the log transform. Another example is the reciprocal transform. A third example is the square root transform.

We use maximum likelihood estimation to estimate λ. Note that $L(\beta_\lambda, \sigma_\lambda^2, \lambda; y) \propto$

$$(\frac{1}{\sigma})^n \exp[-\frac{1}{2\sigma^2} \sum [f_\lambda(y_i) - x_i^T \beta]^2] [\underbrace{\prod f'_\lambda(y_i)}_{\text{Jacobian}}] \tag{170}$$

For fixed λ, we first estimate $\hat{\beta}$ and $\hat{\sigma}^2$ using the usual MLE methods we learnt. So, we first choose $\hat{\beta}$ to minimize the residual sum of

squares in the exponent. Call this S_λ. Maximization with respect to σ^2 gives $\hat{\sigma}^2_\lambda = S_\lambda / n$.

The Likelihood is going to be proportional to $\hat{\sigma}$ times the Jacobian:

$$L(\hat{\beta}_\lambda, \hat{\sigma}^2_\lambda, \lambda; y) \propto S_\lambda^{-n/2} \prod f'_\lambda(y_i) \tag{171}$$

Next, we will take logs and then maximize with respect to λ:

$$\ell = c - \frac{n}{2} \log S_\lambda + \sum \log f'_\lambda(y_i) \tag{172}$$

The above is a general procedure, but an often used family of transformations is the power transformation, proposed in a famous paper by Box and Cox.[12] This family corrects non-normality and/or unequal variance.

[12] George E.P. Box and David R. Cox. An analysis of transformations. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 211–252, 1964

If the response is positive, the transformation is

$$f_\lambda(y) = \begin{cases} \frac{y^\lambda - 1}{\lambda} & \lambda \neq 0 \\ \log y & \lambda = 0 \end{cases} \tag{173}$$

We assume that $f_\lambda(y) \sim N(x_i^T \beta, \sigma^2)$. So we have to just estimate λ by MLE, along with β. Here is how to do it by hand:

Since $f_\lambda = \frac{y^\lambda - 1}{\lambda}$, it follows that $f'_\lambda(y) = y^{\lambda - 1}$.

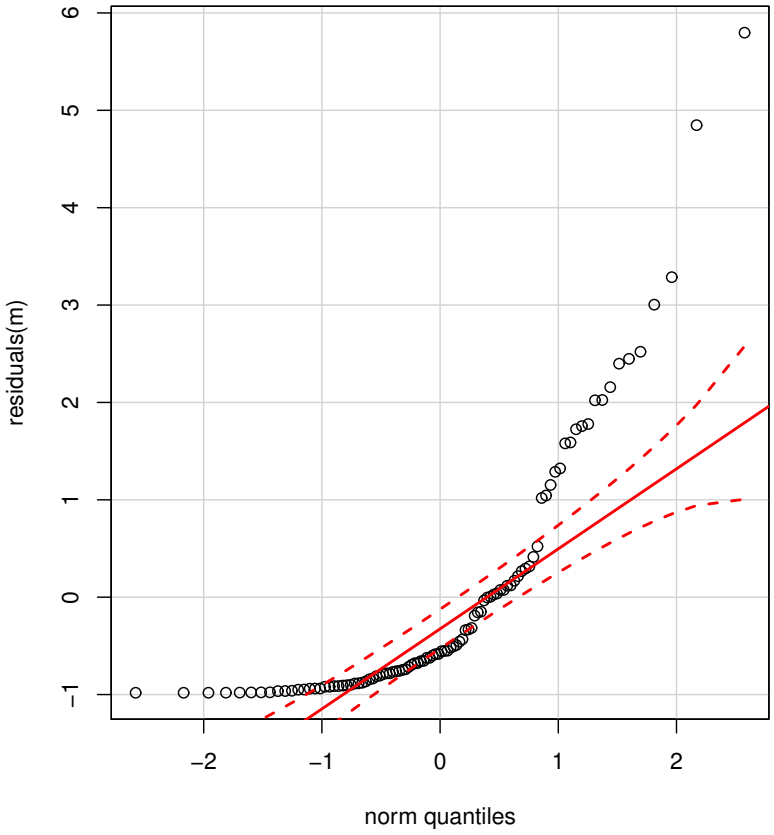
Now, for different λ you can figure out the log likelihoods by hand by solving this equation (remember that this is for a specific data-set and model, i.e., we are given y and can compute S_λ:

$$\ell = c - \frac{n}{2} \log \underset{\uparrow}{S_\lambda} + (\lambda - 1) \sum \log(y_i) \tag{174}$$

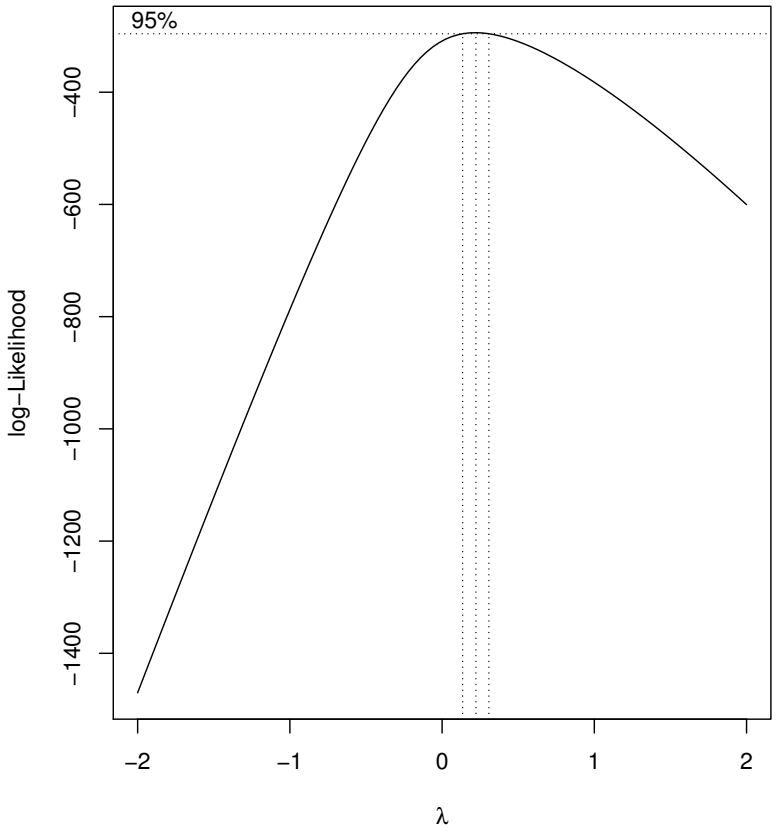
Residual sum of squares

We illustrate this using R. If we have non-normal residuals, we can use the boxcox function to determine the relevant transform. Here, the function estimates that $\lambda = 0$, hence a log transform is suggested.

```
## generate some non-normally distributed data:
data<-rchisq(100,df=1)
m<-lm(data~1)
qqPlot(residuals(m))
```




```
library(MASS)
## suggests log:
boxcox(m)

m<-lm(log(data)~1)
```



9 Generalized Linear Models

9.1 Introduction: Logistic regression

We start with an example data-set that appears in the Dobson et al book: the Beetle dataset.

This data-set shows the number of beetles killed when they were exposed to different doses of some toxic chemical.

```
(beetle<-read.table("datacode/beetle.txt",header=TRUE))

##     dose number killed
## 1 1.6907     59      6
## 2 1.7242     60     13
## 3 1.7552     62     18
## 4 1.7842     56     28
## 5 1.8113     63     52
```

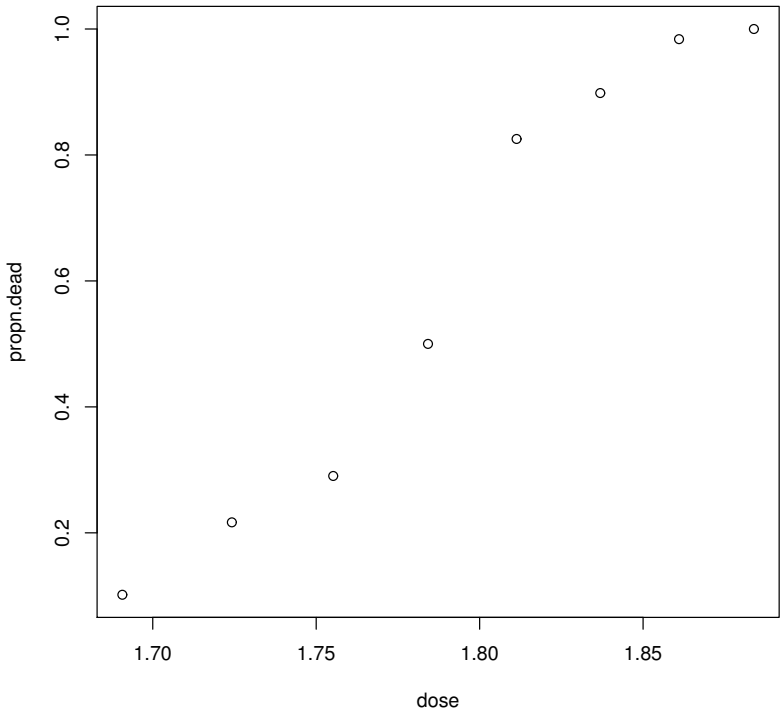
```
## 6 1.8369     59     53
## 7 1.8610     62     61
## 8 1.8839     60     60
```

The research question is: does dose affect probability of killing insects? The first thing we probably want to do is calculate the proportions:

```
(beetle$propn.dead<-beetle$killed/beetle$number)

## [1] 0.1016949 0.2166667 0.2903226 0.5000000 0.8253968 0.8983051 0.9838710
## [8] 1.0000000
```

It's also reasonable to just plot the relationship between dose and proportion of deaths.

```
with(beetle,plot(dose,propn.dead))
```



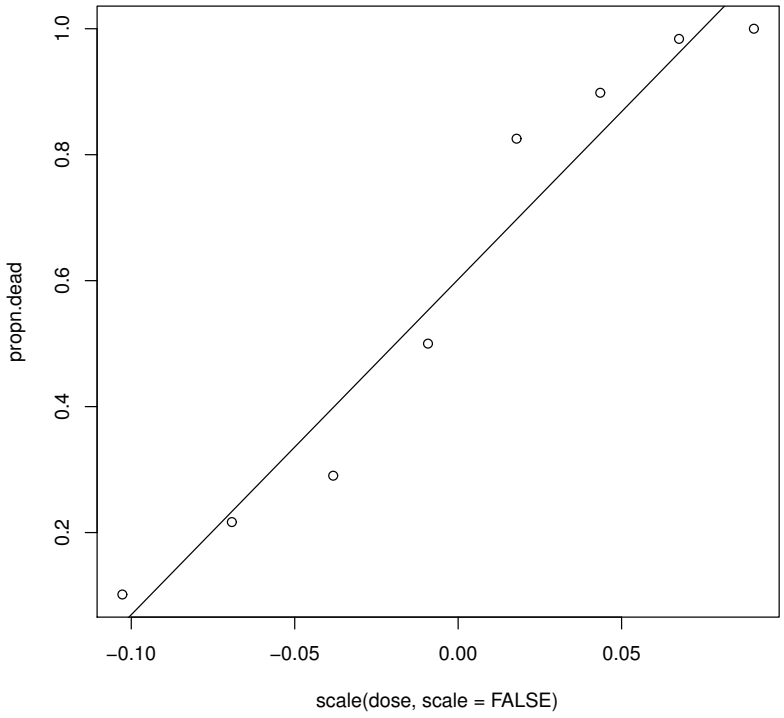
Notice that the y-axis is by definition bounded between 0 and 1.

We could easily fit a linear model to this data-set. We may want to center the predictor, for reasons discussed earlier:

```r
fm<-lm(propn.dead~scale(dose,scale=FALSE),beetle)
summary(fm)
```

```
##
## Call:
## lm(formula = propn.dead ~ scale(dose, scale = FALSE), data = beetle)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.10816 -0.06063  0.00263  0.05119  0.12818
##
## Coefficients:
##                             Estimate Std. Error t value Pr(>|t|)
## (Intercept)                  0.60203    0.03065   19.64 1.13e-06
## scale(dose, scale = FALSE)  5.32494    0.48573   10.96 3.42e-05
##
## Residual standard error: 0.08669 on 6 degrees of freedom
## Multiple R-squared:  0.9524,Adjusted R-squared:  0.9445
## F-statistic: 120.2 on 1 and 6 DF,  p-value: 3.422e-05
```

```r
with(beetle,plot(scale(dose,scale=FALSE),
                 propn.dead))
abline(coef(fm))
```



What's the interpretation of the coefficients?

Clearly the linear model is failing us here. This is the motivation for the generalized linear model.

Instead of using the linear model, we model log odds instead of proportions as a function of dose. Odds are defined as:

$$\frac{p}{1-p} \tag{175}$$

and taking the log will give us log odds.

We are going to model log odds (instead of probability) as a linear function of dose.

$$\log \frac{p}{1-p} = \beta_0 + \beta_1 \text{dose} \tag{176}$$

The model above is called the logistic regression model.

Once we have estimated the β parameters, we can move back from the log odds space to probability space using simple algebra.

Given a model like

$$\log \frac{p}{1-p} = \beta_0 + \beta_1 \text{dose} \tag{177}$$

If we exponentiate each side, we get:

$$\exp \log \frac{p}{1-p} = \frac{p}{1-p} = \exp(\beta_0 + \beta_1 \text{dose}) \tag{178}$$

So now we just solve for p, and get (check this):

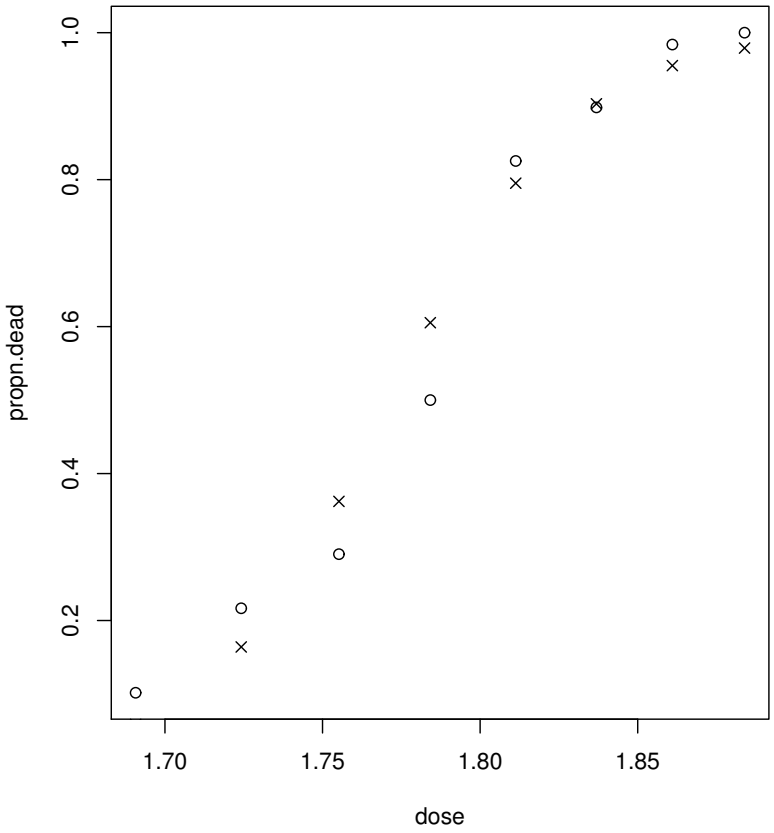
$$p = \frac{\exp(\beta_0 + \beta_1 \text{dose})}{1 + \exp(\beta_0 + \beta_1 \text{dose})} \tag{179}$$

We fit the model in R as follows. Note that as long as I am willing to avoid interpreting the intercept and just interpret the estimate of β_1, there is no need to center the predictor here:

```
fm1<-glm(propn.dead~dose,
         binomial(logit),
         weights=number,
         data=beetle)
summary(fm1)

##
## Call:
## glm(formula = propn.dead ~ dose, family = binomial(logit), data = beetle,
##     weights = number)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.5941  -0.3944   0.8329   1.2592   1.5940
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -60.717      5.181  -11.72   <2e-16
## dose          34.270      2.912   11.77   <2e-16
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 284.202  on 7  degrees of freedom
## Residual deviance:  11.232  on 6  degrees of freedom
## AIC: 41.43
##
## Number of Fisher Scoring iterations: 4
```

We can also plot the observed proportions and the fitted values together; the fit looks pretty good.

```
plot(propn.dead~dose,beetle)
points(fm1$fitted~dose,beetle,pch=4)
```



We can now compute the log odds of death for concentration 1.7552 (for example):

```
## compute log odds of death for
## concentration 1.7552:
x<-as.matrix(c(1, 1.7552))
#log odds:
(log.odds<-t(x)%*%coef(fm1))

##            [,1]
## [1,] -0.5661788
```

We can also obtain the variance-covariance matrix of the fitted coefficients:

```
### compute CI for log odds:
## Get vcov matrix:
(vcovmat<-vcov(fm1))
```

```
##             (Intercept)       dose
## (Intercept)    26.83966 -15.082090
## dose          -15.08209   8.480525

## x^T VCOV x for dose 1.7552:
(var.log.odds<-t(x)%*%vcovmat%*%x)

##           [,1]
## [1,] 0.0216782
```

And using a normal approximation, based on the asymptotic properties discussed in section 7, we can compute the confidence interval for the probability of death given dose 1.7552:

```
##lower
log.odds-1.96*sqrt(var.log.odds)

##            [,1]
## [1,] -0.8547598

##upper
log.odds+1.96*sqrt(var.log.odds)

##            [,1]
## [1,] -0.2775979
```

Note that one should not try to predict outside the range of the design matrix. For example, in the beetle data, the dose ranges from 1.69 to 1.88. We should not try to compute probabilities for dose 2.5, say, since we have no knowledge about whether the relationship remains unchanged beyond the upper bound of our design matrix.

9.2 *Multiple logistic regression: Example from Hindi data*

In the Hindi data, we can compute skipping probability, the probability of skipping a word entirely (i.e., never fixating it). We first have to create a vector that has value 1 if the word has 0 ms total reading time, and 0 otherwise.

```
skip<-ifelse(hindi10$TFT==0,1,0)
hindi10$skip<-skip
fm_skip<-glm(skip ~ word_complex+SC,family=binomial(),hindi10)
```

The above example also illustrates the second way to set up the data for logistic (multiple) regression: the dependent variable can simply be a 1,0 value instead of proportions. So, in the beetle data, you could recode the data to have 1s and 0s instead of proportions. Assuming that

you have recoded the column for status (dead or alive after exposure), the glm function call would be:

```
glm(dead~dose,family=binomial(),beetle)
```

Note that logistic regression assumes independence of each data point; this assumption is violated in the Hindi data.

9.3 Some theory for GLMs

We have considered linear models like

$$E[Y_i] = \mu_i = x_i^T \beta \quad y_i \sim N(\mu_i, \sigma^2) \tag{180}$$

GLMs allow us to stay within the linear modeling framework, even if the relationship betwen response and explanatory variable is not linear.

There is a wider class of distributions beyond the two we have seen (normal, binomial), that are called the **exponential family of distributions**; the normal and binomial fall within this family.

The likelihood function of the exponential family's distributions can be written in very general terms as follows:

$$f(y; \theta_i, \phi) = \exp\left[\frac{y\theta_i - b(\theta_i)}{\phi/w} + c(y, \phi)\right] \tag{181}$$

Example 1: The normal distribution Consider the normal distribution. We can write it in the general form of equation 181.

$$\begin{aligned} f(y) =& \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{(y-\mu)}{\sigma}\right)^2\right] \\ =& \exp\left[\log 1 - \log\sigma\sqrt{2\pi} - \frac{1}{2}\left(\frac{(y-\mu)}{\sigma}\right)^2\right] \\ =& \exp\left[-\frac{1}{2}(\frac{y^2+\mu^2-2y\mu}{\sigma^2}) - \log\sigma\sqrt{2\pi}\right] \end{aligned} \tag{182}$$

A little bit of algebraic manipulation (exercise) will now give us:

$$\begin{aligned} &= \exp\left[\frac{y\mu}{\sigma^2} - \frac{\mu^2}{2\sigma^2} - \frac{y^2}{2\sigma^2} + \frac{\log\sigma\sqrt{2\pi}}{2}\right] \\ &= \exp\left[\frac{y\mu - \mu^2/2}{\sigma^2} + c(y,\phi)\right] \quad \text{i.e., } c(y,\phi) = -\frac{y^2}{2\sigma^2} + \frac{\log\sigma\sqrt{2\pi}}{2} \\ &= \exp\left[\frac{y\theta - b(\theta)}{\phi/w} + c(y,\phi)\right] \end{aligned} \tag{183}$$

Here, $\theta = \mu$, $\phi = \sigma^2$, $w = 1$, and we have $b(\theta) = \mu^2/2$, $c(y, \phi) = -\frac{y^2}{2\sigma^2} + \frac{\log \sigma\sqrt{2\pi}}{2}$.

This general formulation gives us two useful results (not proved here, because that would take us too far afield; but I will try to add the full proof later if there is interest):

1. The first derivative of $b(\theta) = \frac{\mu^2}{2}$, is $b'(\theta) = \mu$. This is a general result for the exponential family:
   $E[y] = b'(\theta) = \mu$
2. The variance of Y is $Var(Y) = \frac{\phi}{w} b''(\theta)$. So, here, we'd get
   $Var(Y) = \frac{\sigma^2}{1} 1 = \sigma^2$

Example 2: Binomial distribution Let's look at another example of how we can write an exponential family distribution in this general form. Consider the binomial distribution, which we will start by writing as below. Here, n is the total number of trials, and y is the proportion of successes. For example, n=10, y=7/10, gives us 7 successes out of 10. This is just another way to parameterize the binomial distribution, although it is not one that you have seen before.

$$ny \sim Binomial\left(n, \frac{\exp(\theta)}{1+\exp(\theta)}\right) \quad \text{i.e., } p = \frac{\exp(\theta)}{1+\exp(\theta)} \tag{184}$$

$$\begin{aligned} f(ny;\theta,\phi) &= \binom{n}{ny} p^{ny}(1-p)^{n-ny} \\ &= \exp\left[\log\binom{n}{ny} + ny\log p + (n-ny)\log(1-p)\right] \\ &= \exp\left[ny\log\frac{p}{1-p} + n\log(1-p) + c(y,\phi)\right] \quad \text{i.e., } c(y,\phi) = \log\binom{n}{ny} \end{aligned} \tag{185}$$

Since $p = \frac{\exp(\theta)}{1+\exp(\theta)}$, we can write

$$n\log(1-p) = n\log\frac{1}{1+\exp(\theta)} = -n\log(1+\exp(\theta)) \tag{186}$$

Also, let $\theta = \log\frac{p}{1-p}$.

Then, we can continue as follows:

$$\begin{aligned} f(ny;\theta,\phi) &= \exp\left[ny\log\frac{p}{1-p} + n\log(1-p) + c(y,\phi)\right] \quad \text{i.e., } c(y,\phi) = \log\binom{n}{ny} \\ &= \exp\left[ny\theta - n\log(1+\exp(\theta)) + c(y,\phi)\right] \\ &= \exp\left[\frac{y\theta - b(\theta)}{\phi/n} + c(y,\phi)\right] \quad \text{i.e., } b(\theta) = n\log(1+\exp(\theta)) \end{aligned} \tag{187}$$

9.4 The canonical link

For each data point Y_i from a distribution that's a member of the exponential family, the general form of the likelihood function is:

$$f(y;\theta_i,\phi) = \exp\left[\frac{y\theta_i - b(\theta_i)}{\phi/w} + c(y,\phi)\right] \tag{188}$$

where $E[Y_i] = \mu_i = h(x_i^T\beta)$. Since we know that $E[Y_i] = b'(\theta_i)$, we can write

$$E(Y_i) = \mu_i = h(x_i^T\beta) = b'(\theta) \tag{189}$$

Now, if we want to get $x_i^T\beta$, we just take the inverse of the function $h(\cdot)$, call it $g(\cdot)$. This gives us something called the canonical link function:

$$x_i^T\beta = h^{-1}(b'(\theta)) = \underset{\text{canonical link}}{\underset{\uparrow}{g}}b'(\theta) \tag{190}$$

For different distributions in the exponential family, the canonical link functions are as follows:

Distribution	$h(x_i^T\beta) = \mu_i$	$g(\mu_i) = \theta_i$
Binomial logit link	$\frac{\exp[\theta_i]}{1+\exp[\theta_i]}$	$\log\frac{y}{1-y}$
Normal identity	θ	$g = h$
Poisson log	$\exp[\theta]$	$\log[\mu]$
Gamma inverse	$-\frac{1}{\theta}$	$-\frac{1}{\mu_i}$
Cloglog cloglog	$1-\exp[-\exp[\theta_i]]$	$\log(-\log(1-\mu_i))$
Probit probit	$\Phi(\theta)$	$\Phi^{-1}(\theta)$ (qnorm)

The big thing about the canonical link is that is expresses θ_i as a linear combination of the parameters: $x_i^T\beta$. You can decide which link to use by plotting $g(\mu_i)$ against the predictor (in case we have only a single predictor x).

9.5 Estimation of parameters

In linear models, we know how to estimate the β parameters:

$$\hat{\beta} = (X^TX)^{-1}X^TY \tag{191}$$

and the covariance matrix is $\sigma^2(X^TX)^{-1}$.

For reasons we won't get into in this course, in GLMs we use **iteratively reweighted least squares**. Here is how it works:

1. Specify an **initial vector of parameters**: $b^{(m)} = (\beta_0, \ldots, \beta_p)^T$, where initially $m = 1$:

```
## eta=xbeta:
eta.i<- -60+35*beetle$dose
```

2. **Specify a weight matrix W** that depends on current parameter estimates:

   If we define:

$$w_{ii} = \frac{n_i \exp[\eta_i]}{(1 + \exp[\eta_i])^2} \tag{192}$$

   we can compute W:

```
n.i <- beetle$number
w.ii.fn<-function(n.i,eta.i){
  (n.i*exp(eta.i))/(1+exp(eta.i))^2
}
w.iis<-w.ii.fn(n.i,eta.i)
##weights matrix:
W<-diag(as.vector(w.iis))
```

3. **Specify a vector z** that depends on the current parameter estimates and response values:

$$z_i = \eta_i + \frac{y_i - \mu_i}{\mu_i(1 - \mu_i)} \quad \mu_i = \frac{exp[\eta_i]}{1 + exp[\eta_i]} \tag{193}$$

```
mu.i<-exp(eta.i)/(1+exp(eta.i))
z.i<-eta.i + ((beetle$propn.dead-mu.i))/
             (mu.i*(1-mu.i))
```

4. Compute new estimate of parameters: $b^{(m+1)} = (X^TWX)^{-1}X^TWz$:

```
##The design matrix:
col1<-c(rep(1,8))
X<-as.matrix(cbind(col1,beetle$dose))
## update coefs:
eta.i<-solve(t(X)%*%W%*%X)%*%
               t(X)%*%W%*%z.i
```

Repeat with updated coefficients; stop at convergence.

If you implement this approach (exercise), you will find that it takes 7 iterations to get convergence. R can do it in four iterations because it uses a different approach.

9.6 Deviance

We saw encountered deviance earlier (page 61) in connection with ANOVA.

The deviance is more generally defined as

$$D = 2[\ell(b_{max}; y) - \ell(b; y)] \tag{194}$$

where $\ell(b_{max}; y)$ is the log likelihood of the saturated model (the model with the maximal number of parameters that can be fit), and $\ell(b; y)$ is the log likelihood of the model with the parameters b. As we saw earlier, D has a chi-squared distribution.

Deviance for the normal distribution The deviance is

$D = \frac{1}{\sigma^2} \sum (y_i - \bar{y})^2$

[See p. 80 onwards in the Dobson et al book for proofs and more detail.]

Deviance for the binomial distribution Deviance is defined as $D = \sum d_i$, where:

$$d_i = -2 \times n_i [y_i \log(\frac{\hat{\mu}_i}{y_i}) + (1 - y_i) \log(\frac{1 - \hat{\mu}_i}{1 - y_i})] \tag{195}$$

The basic idea here is that if the model fit is good, Deviance will have a χ^2 distribution with $N - p$ degrees of freedom. So that is what we will use for assessing model fit.

We will also use deviance for hypothesis testing. The difference in deviance (residual deviance) between two models also has a χ_2 distribution (this should remind you of ANOVA), with dfs being $p - q$, where q is the number of parameters in the first model, and p the number of parameters in the second.

I discuss hypothesis testing first, then evaluating goodness of fit using deviance.

9.7 Hypothesis testing: Residual deviance

Returning to our beetle data, let's say we fit our model:

```
glm1<-glm(propn.dead~dose,binomial(logit),
          weights=number,data=beetle)
```

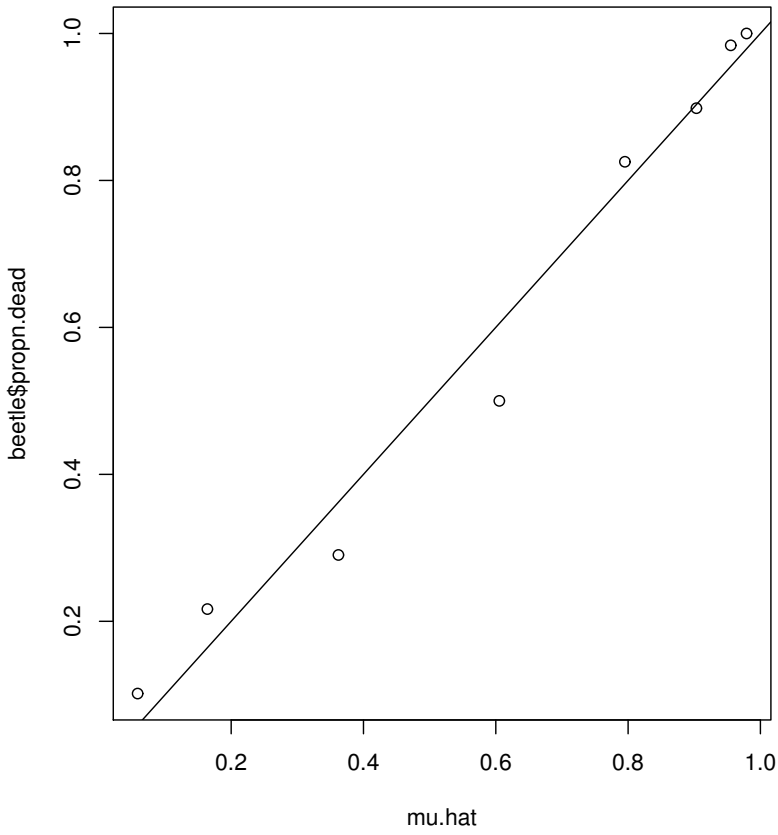
The summary output shows us the number of iterations that led to the parameter estimates:

```
summary(glm1)

##
## Call:
## glm(formula = propn.dead ~ dose, family = binomial(logit), data = beetle,
##     weights = number)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.5941  -0.3944   0.8329   1.2592   1.5940
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -60.717      5.181  -11.72   <2e-16
## dose          34.270      2.912   11.77   <2e-16
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 284.202  on 7  degrees of freedom
## Residual deviance:  11.232  on 6  degrees of freedom
## AIC: 41.43
##
## Number of Fisher Scoring iterations: 4
```

But we also see something called **Null deviance** and **Residual deviance**. These are used to evaluate quality of model fit. Recall that we can compute the fitted values and compare them to the observed values:

```
# beta.hat is (-60.71745 ,   34.27033)
(eta.hat<-  -60.71745 +   34.27033*beetle$dose)

## [1] -2.7766031 -1.6285470 -0.5661668  0.4276728  1.3563987  2.2337192
## [7]  3.0596341  3.8444247

(mu.hat<-exp(eta.hat)/(1+exp(eta.hat)))

## [1] 0.05860168 0.16402950 0.36212179 0.60531781 0.79517377 0.90323690
## [7] 0.95519664 0.97904960
```

```
# compare mu.hat with observed proportions
plot(mu.hat,beetle$propn.dead)
abline(0,1)
```

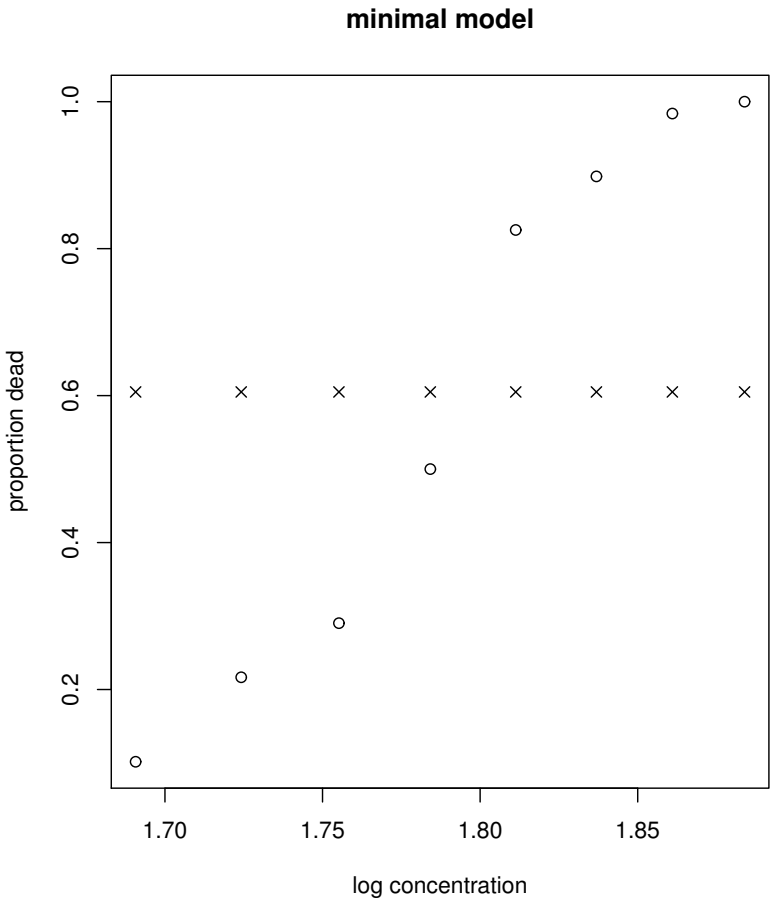


To evaluate whether dose has an effect, we will do something analogous to the model comparison methods we saw earlier. First, fit a model with only an intercept. Notice that the null deviance is 284 on 7 degrees of freedom.

```
null.glm<-glm(propn.dead~1,binomial(logit),
          weights=number,data=beetle)
summary(null.glm)

##
## Call:
## glm(formula = propn.dead ~ 1, family = binomial(logit), data = beetle,
##     weights = number)
##
```

```
## Deviance Residuals:
##    Min      1Q  Median      3Q     Max
## -8.105  -5.294   1.099   5.615   7.766
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  0.42630    0.09327   4.571 4.87e-06
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 284.2  on 7  degrees of freedom
## Residual deviance: 284.2  on 7  degrees of freedom
## AIC: 312.4
##
## Number of Fisher Scoring iterations: 4
```

```
plot(beetle$dose,beetle$propn.dead,xlab="log concentration",
    ylab="proportion dead",main="minimal model")
points(beetle$dose,null.glm$fitted,pch=4)
```

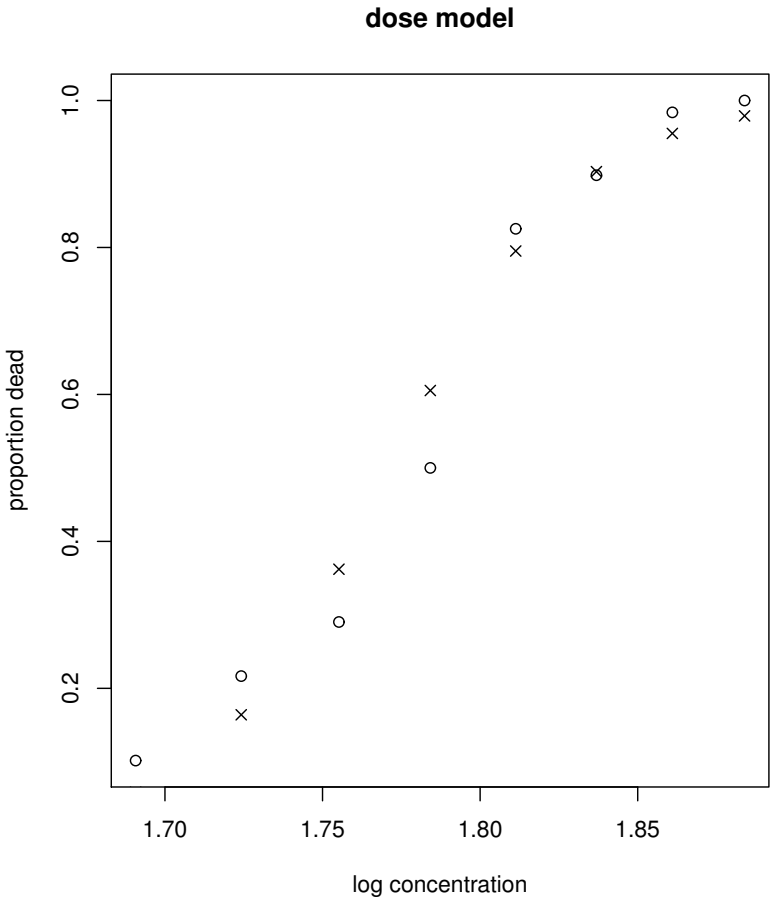


Add a term for dose. Now, the residual deviance is 11.2 on 6 dfs/

```
dose.glm<-glm(propn.dead~dose,binomial(logit),
          weights=number,data=beetle)
summary(dose.glm)

##
## Call:
## glm(formula = propn.dead ~ dose, family = binomial(logit), data = beetle,
##     weights = number)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.5941  -0.3944   0.8329   1.2592   1.5940
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -60.717      5.181  -11.72   <2e-16
```

```
## dose          34.270      2.912   11.77   <2e-16
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 284.202  on 7  degrees of freedom
## Residual deviance:  11.232  on 6  degrees of freedom
## AIC: 41.43
##
## Number of Fisher Scoring iterations: 4
```

```
plot(beetle$dose,beetle$propn.dead,xlab="log concentration",
    ylab="proportion dead",main="dose model")
points(beetle$dose,dose.glm$fitted,pch=4)
```



The change in deviance from the null model is 284.2-11.2=273 on 1 df. Since the critical $\chi^2_1 = 3.84$, we reject the null hypothesis that $\beta_1 = 0$.

You can do the model comparison using the anova function. Note

that no statistical test is calculated; you need to do that yourself.

```
anova(null.glm,dose.glm)

## Analysis of Deviance Table
##
## Model 1: propn.dead ~ 1
## Model 2: propn.dead ~ dose
##   Resid. Df Resid. Dev Df Deviance
## 1         7    284.202
## 2         6     11.232  1   272.97
```

Actually, you don't even need to define the null model; the anova function automatically compares the fitted model to the null model:

```
anova(dose.glm)

## Analysis of Deviance Table
##
## Model: binomial, link: logit
##
## Response: propn.dead
##
## Terms added sequentially (first to last)
##
##
##      Df Deviance Resid. Df Resid. Dev
## NULL                     7    284.202
## dose  1   272.97         6     11.232
```

9.8 *Assessing goodness of fit of a fitted model*

The deviance for a given degrees of freedom v should have a χ^2_v distribution for the model to be adequate. As an example, consider the null model above. The deviance is clearly much larger than the 95th percentile cutoff point of the chi-squared distribution with 7 dfs, so the model is not adequate.

```
deviance(null.glm)

## [1] 284.2024

## critical value:
qchisq(0.95,df=7)

## [1] 14.06714
```

Now consider the model with dose as predictor. The deviance is less than the 95th percentile, so the fit is adequate.

```
deviance(dose.glm)

## [1] 11.23223

qchisq(0.95,df=6)

## [1] 12.59159
```

9.9 *Residuals in GLMs*

In the binomial distribution, Deviance $D = \sum d_i$, where:

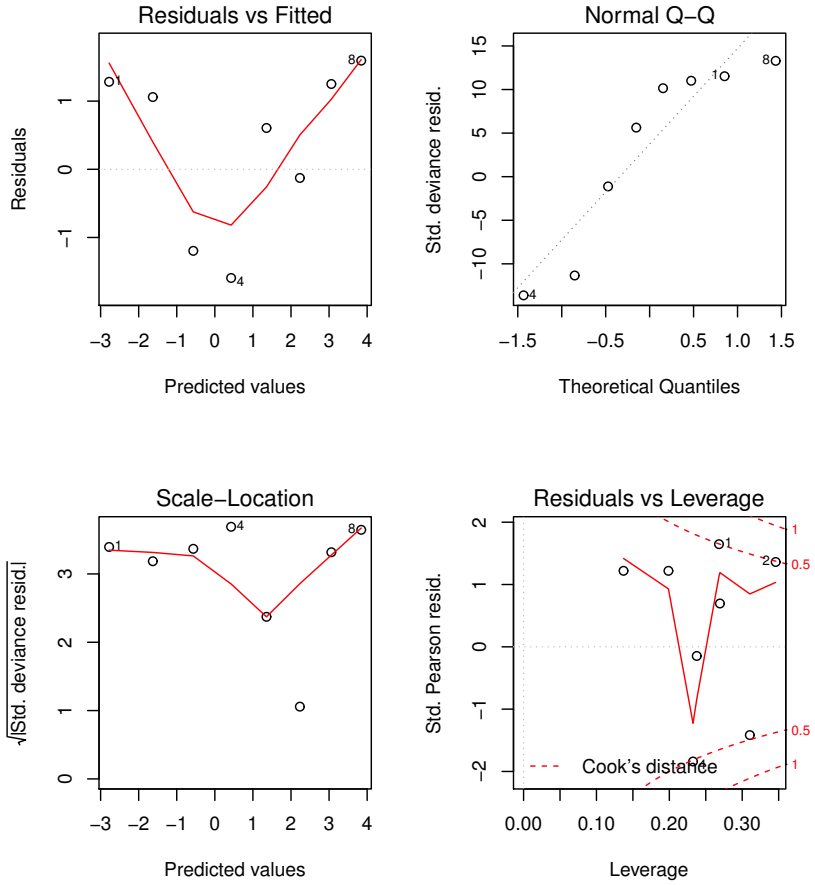
$$d_i = -2 \times n_i[y_i \log(\frac{\hat{\mu}_i}{y_i}) + (1 - y_i) \log(\frac{1 - \hat{\mu}_i}{1 - y_i})] \tag{196}$$

The i-th deviance residual is defined as:

$$e_{D,i} = sgn(y_i - \hat{\mu}_i) \times \sqrt{d_i} \tag{197}$$

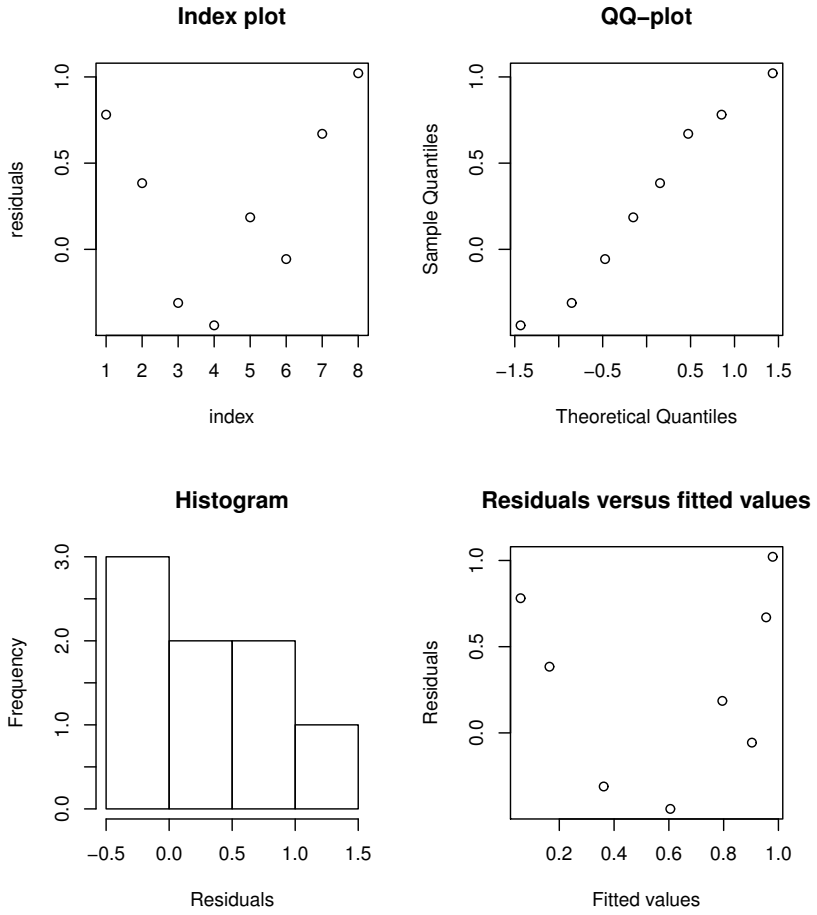
These can be used to check for model adequacy as discussed earlier in the context of linear models. One can just use the plot function inspect the residuals:

```
op<-par(mfrow=c(2,2),pty="s")
plot(dose.glm)
```



Alternatively, one can do this by hand:

```
op<- par(mfrow=c(2,2),pty="s")
plot(dose.glm$resid,
     xlab="index",ylab="residuals",main="Index plot")
qqnorm(dose.glm$resid,main="QQ-plot")
hist(dose.glm$resid,xlab="Residuals",main="Histogram")
plot(dose.glm$fit,dose.glm$resid,xlab="Fitted values",
     ylab="Residuals",
     main="Residuals versus fitted values")
```



10 *Linear mixed models*

In linear modeling, we model the mean of a response $Y_1, \ldots, Y_n$ as a function of a vector of predictors $x_1, \ldots, x_n$. We assume that the Y_i are conditionally independent given $\mathbf{x}, \mathbf{fi}$. When Y's are not marginally independent, we have $Cor(Y_1, Y_2) \neq 0$, or $P(Y_2 \mid Y_1) \neq P(Y_2)$.

Linear mixed models are useful for correlated data where $\mathbf{Y} \mid \mathbf{X}, \mathbf{fi}$ are not independently distributed.

10.1 *Informal presentation of LMMs*

Consider the following fake data set, taken from a textbook (Maxwell and Delaney, p. 497):

```
noisedeg<-read.table("datacode/noisedeg.txt")
```

This is a 2×2 factorial design, where each subject sees a stimulus in a no noise and noise condition; the stimulus is either angled at

0 degrees or 8 degrees. The dependent variable is reaction time (in msecs).

One important point here, which was also true in the Hindi data, is that different subjects have different effects of noise and deg. In the linear models we fit earlier we ignored this.

```
## returning to our noise data (noisedeg):
## here's an important fact about our data:
# different subjects have different means for no.noise and noise
# and different means for the three levels of deg

t(means.noise<-with(noisedeg,tapply(rt,list(subj,noise),mean)))

##           s1 s10  s2  s3  s4  s5  s6  s7  s8  s9
## no.noise 420 450 450 480 480 600 390 480 540 570
## noise    540 600 420 720 630 570 420 630 630 600

t(means.deg<-with(noisedeg,tapply(rt,list(subj,deg),mean)))

##    s1 s10  s2  s3  s4  s5  s6  s7  s8  s9
## 0 450 510 390 570 450 510 360 510 510 510
## 4 510 540 480 630 660 660 450 600 660 660
```

We can view the differential behavior of subjects in a graph (Figures 6 and 7).

Given these differences between subjects, you could fit a separate linear model for each subject, collect together the intercepts and slopes for each subject, and then check if the intercepts and slopes are significantly different from zero.

Try this for one subject (s1):

```
## fit a separate linear model for subject s1:
s1data<-subset(noisedeg,subj=="s1")
lm(rt~noise,s1data)

##
## Call:
## lm(formula = rt ~ noise, data = s1data)
##
## Coefficients:
## (Intercept)   noisenoise
##         420          120
```

Go back and look at the means for s1 for noise and compare them to the coefficients above. Now we can do this for every one of our 10 subjects. I don't print this result out because it's consume a lot of pages.

```r
## We can visualize these differences graphically:

library(lattice)

## noise by subject (data points):
print(xyplot(rt~noise|subj,
        panel=function(x,y,...){panel.xyplot(x,y,type="r")},noisedeg))
```

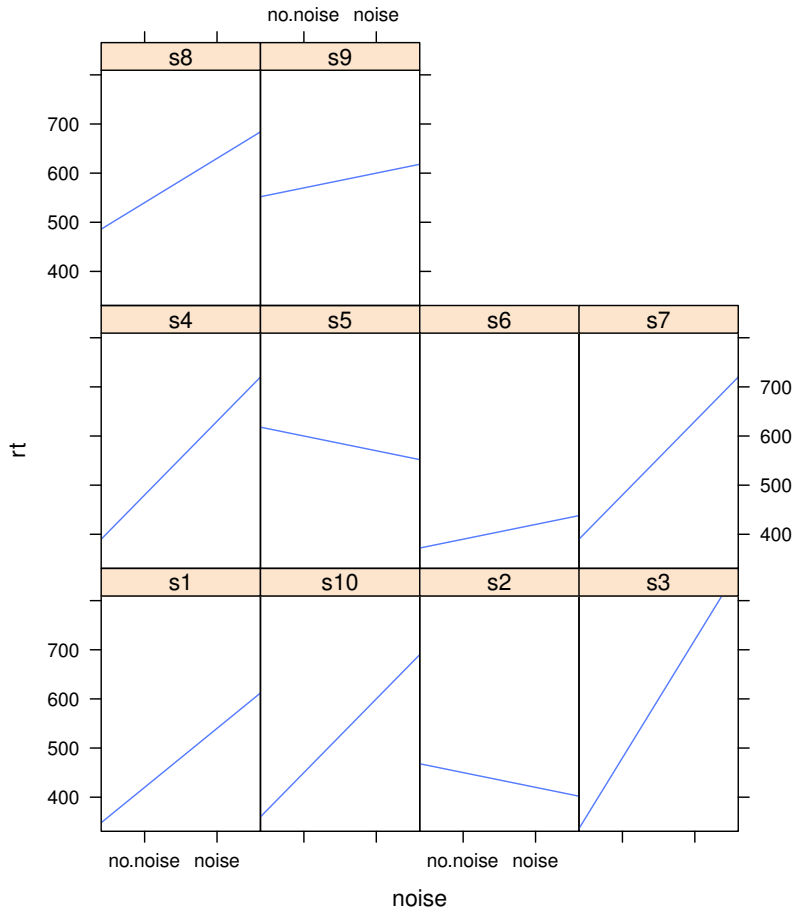
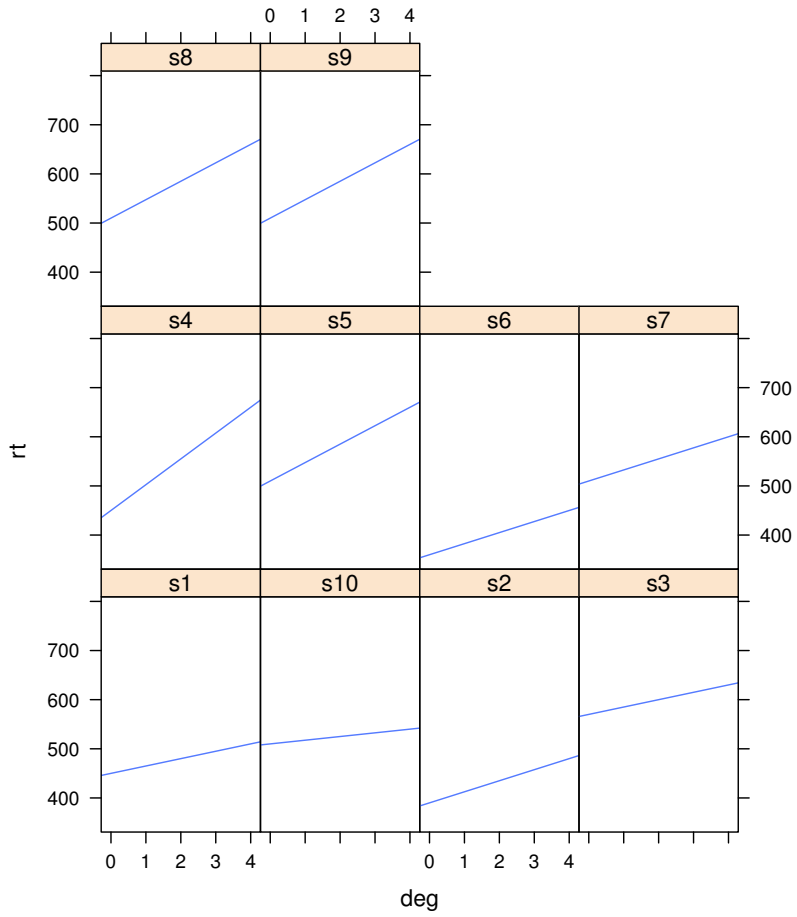


Figure 6: Noise effects by subject.

```
## same as above, but for deg:
print(xyplot(rt~deg|subj,
        panel=function(x,y,...){panel.xyplot(x,y,type="r")},noisedeg))
```

Figure 7: Degree effects by subject.




```
## do the same for each subject using a for-loop
subjects<-paste("s",rep(1:10),sep="")
for(i in subjects){
  sdata<-subset(noisedeg,subj==i)
        lm(rt~noise,sdata)
}
```

There is a function in the package `lme4` that does the above for you: `lmList`.

```
library(lme4)
lmlist.fm1<-lmList(rt~noise|subj,noisedeg)
```

```
print(lmlist.fm1$s1)

##
## Call:
## lm(formula = formula, data = data)
##
## Coefficients:
## (Intercept)   noisenoise
##         420          120
```

One can plot the individual lines for each subject, as well as the linear model mo's line (this shows how each subject deviates in intercept and slope from the model mo's intercept and slopes). See Figure 8.

To find out if there is an effect of noise, you can simply check whether the slopes of the individual subjects' fitted lines taken together are significantly different from zero:

```
t.test(coef(lmlist.fm1)[2])

##
##  One Sample t-test
##
## data:  coef(lmlist.fm1)[2]
## t = 3.2225, df = 9, p-value = 0.01045
## alternative hypothesis: true mean is not equal to 0
## 95 percent confidence interval:
##   26.82139 153.17861
## sample estimates:
## mean of x
##        90
```

The above is called repeated measures regression (see **??** for details). We now transition to the next stage: the linear mixed model.

10.2 Linear mixed model

The **linear mixed model** does something related to the above by-subject fits, but with some crucial differences, as we see below. In the model below, the the statement (1|subj) means that the variance associated with subject intercepts should be estimated, and from that variance the intercepts for each subject should be predicted (I explain in section 10.5 how this prediction is done).

```
## the following command fits a linear model, but in addition estimates between-subject variance:
summary(m0.lmer<-lmer(rt~noise+(1|subj),noisedeg))
```

```
plot(as.numeric(noisedeg$noise)-1,
     noisedeg$rt,axes=F,
     xlab="noise",ylab="rt")
axis(1,at=c(0,1),
     labels=c("no.noise","noise"))
axis(2)

subjects<-paste("s",1:10,sep="")

for(i in subjects){
abline(lmlist.fm1[[i]])
}

abline(lm(rt~noise,noisedeg),lwd=3,col="red")
```

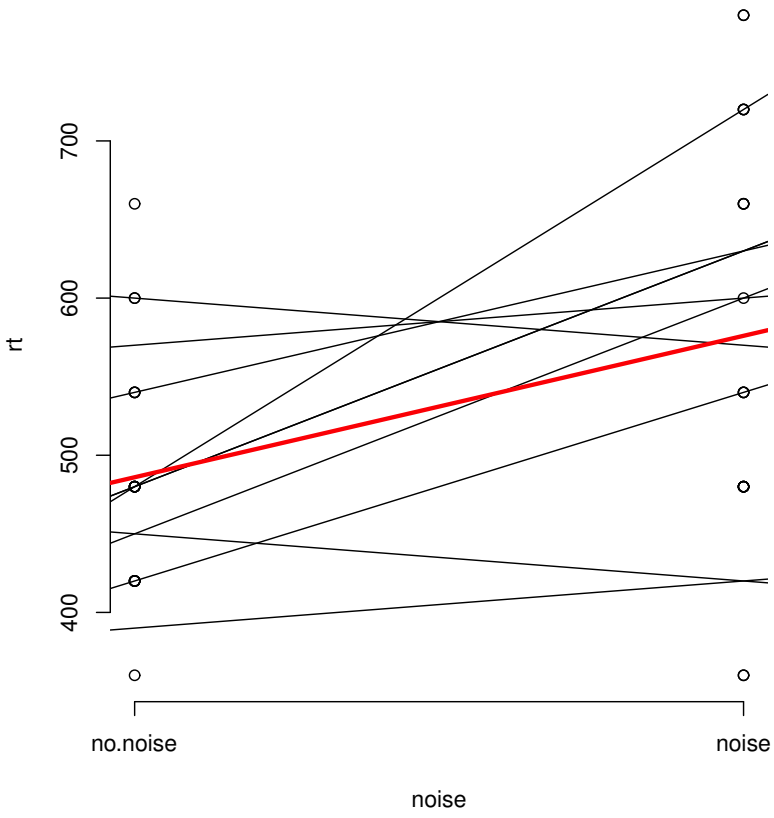


Figure 8: Each subject's intercept and slope line varies about the averager over all subjects (the intercept and slope from the lm function).

```
## Linear mixed model fit by REML ['lmerMod']
## Formula: rt ~ noise + (1 | subj)
##    Data: noisedeg
##
## REML criterion at convergence: 466.1
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -1.7538 -0.5452 -0.1984  0.5529  2.0306
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  subj     (Intercept) 2491     49.91
##  Residual             8876     94.21
## Number of obs: 40, groups:  subj, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)   486.00      26.32  18.463
## noisenoise     90.00      29.79   3.021
##
## Correlation of Fixed Effects:
##            (Intr)
## noisenoise -0.566
```

One thing to notice is that the coefficients of the fixed effects of the above model are identical to those in the linear model mo above. The predicted varying intercepts for each subject can be viewed by typing:

```
ranef(m0.lmer)

## $subj
##     (Intercept)
## s1   -26.972985
## s10   -3.173292
## s2   -50.772677
## s3    36.492862
## s4    12.693169
## s5    28.559631
## s6   -66.639139
## s7    12.693169
## s8    28.559631
## s9    28.559631
```

Or you can display them graphically as shown in Figure 9.

```
print(dotplot(ranef(m0.lmer,condVar=TRUE)))

## $subj
```

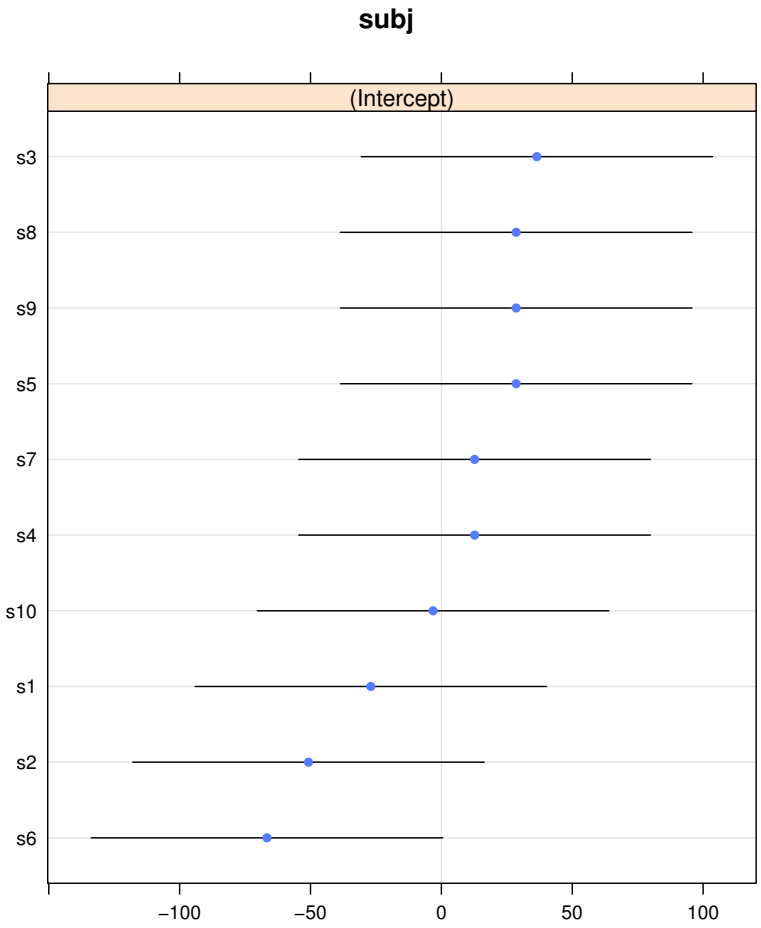


Figure 9: Plotting the varying intercepts.

The model mo.lmer above prints out the following type of linear model; i indexes subjects, j indexes the noise factor (no noise or noise). Since we have two replicates of each noise factor level (one for degree 0 and one for degree 4), the index k indexes the degree level, although the degree factor is not fit in this example (in order to simplify the example).

$$Y_{ijk} = \hat{\beta}_0 + \hat{\beta}_{1j} x_{ijk} + b_i + \epsilon_{ijk} \tag{198}$$

It's just like our linear model except that there are different *predicted* (cf. the lmlist function above, where they are *estimated* for each subject) intercepts b_i for each subject. These are assumed by lmer to come from a normal distribution centered around 0; see [13] for more details. The

[13] A. Gelman and J. Hill. *Data analysis using regression and multilevel/hierarchical models*. Cambridge University Press, Cambridge, UK, 2007

ordinary linear model mo has one intercept β_0 for all subjects, whereas the linear mixed model with varying intercepts mo.lmer has a different intercept $(\beta_0 + b_i)$ for each subject.

We can visualize these different intercepts for each subject as shown below in Figure 10.

Note that, unlike the figure associated with the lmlist.fm1 model above, which also involves fitting separate models for each subject, the model mo.lmer assumes different intercepts for each subject **but the same slope**. We can have lmer fit different intercepts as well as different slopes for each subject:

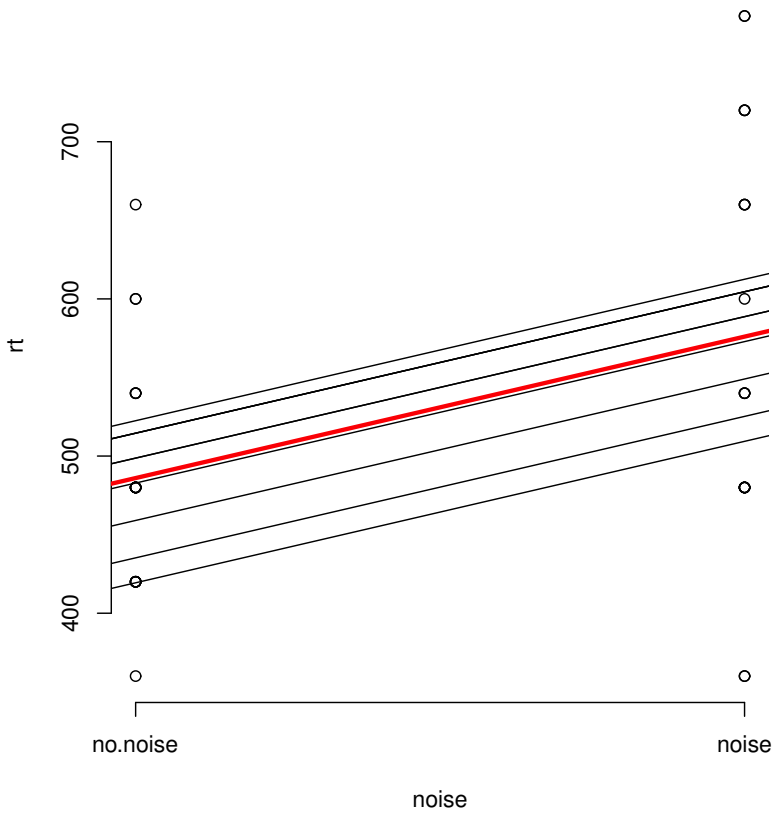
```
summary(m1.lmer<-lmer(rt~noise+(1+noise|subj),noisedeg))

## Linear mixed model fit by REML ['lmerMod']
## Formula: rt ~ noise + (1 + noise | subj)
##    Data: noisedeg
##
## REML criterion at convergence: 465.1
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -1.4441 -0.6729 -0.1930  0.6303  1.9593
##
## Random effects:
##  Groups   Name        Variance Std.Dev. Corr
##  subj     (Intercept) 1093     33.05
##           noisenoise  1408     37.52    1.00
##  Residual             8359     91.43
## Number of obs: 40, groups:  subj, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)   486.00      22.96   21.17
## noisenoise     90.00      31.25    2.88
##
## Correlation of Fixed Effects:
##            (Intr)
## noisenoise -0.410
```

These fits for each subject are visualized below (the red line shows the model with a single intercept and slope, i.e., our old model mo):

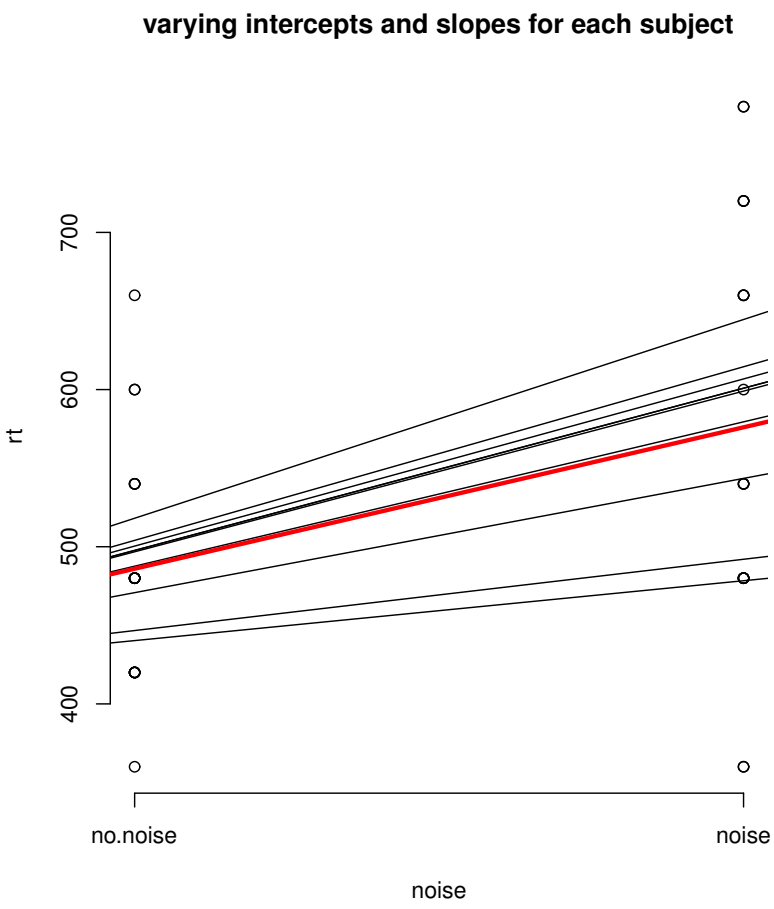
```
(a<-fixef(m1.lmer)[1])

## (Intercept)
##         486
```

```
a<-fixef(m0.lmer)[1]
newa<-a+ranef(m0.lmer)$subj

ab<-data.frame(newa=newa,b=fixef(m0.lmer)[2])

plot(as.numeric(noisedeg$noise)-1,noisedeg$rt,xlab="noise",ylab="rt",axes=F)
axis(1,at=c(0,1),labels=c("no.noise","noise"))
axis(2)
for(i in 1:10){
abline(a=ab[i,1],b=ab[i,2])
}
abline(lm(rt~noise,noisedeg),lwd=3,col="red")
```

Figure 10: Varying intercepts for subjects, with the linear model fit superimposed.



```
(b<-fixef(m1.lmer)[2])

## noisenoise
##         90

newa<-a+ranef(m1.lmer)$subj[1]
newb<-b+ranef(m1.lmer)$subj[2]
## make this into a data frame:
ab<-data.frame(newa=newa,b=newb)

plot(as.numeric(noisedeg$noise)-1,noisedeg$rt,xlab="noise",ylab="rt",axes=F,
main="varying intercepts and slopes for each subject")
axis(1,at=c(0,1),labels=c("no.noise","noise"))
axis(2)

for(i in 1:10){
abline(a=ab[i,1],b=ab[i,2])
}

abline(lm(rt~noise,noisedeg),lwd=3,col="red")
```



Compare this model with the lmlist.fm1 model we fitted earlier; see Figure 11.

xxx

The above graphic shows some crucial differences between the lmlist (repeated measures) model and the lmer model. Note that the fitted line for each subject in the lmer model is much closer to the mo model's fitted (red) line. This is because lmlist uses each subject's data separately (resulting in possibly wildly different models, depending on the variability between subjects), whereas lmer "borrows strength from the mean" and pushes (or "shrinks") the estimated intercepts and slopes of each subject closer to the mean intercepts and slopes (the model mo's intercepts and slopes). Because it shrinks the coefficients towards the means, this is called shrinkage. This is particularly useful when several data points are missing in a particular condition for a particular subject: in an ordinary linear model, estimating coefficients using lmList would lead to very poor estimates for that subject; by contrast, lmer assumes that the estimates for such a subject are not

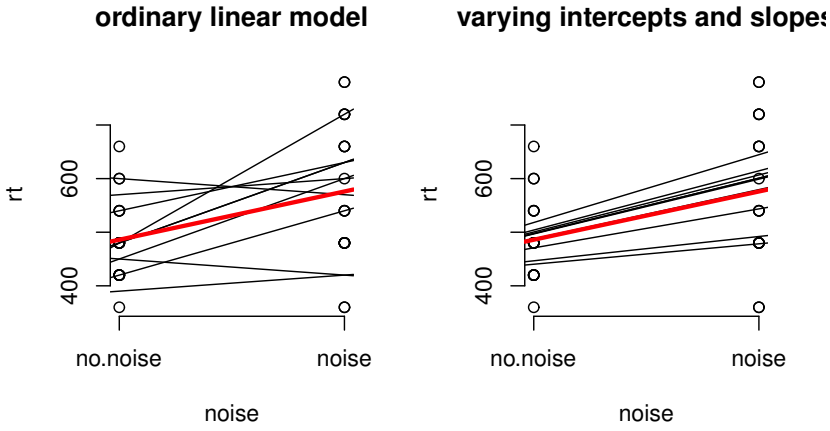


Figure 11: Comparing the lmList and lmer estimates for each subject.

reliable and therefore shrinks that subject's estimate to the mean values. Gelman and Hill provide an example of this (their Laq qui parle example).

10.3 *Some basic types of linear mixed model and their variance components*

Varying intercepts model. The model for a categorical predictor is:

$$Y_{ijk} = \beta_j + b_i + \epsilon_{ijk} \tag{199}$$

$i = 1, \ldots, 10$ is subject id, $j = 1, 2$ is the factor level, k is the number of replicates (here 1). $b_i \sim N(0, \sigma_b^2), \epsilon_{ijk} \sim N(0, \sigma^2)$.

For a continuous predictor:

$$Y_{ijk} = \beta_0 + \beta_1 t_{ijk} + b_{ij} + \epsilon_{ijk} \tag{200}$$

Varying intercepts and slopes (with correlation). The model for a categorical predictor is:

$$Y_{ij} = \beta_1 + b_{1i} + (\beta_2 + b_{2i})x_{ij} + \epsilon_{ij} \quad i = 1, ..., M, j = 1, ..., n_i \tag{201}$$

with $b_{1i} \sim N(0, \sigma_1^2)$, $b_{2i} \sim N(0, \sigma_2^2)$, and $\epsilon_{ij} \sim N(0, \sigma^2)$.
Another way to write such models is:

$$Y_{ijk} = \beta_j + b_{ij} + \epsilon_{ijk} \tag{202}$$

$b_{ij} \sim N(0, \sigma_b)$. The variance σ_b must be a 2×2 matrix:

$$\begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \tag{203}$$

In an lmer model, the output shows the variance covariance matrix of the random effects. Recall the degree noise data:

```
m<-lmer(rt~noise + (1+noise|subj),noisedeg)
summary(m)

## Linear mixed model fit by REML ['lmerMod']
## Formula: rt ~ noise + (1 + noise | subj)
##    Data: noisedeg
##
## REML criterion at convergence: 465.1
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -1.4441 -0.6729 -0.1930  0.6303  1.9593
##
## Random effects:
##  Groups   Name        Variance Std.Dev. Corr
##  subj     (Intercept) 1093     33.05
##           noisenoise  1408     37.52    1.00
##  Residual             8359     91.43
## Number of obs: 40, groups:  subj, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)   486.00      22.96   21.17
## noisenoise     90.00      31.25    2.88
##
## Correlation of Fixed Effects:
##            (Intr)
## noisenoise -0.410
```

Note also that the correlation estimate depends on the parameterization of the fixed effect noise:

```
contrasts(noisedeg$noise)

##          noise
## no.noise     0
## noise        1

## set to sum contrasts:
contrasts(noisedeg$noise)<-contr.sum(2)
contrasts(noisedeg$noise)

##          [,1]
## no.noise    1
## noise      -1

m<-lmer(rt~noise + (1+noise|subj),noisedeg)
summary(m)

## Linear mixed model fit by REML ['lmerMod']
## Formula: rt ~ noise + (1 + noise | subj)
##    Data: noisedeg
##
## REML criterion at convergence: 466.5
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -1.4441 -0.6729 -0.1930  0.6303  1.9593
##
## Random effects:
##  Groups   Name        Variance Std.Dev. Corr
##  subj     (Intercept) 2684.7   51.81
##           noise1       351.9   18.76    -1.00
##  Residual             8359.0   91.43
## Number of obs: 40, groups:  subj, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)   531.00      21.85   24.30
## noise1        -45.00      15.63   -2.88
##
## Correlation of Fixed Effects:
##        (Intr)
## noise1 -0.285
```

So the correlation here is estimated as 1 or -1 depending on the parameterization. This estimate of a perfect correlation is actually a **failure** to estimate the correlation, a consequence of overfitting the model (asking the lmer function to estimate parameters even though you don't have enough data to estimate them). The sensible thing to do here is to fit a model without such a correlation being assumed. There is an important technicality here, that you have to define the contrast as a vector of -1's and 1's (for sum contrast coding), instead of using the noise column in the data frame. The way to tell lmer not to estimate the correlation is to use two vertical bars in the random effects specification.

```
c1<-ifelse(noisedeg$noise=="noise",-1,1)
m<-lmer(rt~c1 + (c1||subj),noisedeg)
summary(m)

## Linear mixed model fit by REML ['lmerMod']
## Formula: rt ~ c1 + ((1 | subj) + (0 + c1 | subj))
##    Data: noisedeg
##
## REML criterion at convergence: 467.5
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -1.7538 -0.5452 -0.1984  0.5529  2.0306
##
## Random effects:
##  Groups   Name        Variance  Std.Dev.
##  subj     (Intercept) 2.491e+03 4.991e+01
##  subj.1   c1          9.521e-13 9.757e-07
##  Residual             8.876e+03 9.421e+01
## Number of obs: 40, groups:  subj, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)    531.0       21.7  24.467
## c1             -45.0       14.9  -3.021
##
## Correlation of Fixed Effects:
##    (Intr)
## c1 0.000
```

There is much more to be said here; see [14] for more.

[14] Douglas Bates, Reinhold Kliegl, Shravan Vasishth, and Harald Baayen. Parsimonious mixed models. ArXiv e-print; submitted to *Journal of Memory and Language*, 2015

10.4 Parameter estimation

There are two basic procedures, likelihood based and REML (restricted or residual ML).

The Likelihood based model fitting procedure. Here are some relevant facts we need to know in order to work out how parameter estimation is done in LMMs using likelihoods.

1. If we have two continuous random variables Y and Z, with density functions $f_Y(y)$ and $f_Z(z)$ and joint density $f_{Y,Z}(y,z)$, then

$$f_Y(y) = \int f_{Y,Z}(y,z)dz. \tag{204}$$

2. The conditional density of $Y \mid Z$ is defined as

$$f_{Y|Z}(y \mid z) = \frac{f_{Y,Z}(y,z)}{f_Z(z)} \tag{205}$$

so we can write

$$f_{Y,Z}(y,z) = f_{Y|Z}(y \mid z) \times f_Z(z). \tag{206}$$

3. Combining equations 204 and 206, we have

$$f_Y(y) = \int f_{Y|Z}(y \mid z) \times f_Z(z)dz \tag{207}$$

Equation 207, where we condition on a second random variable Z (note that Z could be a "non-observable", which is what the varying intercepts and slopes are—they are not observed as data), can be helpful in deriving $f_Y(y)$, if the two densities on the RHS are easy to write down, and the integral can be solved.

Returning to parameter estimation in LMMs, the model is:

$$Y_i = X_i\beta + Z_i\beta_i + \epsilon_i, \quad i = 1, \ldots, M \tag{208}$$

where $b_i \sim N(0, \Psi), \epsilon_i \sim N(0, \sigma^2 I)$. Let θ be the parameters that determine Ψ.

$$\begin{aligned} L(\beta, \theta, \sigma^2 \mid y) =& p(y : \beta, \theta, \sigma^2) \\ =& \prod_i^M p(y_i : \beta, \theta, \sigma^2) \\ =& \prod_i^M \int p(y_i \mid b_i, \beta, \sigma^2) p(b_i : \theta, \sigma^2)\, db_i \end{aligned} \tag{209}$$

we want the density of the observations (y_i) given the parameters β, θ and σ^2 only. In this case, using equation 207 above, with $Y = y_i$ and

$Z = b_i$ is helpful for deriving the density for y_i, because $f(y_i \mid b_i)$ (or $p(y_i \mid b_i, \beta, \sigma^2)$) has a simple form, and so we can get a closed form expression for the integral.

REML estimation (REstricted/REsidual ML). To estimate variance parameters, first fit fixed effects using least squares, and then focus attention on residuals. The **residuals**' distribution depends on σ^2 and variance parameters θ of random effects.

A **likelihood** for these parameters is formed based on the residuals alone. Maximization of this **marginal likelihood** gives estimates of σ^2 and the other variance-covariance parameters which are less biased than the full maximum likelihood estimates.

Once the REML variance-covariance estimates are obtained the **fixed effects are re-estimated by maximum likelihood assuming the random effects parameters are known**.

Alternatively, we can define a restricted likelihood:

$$L_R(\theta, \sigma^2 \mid y) = \int L(\beta, \theta, \sigma^2 \mid y)\, d\beta \tag{210}$$

and maximize this to obtain estimates of these parameters.

Unlike full (max.) likelihood, restricted likelihood is not invariant to parameterization, so we cannot compare models with different fixed effects.

10.5 Computing the BLUPs

In a varying intercepts model, the intercept b_i for subjects $i = 1, \ldots, I$ (assume that each subject has n_i data points) is a latent variable, it cannot be observed. So how is it computed? We can predict these BLUPs using a method called **empirical Bayes estimation**, and generate something called posterior means. This method combines two kinds of information: (a) the data from group i, and (b) the fact that the unobserved b_i is a random variable with mean 0 and variance σ_b^2.

The posterior means $\hat{b}_i$ are given by

$$\hat{b}_i = E[\hat{b}_i \mid y, \beta] = \frac{\sigma_b^2}{\sigma_b^2 + \sigma_e^2 / n_i}(\bar{y}_{\cdot i} - \bar{y}) \tag{211}$$

You have never seen an expression like $\bar{y}_{\cdot i}$, but it just means the group means (that subject's mean score over the n_i data points). The term $\frac{\sigma_b^2}{\sigma_b^2 + \sigma_e^2 / n_i}$ is called a shrinkage factor; it can be at most 1. It will approach 1 when we have n_i approaching infinity, and will be small if n_i is a small number. The implication of this shrinkage factor is that if we have only a few data points for a particular subject, then its value will be shrunk towards the grand mean—the example we saw earlier.

10.6 Correlation of fixed effects

For an ordinary linear model, the covariance matrix (from which we can get the correlation matrix) of $\hat{\beta}$ is:

$$\sigma^2 \times (X^T X)^{-1}. \tag{212}$$

For a mixed effects model, the standard deviations (standard errors) and correlations for the fixed effects estimators are listed at the end of the lmer output. Here is an example from a data-set that measures some dependent variable "wear" as a function of three material types for 10 subjects:

```
BHHshoes<-read.table("datacode/BHHshoes.txt")
lm.full<-lmer(wear~material-1+
                (1|Subject),
              data = BHHshoes)
```

```
Correlation of Fixed Effects:
          matrlA
materialB 0.988
```

Doing this by hand:

$$\hat{\beta}_1 = (Y_{1,1} + Y_{2,1} + \cdots + Y_{10,1})/10 \tag{213}$$

$$\hat{\beta}_2 = (Y_{1,2} + Y_{2,2} + \cdots + Y_{10,2})/10 \tag{214}$$

```
b1.vals<-subset(BHHshoes,
                material=="A")$wear
b2.vals<-subset(BHHshoes,
                material=="B")$wear

vcovmatrix<-var(cbind(b1.vals,b2.vals))

## get covariance from off-diagonal:
covar<-vcovmatrix[1,2]
sds<-sqrt(diag(vcovmatrix))
## correlation of fixed effects:
covar/(sds[1]*sds[2])

##   b1.vals
## 0.9882255

#cf:
covar/((0.786*sqrt(10))^2)
```

```
## [1] 0.9875248
```

11 Bayesian data analysis: Some introductory ideas

Recall Bayes rule:

Theorem 1 ***Bayes' Rule***. *Let B_1, B_2, ..., B_n be mutually exclusive and exhaustive and let A be an event with $\mathbb{P}(A) > 0$. Then*

$$\mathbb{P}(B_k|A) = \frac{\mathbb{P}(B_k)\mathbb{P}(A|B_k)}{\sum_{i=1}^{n} \mathbb{P}(B_i)\mathbb{P}(A|B_i)}, \quad k = 1, 2, \ldots, n. \tag{215}$$

When A and B are observable events, we can state the rule as follows:

$$p(A \mid B) = \frac{p(B \mid A)p(A)}{p(B)} \tag{216}$$

Note that $p(\cdot)$ is the probability of an event.

When looking at probability distributions, we will encounter the rule in the following form.

$$f(\theta \mid \text{data}) = \frac{f(\text{data} \mid \theta)f(\theta)}{f(y)} \tag{217}$$

Here, $f(\cdot)$ is a probability density, not the probability of a single event. $f(y)$ is called a "normalizing constant", which makes the left-hand side a probability distribution.

$$f(y) = \int f(x, \theta)\, d\theta = \int \underset{\substack{\uparrow \\ \textit{likelihood}}}{f(y \mid \theta)} \underset{\substack{\uparrow \\ \textit{prior}}}{f(\theta)}\, d\theta \tag{218}$$

If θ is a discrete random variable taking one value from the set $\{\theta_1, \ldots, \theta_n\}$, then

$$f(y) = \sum_{i=1}^{n} f(y \mid \theta_i)P(\theta = \theta_i) \tag{219}$$

Without the normalizing constant, we have the relationship:

$$f(\theta \mid \text{data}) \propto f(\text{data} \mid \theta)f(\theta) \tag{220}$$

Note that the likelihood $L(\theta; \text{data})$ (our data is fixed) is proportional to $f(\text{data} \mid \theta)$, and that's why we can refer to $f(\text{data} \mid \theta)$ as the likelihood in the following manner:

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior} \tag{221}$$

Our central goal is going to be to derive the posterior distribution and then summarize its properties (mean, median, 95% credible interval, etc.). Usually, we don't need the normalizing constant to understand the properties of the posterior distribution. That's why Bayes theorem is often stated in terms of the proportionality shown above.

"To a Bayesian, the best information one can ever have about θ is to know the posterior density." p. 31 of Christensen et al's book.

Incidentally, this is supposed to be the moment of great divide between frequentists and Bayesians: the latter assign a probability distribution to the parameter, the former treat the parameter as a point value.

Two examples will clarify how we can use Bayes' rule to obtain the posterior.

11.1 Example 1: Proportions

This is a contrived example, just meant to provide us with an entry point into Bayesian data analysis. Suppose that an aphasic patient answered 46 out of 100 questions correctly in a particular task. The research question is, what is the probability that their average response is greater than 0.5, i.e., above chance.

The likelihood function will tell us $P(\text{data} \mid \theta)$:

```
dbinom(46, 100, 0.5)

## [1] 0.0579584
```

Note that

$$P(\text{data} \mid \theta) \propto \theta^{46}(1-\theta)^{54} \tag{222}$$

So, to get the posterior, we just need to work out a prior distribution $f(\theta)$.

$$f(\theta \mid \text{data}) \propto f(\text{data} \mid \theta) \underbrace{f(\theta)}_{prior} \tag{223}$$

For the prior, we need a distribution that can represent our uncertainty about the parameter p. The beta distribution (a generalization of the continuous uniform distribution) is commonly used as prior for proportions.

The pdf is[15]

$$f(x) = \begin{cases} \frac{1}{B(a,b)} x^{a-1}(1-x)^{b-1} & \text{if } 0 < x < 1 \\ 0 & \text{otherwise} \end{cases}$$

where

$$B(a,b) = \int_0^1 x^{a-1}(1-x)^{b-1}\,dx$$

We say that the Beta distribution is conjugate to the binomial density; i.e., the two densities have similar functional forms.

[15] Incidentally, there is a connection between the beta and the gamma:

$$B(a,b) = \int_0^1 x^{a-1}(1-x)^{b-1}\,dx = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

which allows us to rewrite the beta PDF as

$$f(x) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} x^{a-1}(1-x)^{b-1}, \quad 0 < x < 1. \tag{224}$$

Here, x refers to the probability p.

In R, we write $X \sim \texttt{beta}(\texttt{shape1} = \alpha, \texttt{shape2} = \beta)$. The associated R function is $\texttt{dbeta}(\texttt{x}, \texttt{shape1}, \texttt{shape2})$.

The mean and variance are

$$E[X] = \frac{a}{a+b} \text{ and } Var(X) = \frac{ab}{(a+b)^2(a+b+1)}. \quad (225)$$

The Beta distribution's parameters a and b can be interpreted as (our beliefs about) prior successes and failures, and are called **hyper-parameters**. Once we choose values for a and b, we can plot the beta pdf. in Figure 12, I show the Beta pdf for three sets of values of a,b.

As the figure shows, as the a,b values are increased, the shape begins to resemble the normal distribution.

If we don't have much prior information, we could use a=b=2; this gives us a uniform prior; this is called an uninformative prior or non-informative prior (although having no prior knowledge is, strictly speaking, not uninformative). If we have a lot of prior knowledge and/or a strong belief that p has a particular value, we can use a larger a,b to reflect our greater certainty about the parameter. Notice that the larger our parameters a and b, the smaller the spread of the distribution; this makes sense because a larger sample size (a greater number of successes a, and a greater number of failures b) will lead to more precise estimates.

The central point is that the Beta distribution can be used to define the prior distribution of p.

Just for the sake of argument, let's take four different beta priors, each reflecting increasing certainty.

1. Beta(a=2,b=2)
2. Beta(a=3,b=3)
3. Beta(a=6,b=6)
4. Beta(a=21,b=21)

Each (except perhaps the first) reflects a belief that p=0.5, with varying degrees of (un)certainty. Now we just need to plug in the likelihood and the prior:

$$f(\theta \mid \text{data}) \propto f(\text{data} \mid \theta) f(\theta) \quad (226)$$

The four corresponding posterior distributions would be:

$$f(\theta \mid \text{data}) \propto [p^{46}(1-p)^{54}][p^{2-1}(1-p)^{2-1}] = p^{47}(1-p)^{55} \quad (227)$$

$$f(\theta \mid \text{data}) \propto [p^{46}(1-p)^{54}][p^{3-1}(1-p)^{3-1}] = p^{48}(1-p)^{56} \quad (228)$$

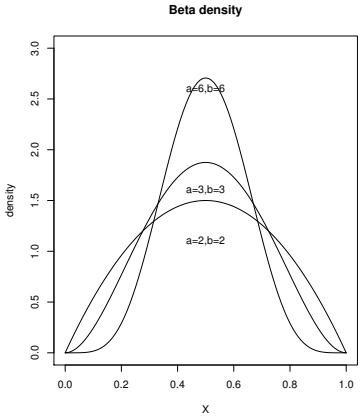


Figure 12: Examples of the beta distribution with different parameter values.

$$f(\theta \mid \text{data}) \propto [p^{46}(1-p)^{54}][p^{6-1}(1-p)^{6-1}] = p^{51}(1-p)^{59} \quad (229)$$

$$f(\theta \mid \text{data}) \propto [p^{46}(1-p)^{54}][p^{21-1}(1-p)^{21-1}] = p^{66}(1-p)^{74} \quad (230)$$

We can now visualize each of these triplets of priors, likelihoods and posteriors. Note that I use the Beta to model the likelihood because this allows me to visualize all three (prior, lik., posterior) in the same plot. The likelihood function is as shown in Figure 13.

We can represent the likelihood in terms of the beta as well:

As an exercise, you should try to plot the priors, likelihoods, and posterior distributions in the four cases above. I do the first case for you below, but I don't plot the result.

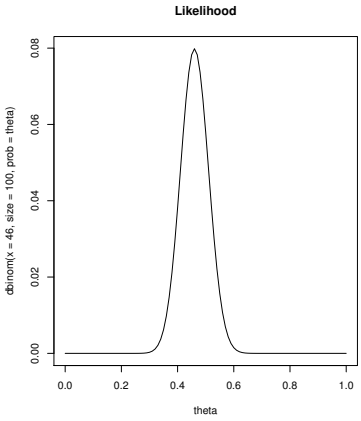
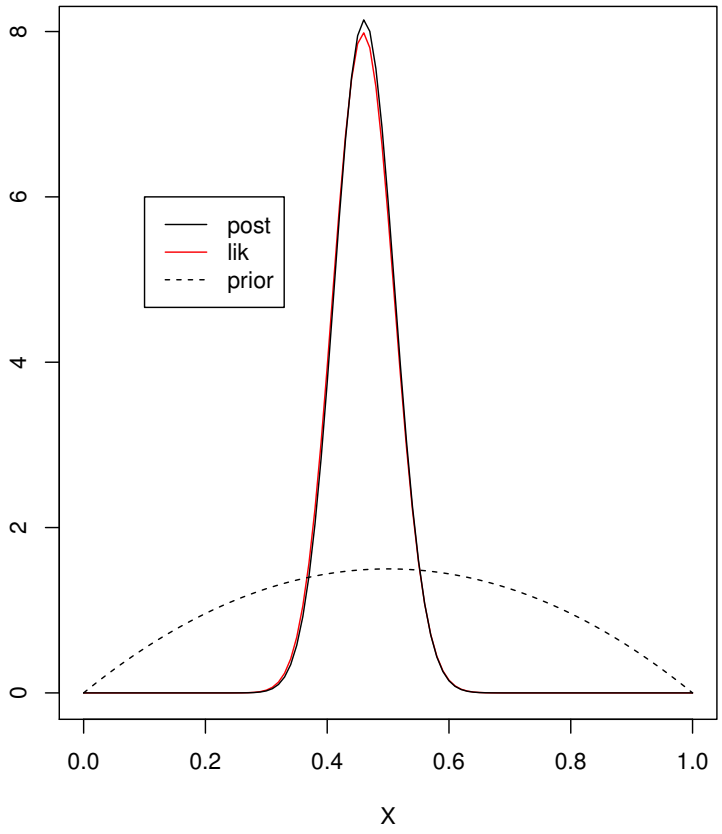


Figure 13: Binomial likelihood function.



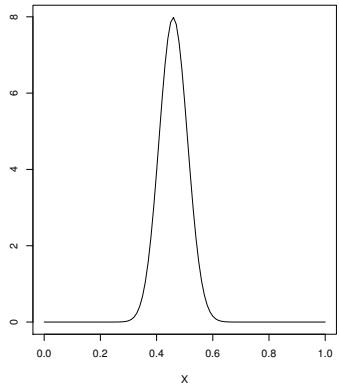


Figure 14: Using the beta distribution to represent a binomial.

11.2 Example 2: Proportions

This example is taken from a Copenhagen course on Bayesian data analysis that I attended in 2012.

For a single Bernoulli trial, the **likelihood** for possible parameters value θ_j (which we, for simplicity, fix at four values, 0.2, 0.4, 0.6, 0.8.) is:[16]

[16] See section 1.1 for the definition of the binomial distribution. The Bernoulli distribution is the binomial with n=1.

$$p(y \mid \theta_j) = \theta_j^y (1 - \theta_j)^{1-y} \tag{231}$$

```
y<-1
n<-1

thetas<-seq(0.2,0.8,by=0.2)

likelihoods<-rep(NA,4)
for(i in 1:length(thetas)){
  likelihoods[i]<-dbinom(y,n,thetas[i])
}
```

Note that these do not sum to 1:

```
sum(likelihoods)

## [1] 2
```

Question: How can we make them sum to 1? I.e., how can we make the likelihood a proper probability mass function? Think about this.

Let the **prior** distribution of the parameters be $p(\theta_j)$; let this be a uniform distribution over the possible values of θ_j.

```
(priors<-rep(0.25,4))

## [1] 0.25 0.25 0.25 0.25
```

The prior is a proper probability distribution.

For any outcome y (which could be 1 or 0—this is a single trial), the posterior probability of success (a 1) is related to the prior and likelihood by the relation:

$$p(\theta_j \mid y) \propto p(\theta_j) \theta_j^y (1 - \theta_j)^{1-y} \tag{232}$$

To get the posterior to be a proper probability distribution, you have to make sure that the RHS sums to 1.

```
liks.times.priors<-likelihoods * priors

## normalizing constant:
sum.lik.priors<-sum(liks.times.priors)

posteriors<- liks.times.priors/sum.lik.priors
```

Note that the posterior distribution sums to 1, because we **normalized** it.

Now suppose our sample size was 20, and the number of successes 15. What does the posterior distribution look like now?

```
n<-20
y<-15

priors<-rep(0.25,4)

likelihoods<-rep(NA,4)
for(i in 1:length(thetas)){
  likelihoods[i]<-dbinom(y,n,thetas[i])
}

liks.priors<-likelihoods * priors

sum.lik.priors<-sum(liks.priors)

(posteriors<- liks.priors/sum.lik.priors)

## [1] 6.645594e-07 5.167614e-03 2.979907e-01 6.968411e-01
```

Now suppose that we had a non-zero prior probability to extreme values (0,1) to θ. The prior is now defined over six values, not four, so the probability distribution on the priors changes accordingly to $1/6$ for each value of θ.

Given the above situation of n=20, y=15, what will change in the posterior distribution compared to what we just computed:

```
posteriors

## [1] 6.645594e-07 5.167614e-03 2.979907e-01 6.968411e-01
```

Let's find out what the posteriors will look like:

```
thetas<-seq(0,1,by=0.2)
priors<-rep(1/6,6)
```

```
y<-15
n<-20

likelihoods<-rep(NA,6)
for(i in 1:length(thetas)){
  likelihoods[i]<-dbinom(y,n,thetas[i])
}

liks.priors<-likelihoods * priors

sum.lik.priors<-sum(liks.priors)

(posteriors<- liks.priors/sum.lik.priors)

## [1] 0.000000e+00 6.645594e-07 5.167614e-03 2.979907e-01 6.968411e-01
## [6] 0.000000e+00
```

How would the posteriors change if we had only one trial (a Bernoulli trial)? Let's find out:

```
thetas<-seq(0,1,by=0.2)
priors<-rep(1/6,6)

y<-1
n<-1

j<-6 ## no. of thetas
likelihoods<-rep(NA,6)
for(i in 1:length(thetas)){
  likelihoods[i]<-dbinom(y,n,thetas[i])
}

liks.priors<-likelihoods * priors

sum.lik.priors<-sum(liks.priors)

posteriors<- liks.priors/sum.lik.priors
```

We have been using discrete prior distributions so far. We might want to use a continuous prior distribution if we have prior knowledge that, say, the true value lies between 0.2 and 0.6, with mean 0.4. If our prior should have mean 0.4 and sd 0.1, we can figure out what the corresponding parameters of the beta distribution should be. (Look up the mean and variance of the beta distribution, and solve for the parameters.) You should be able to prove analytically that a= 9.2, b=13.8.

Let's plot the prior (Figure 15). Then plot the likelihood (Figure 16). Recall that the likelihood is a function of the parameters θ.

This likelihood can equally well be presented as a Beta distribution because the Beta distribution's parameters a and b can be interpreted as prior successes and failures. See Figure 17.

Since we multiply the Beta distribution representing the prior and the beta distribution representing the likelihood:

$$Beta(9.2, 13.8) * Beta(15, 5) = Beta(a = 9.2 + 15, b = 13.8 + 5) \quad (233)$$

We can also plot all three (prior, likelihood, posterior) in one figure. That's an exercise for you.

As a further exercise, you may want to write a generic function that, for a given set of values for the prior (given mean's and sd's), and given the data (number of successes and failures), plots the appropriate posterior (alongside the priors and likelihood).

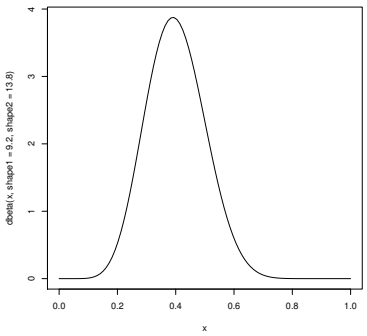


Figure 15: The prior in terms of the beta distribution.

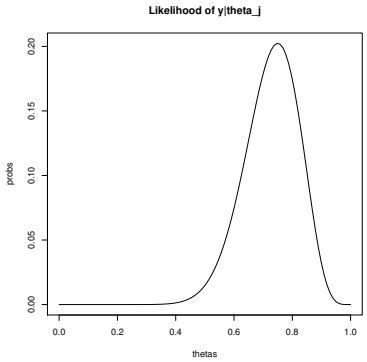


Figure 16: Likelihood.

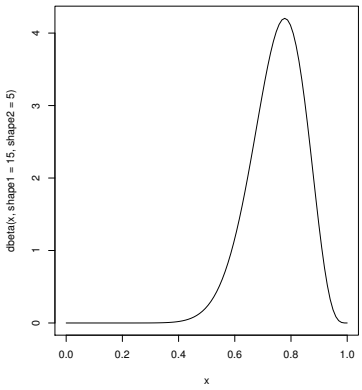


Figure 17: Likelihood in terms of the beta.

11.3 Exercise: The proportion of female births in France

Here is another exercise to help you solidify your understanding of the above concepts. It is taken from the Copenhagen course of 2012 that I mentioned earlier. I quote it verbatim.

"The French mathematician Pierre-Simon Laplace (1749-1827) was the first person to show definitively that the proportion of female births in the French population was less then 0.5, in the late 18th century, using a Bayesian analysis based on a uniform prior distribution[17]). Suppose you were doing a similar analysis but you had more definite prior beliefs about the ratio of male to female births. In particular, if θ represents the proportion of female births in a given population, you are willing to place a Beta(100,100) prior distribution on θ.

[17]

1. Show that this means you are more than 95% sure that θ is between 0.4 and 0.6, although you are ambivalent as to whether it is greater or less than 0.5.

2. Now you observe that out of a random sample of $1,000$ births, 511 are boys. What is your posterior probability that $\theta > 0.5$?"

Here is yet another exercise, taken from Lunn et al.[18], their example 3.1.1. Suppose that 1 in 1000 people in a population are (or is) expected to get HIV. Suppose a test is administered on a suspected HIV case, where the test has a true positive rate (the proportion of positives that are actually HIV positive) of 95% and true negative rate (the proportion of negatives are actually HIV negative) 98%. Use Bayes theorem to find out the probability that a patient testing positive actually has HIV.

[18] David Lunn, Chris Jackson, David J Spiegelhalter, Nicky Best, and Andrew Thomas. *The BUGS book: A practical introduction to Bayesian analysis*, volume 98. CRC Press, 2012

Next, we turn to a key idea in Bayesian data analysis: **the posterior is a compromise between the prior and the likelihood**. Let's look at some specific examples.

11.4 The posterior is the weighted mean of the prior mean and the MLE

Suppose we are modeling the number of times that a speaker says the word "the" per day.

The number of times x that the word is uttered in one day can be modeled by a Poisson distribution:

$$f(x \mid \theta) = \frac{\exp(-\theta)\theta^x}{x!} \tag{234}$$

where the rate θ is unknown, and the numbers of utterances of the target word on each day are independent given θ.

Let's say we are told that the prior mean of θ is 100 and prior variance for θ is 225. This expresses a prior belief, based for example on prior knowledge (existing data), expert opinion or the like.

We can fit a Gamma density prior for θ based on the above information.

It is known from standard statistical theory that for a Gamma density with parameters a, b, the mean is $\frac{a}{b}$ and the variance is $\frac{a}{b^2}$. Since we are given values for the mean and variance, we can solve for a,b, which gives us the gamma density.

If $\frac{a}{b} = 100$ and $\frac{a}{b^2} = 225$, it follows that $a = 100 \times b = 225 \times b^2$ or $100 = 225 \times b$, i.e., $b = \frac{100}{225}$.

This means that $a = \frac{100 \times 100}{225} = \frac{10000}{225}$. Therefore, the Gamma distribution for the prior is as shown below (also see Fig 18):

$$\theta \sim Gamma(\frac{10000}{225}, \frac{100}{225}) \tag{235}$$

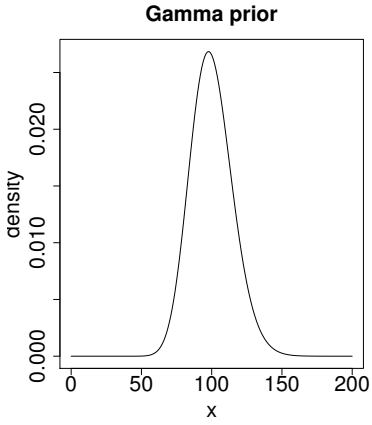


Figure 18: The gamma prior for θ.

A distribution for a prior is **conjugate** if, multiplied by the likelihood, it yields a posterior that has the distribution of the same family as the prior.

It turns out that the Gamma distribution is a conjugate prior for the Poisson distribution. That's why we chose a prior expressed in terms of the Gamma.

For the Gamma distribution to be a conjugate prior for the Poisson, the posterior needs to have the general form of a Gamma distribution.

Given that

$$\text{Posterior} \propto \text{Prior Likelihood} \tag{236}$$

and given that the likelihood is:

$$\begin{aligned} L(\mathbf{x} \mid \theta) =& \prod_{i=1}^{n} \frac{\exp(-\theta)\theta^{x_i}}{x_i!} \\ =& \frac{\exp(-n\theta)\theta^{\sum_i^n x_i}}{\prod_{i=1}^n x_i!} \end{aligned} \tag{237}$$

we can compute the posterior as follows:

$$\text{Posterior} = \left[\frac{\exp(-n\theta)\theta^{\sum_i^n x_i}}{\prod_{i=1}^n x_i!}\right]\left[\frac{b^a\theta^{a-1}\exp(-b\theta)}{\Gamma(a)}\right] \tag{238}$$

Disregarding the terms $x!, \Gamma(a), b^a$, which do not involve θ, we have

$$\begin{aligned} \text{Posterior} \propto& \exp(-n\theta)\theta^{\sum_i^n x_i}\theta^{a-1}\exp(-b\theta) \\ =& \theta^{a-1+\sum_i^n x_i}\exp(-\theta(b+n)) \end{aligned} \tag{239}$$

We can figure out the parameters of the posterior distribution, and show that it will be a Gamma distribution. Note that the Gamma distribution in general is $Gamma(a,b) \propto \theta^{a-1}\exp(-\theta b)$. So it's enough to state the above as a Gamma distribution with some parameters a*, b*.

If we equate $a^* - 1 = a - 1 + \sum_i^n x_i$ and $b^* = b + n$, we can rewrite the above as:

$$\theta^{a^*-1}\exp(-\theta b^*) \tag{240}$$

This means that $a^* = a + \sum_i^n x_i$ and $b^* = b + n$. We can find a constant k such that the above is a proper probability density function, i.e.:

$$\int_{-\infty}^{\infty} k\theta^{a^*-1}\exp(-\theta b^*) = 1 \tag{241}$$

Thus, the posterior has the form of a Gamma distribution with parameters $a^* = a + \sum_i^n x_i, b^* = b + n$. Hence the Gamma distribution is a conjugate prior for the Poisson.

11.5 Example: The Poisson-Gamma conjugate case

Returning to our specific example, if we are given that the number of "the" utterances is $115, 97, 79, 131$, we can derive the posterior distribution as follows.

The prior is Gamma(a=10000/225,b=100/225). The data are as given; this means that $\sum_i^n x_i = 422$ and sample size $n = 4$. It follows that the posterior is

$$\begin{aligned} Gamma(a^* = a + \sum_i^n x_i, b^* = b + n) =& Gamma(10000/225 + 422, 4 + 100/225) \\ =& Gamma(466.44, 4.44) \end{aligned} \tag{242}$$

The mean and variance of this distribution can be computed using the fact that the mean is $\frac{a*}{b*} = 466.44/4.44 = 104.95$ and the variance is $\frac{a*}{b*^2} = 466.44/4.44^2 = 23.61$.

We can do this in R as follows.

```r
## load data:
data<-c(115,97,79,131)

a.star<-function(a,data){
  return(a+sum(data))
}
```

```
b.star<-function(b,n){
  return(b+n)
}

new.a<-a.star(10000/225,data)
new.b<-b.star(100/225,length(data))

## post. mean
post.mean<-new.a/new.b
## post. var:
post.var<-new.a/(new.b^2)

new.data<-c(200)

new.a.2<-a.star(new.a,new.data)
new.b.2<-b.star(new.b,length(new.data))

## new mean
new.post.mean<-new.a.2/new.b.2
## new var:
new.post.var<-new.a.2/(new.b.2^2)
```

11.6 *Using JAGS for the Poisson-Gamma conjugate example*

This is also a good place to introduce an important programming language for Bayesian data analysis. One such language is JAGS [19]. I present below the JAGS version of the closed-form solution we computed above.

[19] Martyn Plummer. Jags version 3.3.0 manual. *International Agency for Research on Cancer. Lyon, France*, 2012

```
## specify data:
dat<-list(y=c(115,97,79,131))

## model specification:
cat("
model
   {
for(i in 1:4){
  y[i] ~ dpois(theta)
}
  ##prior
  ## gamma params derived from given info:
  theta ~ dgamma(10000/225,100/225)
}",
```

```
    file="datacode/poissonexample.jag" )

## specify variables to track
## the posterior distribution of:
track.variables<-c("theta")

## load rjags library:
library(rjags,quietly=T)

## Linked to JAGS 3.4.0
## Loaded modules:  basemod,bugs

## define model:
pois.mod <- jags.model(
    data = dat,
    file = "datacode/poissonexample.jag",
    n.chains = 4,
    n.adapt =2000 ,quiet=T)

## run model:
pois.res <- coda.samples( pois.mod,
               var = track.variables,
               n.iter = 50000,
               thin = 50 )
```

We can also visualize the results as shown in Figure 19.

According to the JAGS model, the mean is 104.93, and the variance is 22.3. This matches up well with the above analytically derived results. I got these results by typing:

```
print(summary(pois.res))

##
## Iterations = 50:50000
## Thinning interval = 50
## Number of chains = 4
## Sample size per chain = 1000
##
## 1. Empirical mean and standard deviation for each variable,
##    plus standard error of the mean:
##
##           Mean             SD       Naive SE Time-series SE
##      104.93218        4.72220        0.07466        0.07170
##
## 2. Quantiles for each variable:
```

```
## summarize and plot:
plot(pois.res)
```

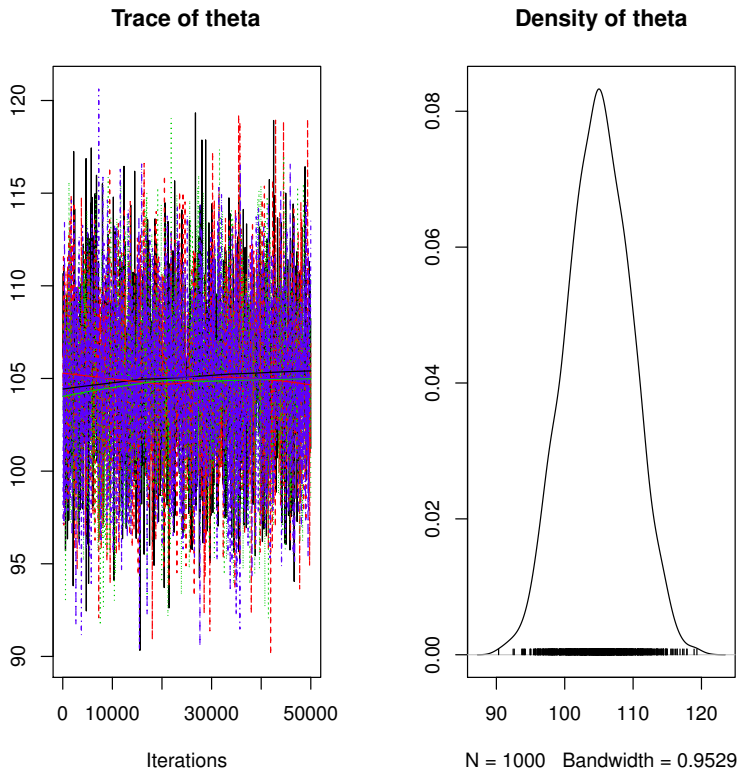


Figure 19: Plot showing the results of the JAGS model fit.

```
##
##  2.5%   25%   50%   75% 97.5%
##  95.8 101.7 104.9 108.2 114.1
```

The plot in Figure 19 shows, on the left hand side, the sampling from the posterior distribution done by JAGS. The word "sampling" here means that given some probability distribution function, we can can sample from it using some standard computational statistical methods (e.g., Gibbs sampling, Metropolis-Hastings sampling, Hamiltonian Monte Carlo). Recall that we know how to sample from the normal distribution or the like, using the `rnorm` function; the JAGS software makes it possible to sample from a probability density function that we know up to proportionality and may not have some built-in R function for. In this course, we don't have time to discuss these methods, but see the the Dobson et al book for discussion, and also see my lecture notes on BDA (this course is taught in winter semesters). If you see "fat hairy caterpillars" in the left-hand side plot, this means that JAGS

is starting to sample from the target distribution and has converged as regards sampling from the posterior distribution.

The right-hand side plot in Figure 19 shows the posterior distribution of the parameter of interest.

We can plot the prior, likelihood, and posterior associated with the above model fit in a single figure (see Figure 20).

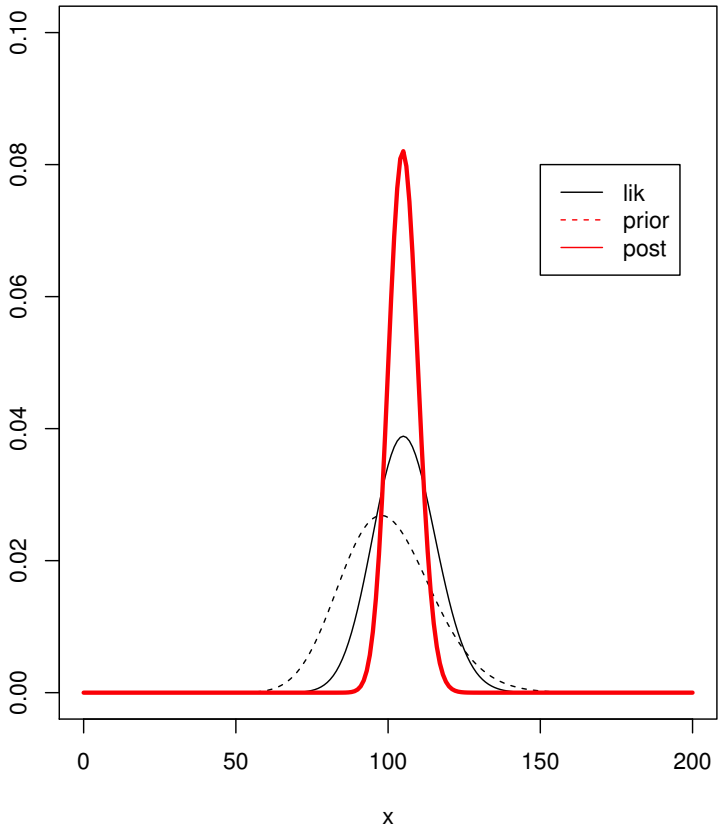


Figure 20: The broken line is the prior (Gamma), the solid black line is the likelihood, and the thick red line is the posterior.

11.7 *The posterior in the Poisson-Gamma case as a weighted sum*

In this example too, we can express the posterior mean as a weighted sum of the prior mean and the maximum likelihood estimate of θ.

The posterior mean is:

$$\frac{a*}{b*} = \frac{a + \sum x_i}{n + b} \tag{243}$$

This can be rewritten as

$$\frac{a*}{b*} = \frac{a + n\bar{x}}{n + b} \tag{244}$$

Dividing both the numerator and denominator by b:

$$\frac{a*}{b*} = \frac{(a + n\bar{x})/b}{(n + b)/b} = \frac{a/b + n\bar{x}/b}{1 + n/b} \tag{245}$$

Since a/b is the mean m of the prior, we can rewrite this as:

$$\frac{a/b + n\bar{x}/b}{1 + n/b} = \frac{m + \frac{n}{b}\bar{x}}{1 + \frac{n}{b}} \tag{246}$$

We can rewrite this as:

$$\frac{m + \frac{n}{b}\bar{x}}{1 + \frac{n}{b}} = \frac{m \times 1}{1 + \frac{n}{b}} + \frac{\frac{n}{b}\bar{x}}{1 + \frac{n}{b}} \tag{247}$$

This is a weighted average: setting $w_1 = 1$ and $w_2 = \frac{n}{b}$, we can write the above as:

$$m\frac{w_1}{w_1 + w_2} + \bar{x}\frac{w_2}{w_1 + w_2} \tag{248}$$

A n approaches infinity, the weight on the prior mean m will tend towards 0, making the posterior mean approach the maximum likelihood estimate of the sample.

This brings us to the key point: **as sample size increases, the likelihood will dominate in determining the posterior mean**.

Regarding variance, since the variance of the posterior is:

$$\frac{a*}{b*^2} = \frac{(a + n\bar{x})}{(n + b)^2} \tag{249}$$

as n approaches infinity, the posterior variance will approach zero, which makes sense: more data will reduce variance (uncertainty).

11.8 Exercise: Using the posterior as a prior for new data

Here is an exercise you can do to understand the concepts above a bit better. If we have additional data from two weeks, with a count of 200, $\sum x_i = 422 + 200 = 622$ and $n = 6$ (not 5, because it is two weeks' data).[20] The task is to find the new posterior distribution given this new data. Try doing this yourself first before reading on.

Solution: The posterior would be a Gamma distribution with parameters: $a^{**} = a + \sum_i^6 x_i = 10000/225 + 622 = 666.44$ and $b^{**} = b + 6 = 100/225 + 6 = 6.44$. In other words, the mean of the posterior is 103.41 and the variance is 16.05.

We can verify this using JAGS.

[20] One can also demonstrate this by multiplying the likelihood of the five data points; for the two weeks' measurement, the likelihood would be proportional to $\exp(-2\theta)(2\theta)^x$. Given that $n = 4$ for the original data, this likelihood for the new data has the effect that the likelihood ends up being proportional to $\exp(-\theta(n+2))(\theta)^{\sum x}$.

```
dat2<-list(y=c(115,97,79,131,200))

## model specification:
cat("
model
   {
for(i in 1:4){
  y[i] ~ dpois(theta)
}
  y[5] ~ dpois(2*theta)

  ##prior
  ## gamma params derived from given info:
  theta ~ dgamma(10000/225,100/225)
}",
    file="datacode/poisexample2.jag" )

## specify variables to track
## the posterior distribution of:
track.variables<-c("theta")

## define model:
poisex2.mod <- jags.model(
    data = dat2,
    file = "datacode/poisexample2.jag",
    n.chains = 4,
    n.adapt =2000 ,quiet=T)

## run model:
poisex2.res <- coda.samples( poisex2.mod,
               var = track.variables,
               n.iter = 100000,
               thin = 50 )
```

JAGS returns the mean as 103.44, and the variance as 16.37. This is quite close to the analytically computed values.

Again, I got this summary by typing:

```
print(summary(poisex2.res))

##
## Iterations = 50:1e+05
## Thinning interval = 50
## Number of chains = 4
```

```
## Sample size per chain = 2000
##
## 1. Empirical mean and standard deviation for each variable,
##    plus standard error of the mean:
##
##           Mean             SD       Naive SE Time-series SE
##      103.43674        4.04577        0.04523        0.04603
##
## 2. Quantiles for each variable:
##
##   2.5%    25%    50%    75%  97.5%
##  95.82 100.66 103.38 106.11 111.58
```

We can also use the posterior distribution from the old data as our prior for the new data. The posterior distribution given the old data is $Gamma(a = 466.44, b = 4.44)$. The new data is a count of 200 over two weeks, therefore the likelihood is proportional to:

$\exp(-2\theta)(2\theta)^{200}$

Multiplying the prior (the above posterior) with the likelihood, we get:

$$\begin{aligned}[\theta^{466.44-1}\exp(-4.44\theta)][\exp(-2\theta)(2\theta)^{200}] =& \theta^{666.44-1}\exp(-4.44\theta - 2\theta) \\ =& \theta^{666.44-1}\exp(-6.44\theta)\end{aligned} \tag{250}$$

In other words, the posterior is $Gamma(666.44, 6.44)$.

This is identical to the posterior we obtained above by combining the data. This situation will always be true when we have conjugate priors: **the result will be the same regardless of whether we take all the data together or successively fit new data, using the posterior of the previous fit as our prior**. This is because the multiplication of the terms will always give the same result regardless of how they are rearranged.

In the above example, we can again express the posterior mean as a weighted sum of the prior mean and the maximum likelihood estimate of θ.

The posterior mean is:

$$\frac{a*}{b*} = \frac{a + \sum x_i}{n + b} \tag{251}$$

This can be rewritten as

$$\frac{a*}{b*} = \frac{a + n\bar{x}}{n + b} \tag{252}$$

Dividing both the numerator and denominator by b:

$$\frac{a*}{b*} = \frac{(a + n\bar{x})/b}{(n + b)/b} = \frac{a/b + n\bar{x}/b}{1 + n/b} \tag{253}$$

Since a/b is the mean m of the prior, we can rewrite this as:

$$\frac{a/b + n\bar{x}/b}{1 + n/b} = \frac{m + \frac{n}{b}\bar{x}}{1 + \frac{n}{b}} \tag{254}$$

We can rewrite this as:

$$\frac{m + \frac{n}{b}\bar{x}}{1 + \frac{n}{b}} = \frac{m \times 1}{1 + \frac{n}{b}} + \frac{\frac{n}{b}\bar{x}}{1 + \frac{n}{b}} \tag{255}$$

This is a weighted average: setting $w_1 = 1$ and $w_2 = \frac{n}{b}$, we can write the above as:

$$m\frac{w_1}{w_1 + w_2} + \bar{x}\frac{w_2}{w_1 + w_2} \tag{256}$$

A n approaches infinity, the weight on the prior mean m will tend towards 0, making the posterior mean approach the maximum likelihood estimate of the sample.

This makes sense: as sample size increases, the likelihood will dominate in determining the posterior mean.

Regarding variance, since the variance of the posterior is:

$$\frac{a*}{b*^2} = \frac{(a + n\bar{x})}{(n + b)^2} \tag{257}$$

as n approaches infinity, the posterior variance will approach zero, which makes sense: more data will reduce variance (uncertainty).

This ends our introduction to Bayesian data analysis. We turn next to our main topic: linear modeling in a Bayesian framework.

12 *Fitting Linear Models and Linear Mixed Models in a Bayesian setting*

I will add notes here later, but for next week, please read the ArXiv preprint by Sorensen and Vasishth [21].

[21] Tanner Sorensen and Shravan Vasishth. Bayesian linear mixed models using Stan: A tutorial for psychologists, linguists, and cognitive scientists. ArXiv e-print, 2015

Acknowledgements

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