Lab 6

Ben Bolker, modified at several places by Bob Douma and Alejandro Morales. Bayesian part by Alejandro Morales Sierra.

19 October 2018

Learning goals

You will learn how to:

1. Program the likelihood function of a model.
2. Estimate the parameters of a model through maximum likelihood.
3. Estimate the confidence intervals of the model parameters through profiling and the quadratic approximation.
4. Estimate parameters in a Bayesian framework and how parameter uncertainty can be assessed (time permitting and when of interest to you).

Fitting models to data

In this exercise you will learn how to fit models to data through means of maximum likelihood and compare the likelihood of different models (hypotheses). Fitting a model to data through likelihood requires that you take four steps:

1. Specify how the dependent variable depends on the independent variable, i.e. specify a function how the mean of y depends on the value of x.
2. Specify a probability distribution to describe the deviations of the observations from the mean
3. Choose the parameters of the deterministic model and the probability model such that the negative log likelihood is lowest.
4. Compare the likelihood of alternative models (change the deterministic function or the stochastic function) and compare with AIC(c) or BIC which model is most parsimonious.

To fit a model through means of maximum likelihood you need to specify a function that calculate the negative log likelihood (NLL) based on the data and the parameter values. For example to calculate the NLL of a linear model and a normal distribution the following function works:

```
nll = function(par,y,x){
  a = par[1]
  b = par[2]
  sd = par[3]
  # this calculates the mean y for a given value of x: the deterministic function
  mu = a+b*x
  # this calculates the likelihood of the function given the probability
  # distribution, the data and mu and sd
  nll = -sum(dnorm(y,mean=mu,sd=sd,log=T))
  return(nll)
}
```

Note that `-sum(log(dnorm(y,mean=mu,sd=sd)))` should not be used as it may lead to underflow (the computer cannot store very very small probabilities) and therefore to optimisation problems.

Next we specify a function to find the maximum likelihood estimate

```
par=c(a=1,b=1,c=1) # initial parameters
opt1 = optim(par=par,nll,x=x,y=y) # y represents the data, x the independent variable
```

It can also be done through `mle2`

```
nll.mle = function(a,b,sd){
  # this calculates the mean y for a given value of x: the deterministic function
  mu = a+b*x
  # this calculates the likelihood of the function given the probability
  # distribution, the data and mu and sd
  nll = -sum(dnorm(y,mean=mu,sd=sd,log=T))
  return(nll)
}
```

```
# the data should be supplied through data and the parameters through list().
mle2.1 = mle2(nll.mle,start=list(a=1,b=1,sd=1),data=data.frame(x,y))
summary(mle2.1)
```

Made-up data: negative binomial

The simplest thing to do to convince yourself that your attempts to estimate parameters are working is to simulate the "data" yourself and see if you get close to the right answers back.

Start by making up some negative binomial `data`: first, set the random-number seed so we get consistent results across different `R` sessions:

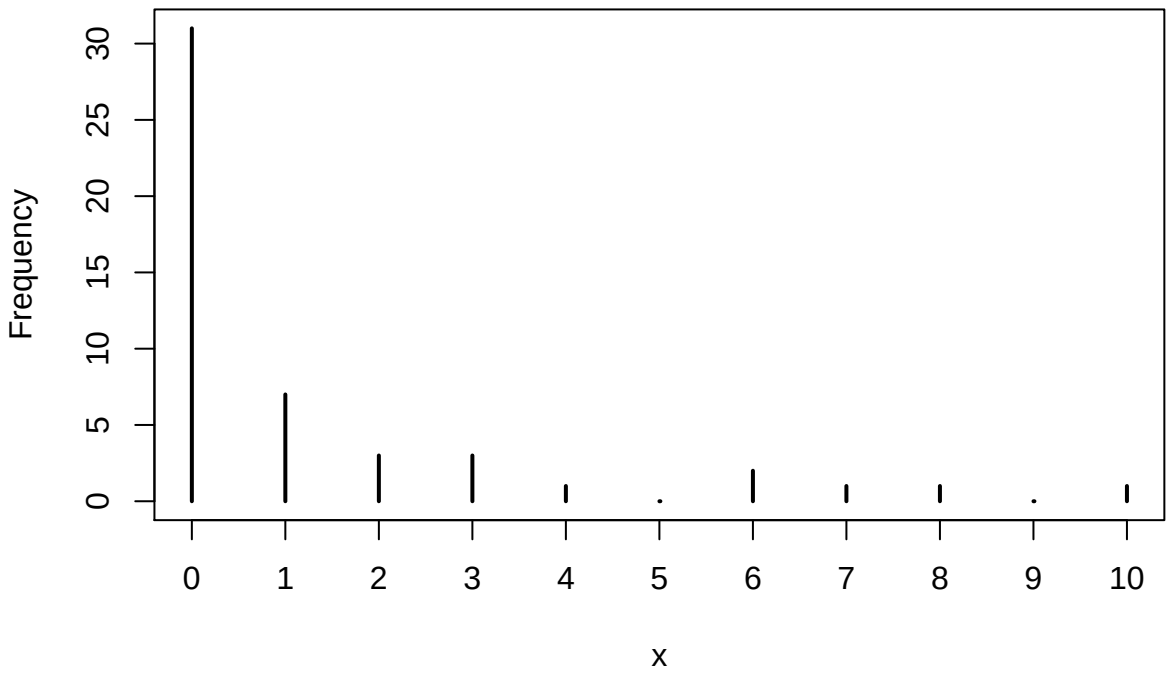
```
set.seed(1001)
```

Generate 50 values with $\mu = 1$, $k = 0.4$ (save the values in variables in case we want to use them again later, or change the parameters and run the code again):

```
mu.true=1
k.true=0.4
x = rnbinom(50,mu=mu.true,size=k.true)
```

Take a quick look at what we got:

```
plot(table(factor(x,levels=0:max(x))),
     ylab="Frequency",xlab="x")
```



(reminder: I won't always draw the pictures, but it's good to make a habitat of examining your variables (with `summary()` etc. and graphically) as you go along to make sure you know what's going on!)

Negative log-likelihood function for a simple draw from a negative binomial distribution: the first parameter, `p`, will be the vector of parameters, and the second parameter, `dat`, will be the data vector (in case we want to try this again later with a different set of data; by default we'll set it to the 'x} vector we just drew randomly).

```
NLLfun1 = function(p,dat=x) {
  mu=p[1]
  k=p[2]
  -sum(dnbinom(x,mu=mu,size=k,log=TRUE))
}
```

Calculate the negative log-likelihood for the true values. I have to combine these values into a vector with `c()` to pass them to the negative log-likelihood function. Naming the elements in the vector is optional but will help keep things clear as we go along:

```
nll.true=NLLfun1(c(mu=mu.true,k=k.true)); nll.true
```

The NLL for other parameter values that I know are way off ($\mu = 10$, $k = 10$):

```
NLLfun1(c(mu=10,k=10))
```

```
## [1] 291.4351
```

Much higher negative log-likelihood, as it should be.

Find the method-of-moments estimates for μ and k:

```
m = mean(x)
v = var(x)
mu.mom = m
k.mom = m/(v/m-1)
```

Negative log-likelihood estimate for method of moments parameters:

```
nll.mom=NLLfun1(c(mu=mu.mom,k=k.mom)); nll.mom
```

```
## [1] 72.08996
```

Despite the known bias, this estimate is better (lower negative log-likelihood) than the "true" parameter values. The Likelihood Ratio Test would say, however, that the difference in likelihoods would have to be greater than $\chi^2_2(0.95)/2$ (two degrees of freedom because we are allowing both μ and k to change):

```
ldiff=nll.true-nll.mom;ldiff
```

```
## [1] 0.5576733
```

```
qchisq(0.95,df=2)/2
```

```
## [1] 2.995732
```

So — better, but not significantly better at $p = 0.05$. `pchisq(2*ldiff,df=2,lower.tail=FALSE)` would tell us the exact p-value if we wanted to know.)

But what is the MLE? Use `optim` with the default options (Nelder-Mead simplex method) and the method-of-moments estimates as the starting estimates (`par`):

```
O1 = optim(fn=NLLfun1,par=c(mu=mu.mom,k=k.mom),hessian=TRUE);
O1
```

```
## $par
##        mu         k
## 1.2602356 0.2884793
##
## $value
## [1] 71.79646
##
## $counts
## function gradient
##       45       NA
##
## $convergence
## [1] 0
##
## $message
## NULL
##
## $hessian
##             mu            k
## mu 7.387808317  0.004901576
## k  0.004901576 97.372581394
```

The optimization result is a list with elements:

- the best-fit parameters (`O1$par`, with parameter names because we named the elements of the starting vector—see how useful this is?);}
- the minimum negative log-likelihood (`O1$value`);

- information on the number of function evaluations (`O1$counts`; the `gradient` part is `NA` because we didn't specify a function to calculate the derivatives (and the Nelder-Mead algorithm wouldn't have used them anyway)
- information on whether the algorithm thinks it found a good answer `O1$convergence`, which is zero if `R` thinks everything worked and uses various numeric codes (see `?optim` for details) if something goes wrong;
- `O1$message` which may give further information about the when the fit converged or how it failed to converge;
- because we set `hessian=TRUE`, we also get `O1$hessian`, which gives the (finite difference approximation of) the second derivatives evaluated at the MLE.

The minimum negative log-likelihood (`round(O1$value,2)`) is better than either the negative log-likelihood corresponding to the method-of-moments parameters (`round(nll.mom,2)`) or the true parameters (`round(nll.true,2)`), but all of these are within the LRT cutoff.

Now let's find the likelihood surface, the profiles, and the confidence intervals.

The likelihood surface is straightforward: set up vectors of μ and k values and run `for` loops, set up a matrix to hold the results, and run `for` loops to calculate and store the values. Let's try μ from 0.4 to 3 in steps of 0.05 and k from 0.01 to 0.7 in steps of 0.01. (I initially had the μ vector from 0.1 to 2.0 but revised it after seeing the contour plot below.)

```
muvec = seq(0.4,3,by=0.05)
kvec = seq(0.01,0.7,by=0.01)
```

The matrix for the results will have rows corresponding to μ and columns corresponding to k:

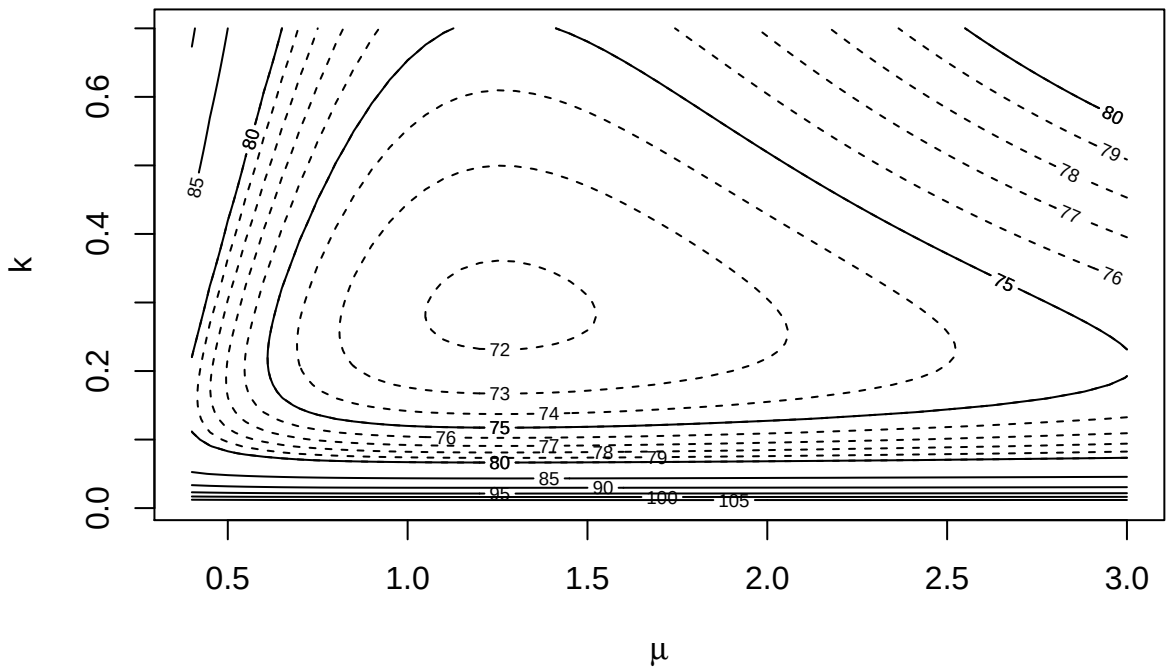
```
resmat = matrix(nrow=length(muvec),ncol=length(kvec))
```

Run the `for` loops:

```
for (i in 1:length(muvec)) {
  for (j in 1:length(kvec)) {
    resmat[i,j] = NLLfun1(c(muvec[i],kvec[j]))
  }
}
```

Drawing a contour: the initial default choice of contours doesn't give us fine enough resolution (it picks contours spaced 5 apart to cover the range of the values in the matrix), so I added levels spaced 1 log-likelihood unit apart from 70 to 80 by doing a second `contour` plot with `add=TRUE`.

```
contour(muvec,kvec,resmat,xlab=expression(mu),ylab="k")
contour(muvec,kvec,resmat,levels=70:80,lty=2,add=TRUE)
```



Maximum likelihood and covariates

The following steps will lead you through the model fitting procedure when we have a covariate.

1. Take the first dataset (or another one from the six that we have been working with before) and tweak the above functions such that it matches with the deterministic and stochastic model that you have chosen. In case you got stuck in the previous exercises where you had to choose a deterministic function and a stochastic function see next page for suggestions.

   hint: In a previous exercise you have eyeballed the parameter values of the functions, you can use these as starting values.

   hint: In case you get convergence problems, further adapt your starting values, or choose a different optimizer. For example Nelder-Mead is a robust one, e.g. `method = "Nelder-Mead"`.

2. Change the determinstic function for a possible alternative determinstic function
3. Compare the likelihoods of the data given both models
4. Apply model selection criteria and conclude which model fits that data best.
5. Does the model makes sense from a biological perspective?

Optional and time permitting:
6. Repeat the above procedure for the other 5 datasets

```
library(bbmle)
```

```
## Loading required package: stats4
```

```
shapes1= read.csv("D:/BobDouma/Education/CSA-34306 Ecological Models and Data in R/2017-2018/tutorials/
plot(shapes1)

x = shapes1$x
y = shapes1$y

nll.mle = function(a,b,sd){
  # this calculates the mean y for a given value of x: the deterministic function
  mu = a*(1-exp(-b*x))
  # this calculates the likelihood of the function given the probability
  # distribution, the data and mu and sd
  nll = -sum(dnorm(y,mean=mu,sd=sd,log=T))
  return(nll)
}


mle2.1 = mle2(nll.mle,start=list(a=25,b=0.0080,sd=1),data=shapes1,method="Nelder-Mead")
summary(mle2.1)
```

```
## Maximum likelihood estimation
##
## Call:
## mle2(minuslogl = nll.mle, start = list(a = 25, b = 0.008, sd = 1),
##     method = "Nelder-Mead", data = shapes1)
##
## Coefficients:
##      Estimate Std. Error z value     Pr(z)
## a  2.2848e+01 3.8002e-01 60.1231 < 2.2e-16 ***
## b  8.9681e-03 9.1372e-04  9.8149 < 2.2e-16 ***
## sd 2.0655e+00 1.9697e-01 10.4865 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## -2 log L: 235.8625
```

```
logLik(mle2.1)
```

```
## 'log Lik.' -117.9313 (df=3)
```

```
confint(mle2.1)
```

```
## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced
```

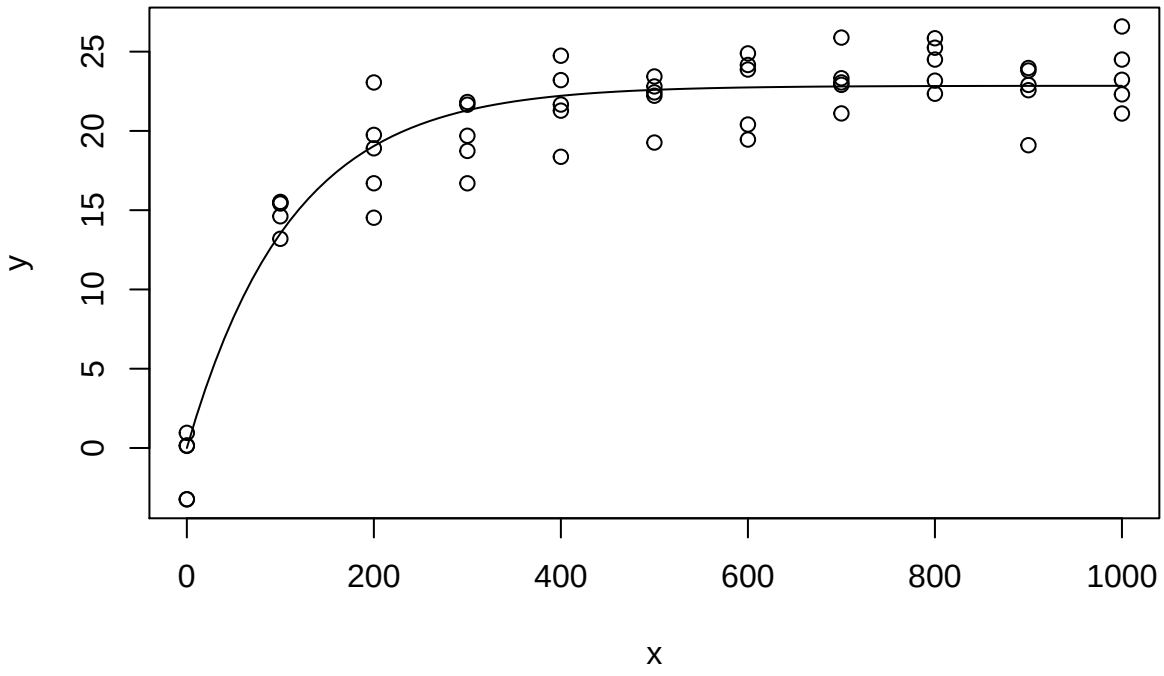
```
##           2.5 %      97.5 %
## a  22.103948268 23.62291449
## b   0.007380406  0.01111318
## sd  1.732263911  2.52072347
```

```
coef(mle2.1)
```

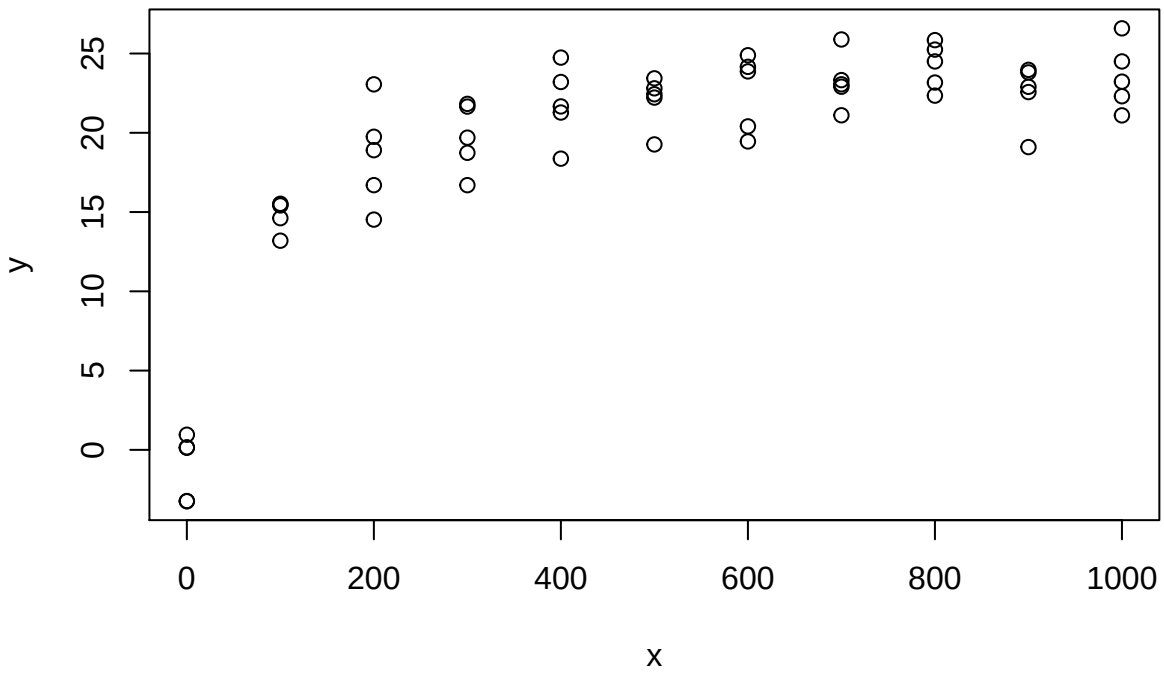
```
##           a           b          sd
```

```
## 22.84786012  0.00896807  2.06549462
```

```
plot(shapes1)
curve(coef(mle2.1)[1]*(1-exp(-coef(mle2.1)[2]*x)),add=T)
```



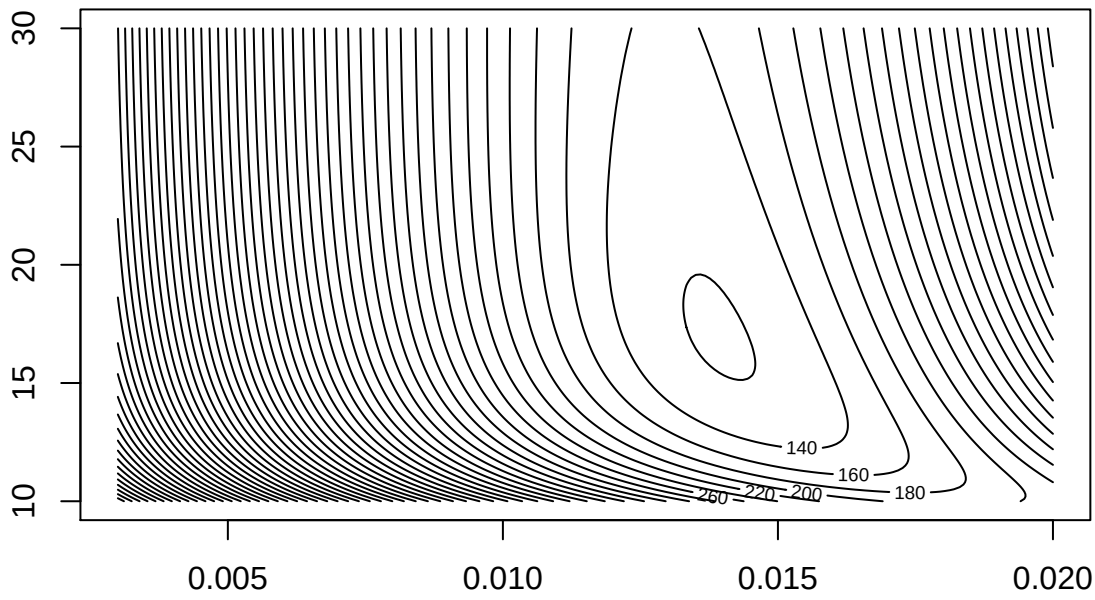

```
library(reshape2)
shapes1= read.csv("D:/BobDouma/Education/CSA-34306 Ecological Models and Data in R/2017-2018/tutorials/
plot(shapes1)
```




```
# likelihood surface
a1 = seq(10,30,length.out = 200)
b1= seq(0.003,0.02,length.out=200)

nll.grid = expand.grid(a1,b1)
nll.grid$NLL = NA
no = 0
for (i in 1:length(a1)){
  for (j in 1:length(b1)){
    no = no + 1
    nll.grid[no,1] = a1[i]
    nll.grid[no,2] = b1[j]
    nll.grid[no,3] = nll.mle(a=a1[i],b=b1[j],sd=2.06)
  }
}
z1 = as.matrix(dcast(nll.grid,Var1~Var2)[,-1])
```

```
## Using NLL as value column: use value.var to override.
```

```
contour(b1,a1,z1,nlevels=60)
```

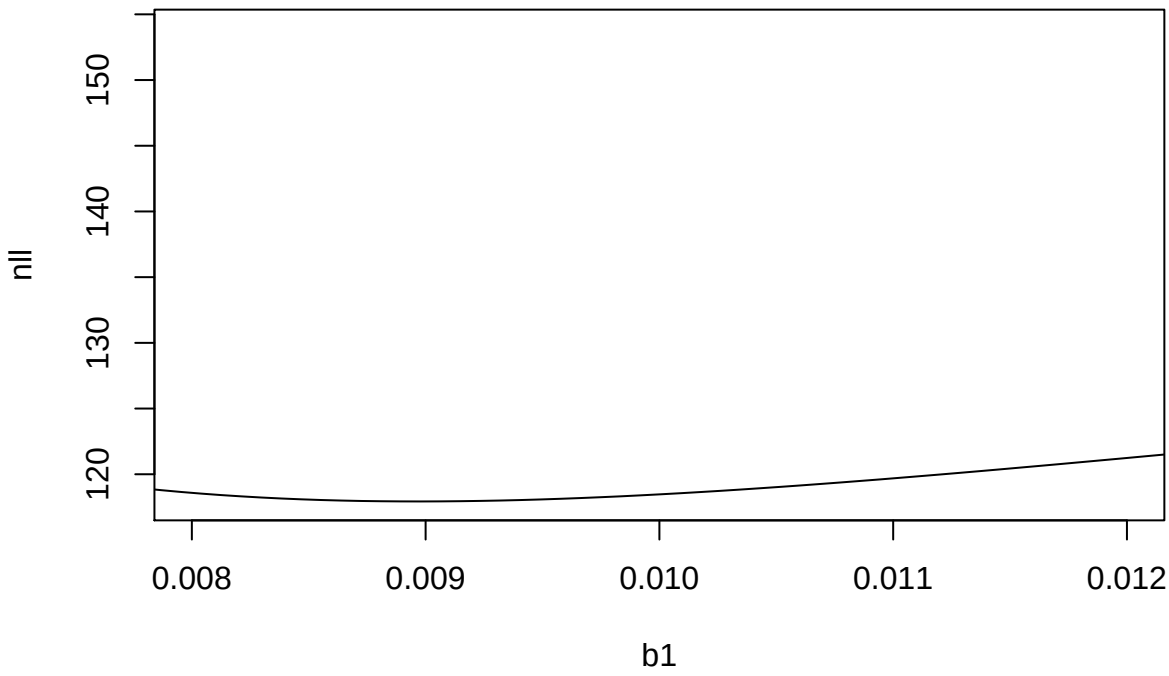



```
# profile
nll.mle1 = function(a,sd){
  # this calculates the mean y for a given value of x: the deterministic function
  mu = a*(1-exp(-b*x))
  # this calculates the likelihood of the function given the probability
  # distribution, the data and mu and sd
  nll = -sum(dnorm(y,mean=mu,sd=sd,log=T))
  return(nll)
}

nll = numeric(length(b1))
for (i in 1:length(b1)){
  b = b1[i]
  mle.21 = mle2(nll.mle1,start=list(a=25,sd=7.96),data=shapes1,method="Nelder-Mead")
  nll[i] = -logLik(mle.21)
}
```

```
## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced
```

```
## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced
```

```
plot(nll~ b1,type="l",xlim=c(0.008,0.012))
```




```
which.min(nll)
```

```
## [1] 71
```

```
# cutoff
-logLik(mle2.1) + qchisq(0.95, 1)/2
```

```
## 'log Lik.' 119.852 (df=3)
```

```
which(nll < 119.852)
```

```
##  [1] 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75
## [24] 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95
```

```r
b1[c(53,95)]
```

```
## [1] 0.007442211 0.011030151
```

```r
plot(nll~ b1,type="l",xlim=c(0.007,0.0110),ylim=c(116,125))
abline(v=c(0.00744,0.01103),lty=2)
abline(v=0.008968,lty=1,lwd=2)
abline(v=c(0.00738,0.01103),lty=2,col="red")

c = mle2.1@details$hessian/2
b = coef(mle2.1)[2]
a = -logLik(mle2.1)

se.mu = sqrt(diag(solve(mle2.1@details$hessian))[2])
b + c(-1,1)*qnorm(0.975) * se.mu
```

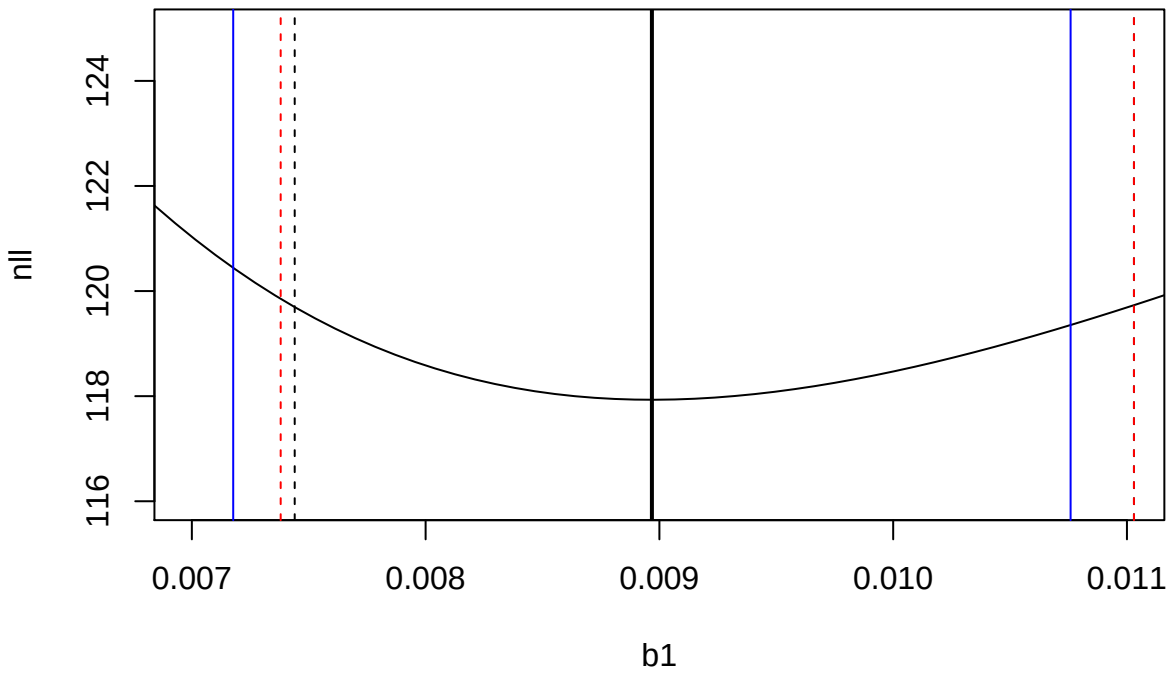
```
## [1] 0.007177214 0.010758926
```

```r
confint(mle2.1)
```

```
## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced
```

```
##           2.5 %      97.5 %
## a  22.103948268 23.62291449
## b   0.007380406  0.01111318
## sd  1.732263911  2.52072347
```

```r
abline(v=c(0.007177,0.0107589),col="blue")
```



Optimisation problems and assessing the confidence limits of parameter estimates

Fitting a model to data requires you to specify a relationship between variables. After specifying this relationship we need to fit parameters of this model that best fits the data. This fitting is done through computer algorithms (optimizers). However, sometimes it may be hard to fit a model to data. After having found the best fitting model, you want to assess how certain you are about the parameter estimates. For assessing the uncertainty of model parameters several methods exist that have pros and cons.

This exercise has two purposes. First you will learn that an innocent looking function can be challenging to fit. Second, you will learn to assess the uncertainty in the parameter values. For assessing the uncertainty in the parameter estimates there are two methods: the profiling method and the quadratic approximation. Bolker recommends to use the likelihood profile for assessing the uncertainty in the parameters because this one is more accurate than the one based on the Hessian matrix.

1. Take the first dataset of the six datasets you have worked with earlier on. Assume that the function was generated by the monomolecular function $a(1 - e^{(-bx)}$. Fit this model with normally distributed errors through this data with `mle2` and optim method `Nelder-Mead`. Choose four different starting points of the optimisation: `start_a = c(5,10,20,30)`, `start_b = c(0.001,0.005,0.01,0.1)` and compare the NLL of those four optimisations. Plot the curves into the plot with data and try to understand what happened.

2. To understand the behaviour of the optimisation routine we will plot the likelihood surface over a range of values of a and b. For a choose a number of parameter values in the range of 0-40 and for b choose a number of values in the range 0.1-10. Calculate for each combination the NLL and plot the NLL surface using `contour` plot. For more insight into the functioning of what the optimisation method did,

you can add the starting points that you gave to mle2 and the best fitting points, use `points()` for this. Do you have a clue why the optimisation did not find the minimum point in the landscape? Now zoom in and choose values for b in the range of 0.001-0.03 and check again the NLL surface.

hint: See Bolker Lab 6 for inspiration on coding.

hint: You can use a for a double for-loop to run over all parameters

hint: Store the NLL results in a matrix (you can make a 100x100 matrix by `matrix(NA,nrow=100,ncol=100)`).

3. Calculate the confidence intervals of the parameters through constructing the likelihood profile. Consult page 106 of Bokler or Lab 6 for how to calculate the confidence intervals based on the likelihood profile. Use the following pseudocode to achieve this:

   a. Adapt the likelihood function such that one parameter is not optimised but chosen by you, say parameter a.
   b. Vary a of a range and optimise the other parameteters.
   c. Plot the NLL as a function of parameter a.
   d. Find the values of a that enclose $-L + \chi^2(1-\alpha)/2$. In `R` this can be done through `qchisq(0.95,1)/2`.
   e. Compare your results with the results from the `R` function `confint()`. `confint()` uses the profiling method along with interpolation methods.

4. *(time permitting)* Calculate the confidence intervals through the quadratic approximation. Take the following steps to achieve this:

   a. Get the standard error of the parameter estimates through `vcov`. Note that `vcov` return the variance/covariance matrix
   b. Calculate the interval based on the fact that the 95% limits are 1.96 (qnorm(0.975,0,1)) standard deviation units away from the mean.

5. *(time permitting)* Plot the confidence limits of the both method and compare the results. Is there a big difference between the methods?

6. To assess the uncertainty in the predictions from the model you can construct population prediction intervals (PPIs, see 7.5.3 Bolker). Population prediction intervals shows the interval in which a new observation will likely fall. To construct the PPI take the following steps

   a. Simulate a number of parameter values taken the uncertainty in the parameter estimates into account.

      hint: If the fitted mle object is called `mle2.obj`, then you can extract the variance-covariance matrix by using `vcov(mle2.obj)`. You can extract the mean parameter estimates by using `coef(mle2.obj)`. Now you are ready to simulate 1000 combinations of parameter values through `z = mvrnorm(1000,mu=coef(mle2.obj),Sigma=vcov(mle2.obj))`. `mvrnorm` is a function to randomly draw values from a multivariate normal distribution.

   b. Predict the mean response based on the simulated parameter values and the values of x

      hint: make a for-loop and predict for each simulated pair of parameter values the mean for a given x. Thus `mu = z[i,1]*(1-exp(-z[i,2]*x))`

   c. Draw from a normal distribution with a mean that was predicted in the previous step and the sd that you simulated in step a.

      hint: `pred = rnorm(length(mu),mean=mu,sd=z[i,3])`. Store pred in a matrix with each simulated dataset in a seperate row.

   d. Calculate for each value of x the 2.5% and the 97.5% quantiles

      hint: If the predictions are stored in a matrix `mat`, you can use `apply(mat,2,quantile,0.975)` to get the upper limit.

```r
#shapes1= read.csv("shapes1.csv")
plot(shapes1)

nll.mle = function(a,b,sd){
  # this calculates the mean y for a given value of x: the deterministic function
  mu = a*(1-exp(-b*shapes1$x))
  # this calculates the likelihood of the function given the probability
  # distribution, the data and mu and sd
  nll = -sum(dnorm(shapes1$y,mean=mu,sd=sd,log=T))
  return(nll)
}

library(bbmle)

# Try 4 different starting points
mle2.1 = vector("list", 4)
start_a = c(5,10,20,30)
start_b = c(0.001,0.005,0.01,0.1)
for(i in 1:4) {
  mle2.1[[i]] = mle2(nll.mle,start=list(a=start_a[i],b = start_b[i], sd=1), method="Nelder-Mead")
}
```

```
## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced
```

```r
# Check the best fit (in this case it is 3rd starting point)
for(i in 1:4) {
  print(logLik(mle2.1[[i]]))
}
```

```
## 'log Lik.' -141.8482 (df=3)
## 'log Lik.' -141.8481 (df=3)
## 'log Lik.' -117.9313 (df=3)
## 'log Lik.' -141.8482 (df=3)
```

```r
# Extract the best fit for the rest of the analysis
best_mle2.1 = mle2.1[[3]]
summary(best_mle2.1)
```

```
## Maximum likelihood estimation
##
## Call:
## mle2(minuslogl = nll.mle, start = list(a = start_a[i], b = start_b[i],
##     sd = 1), method = "Nelder-Mead")
##
## Coefficients:
##      Estimate Std. Error z value     Pr(z)
## a  2.2848e+01 3.8005e-01 60.1178 < 2.2e-16 ***
## b  8.9698e-03 9.1421e-04  9.8115 < 2.2e-16 ***
## sd 2.0656e+00 1.9700e-01 10.4855 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## -2 log L: 235.8625
```

```r
logLik(best_mle2.1)
```

```
## 'log Lik.' -117.9313 (df=3)
```

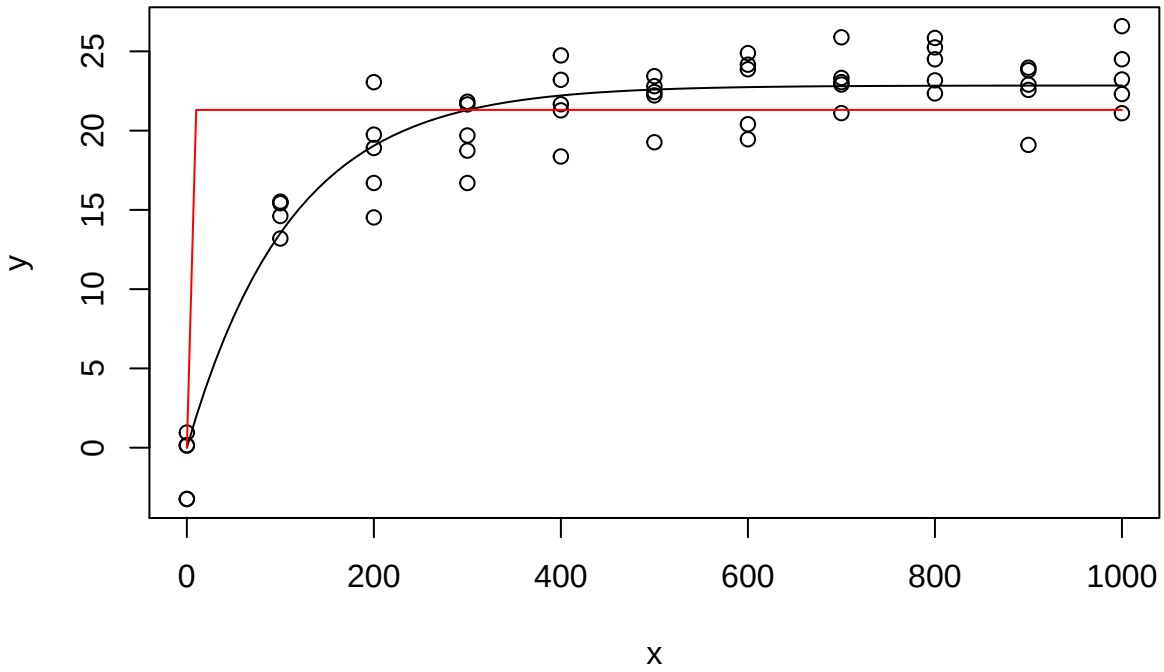
```r
confint(best_mle2.1)
```

```
## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced
##           2.5 %      97.5 %
## a  22.103944203 23.62291394
## b   0.007380444  0.01111312
## sd  1.732265956  2.52072547
```

```r
coef(best_mle2.1)
```

```
##            a            b           sd
## 22.847710401  0.008969762  2.065621124
```

```r
plot(shapes1)
curve(coef(best_mle2.1)[1]*(1-exp(-coef(best_mle2.1)[2]*x)),add=T)
curve(coef(mle2.1[[1]])[1]*(1-exp(-coef(mle2.1[[1]])[2]*x)),add=T, col = 2)
```



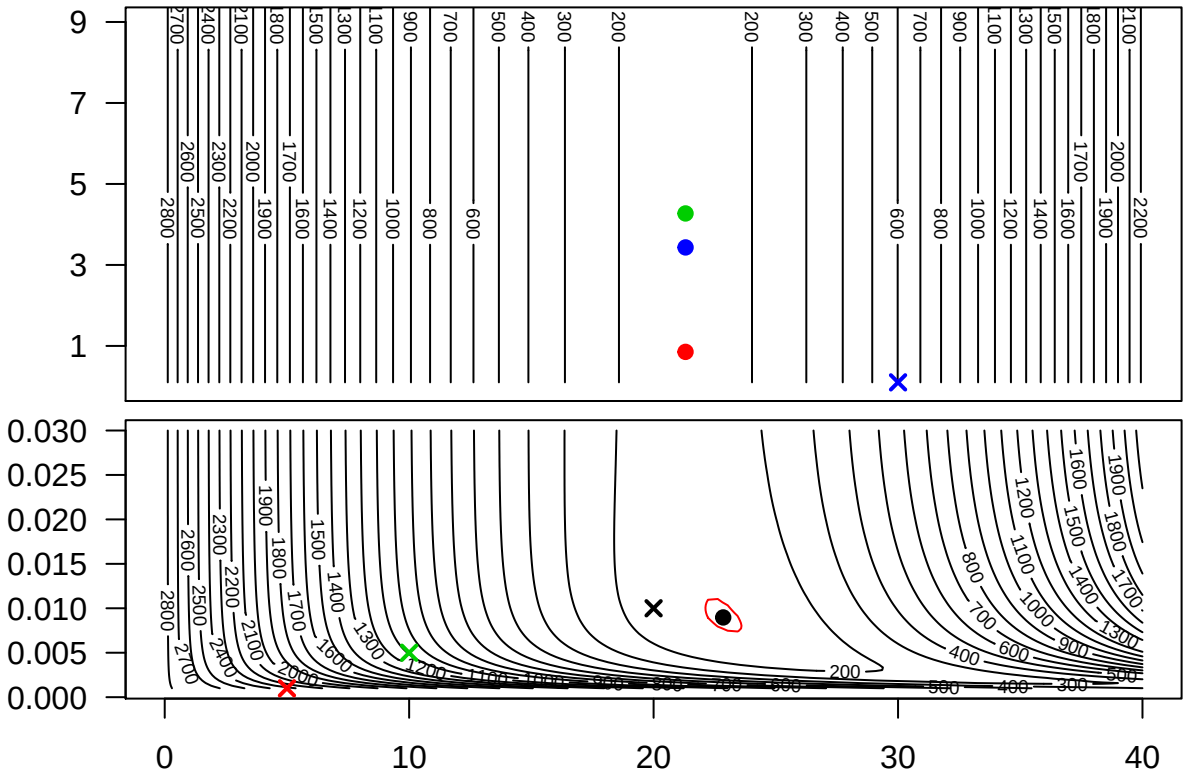
```r
# likelihood surface
a1 = seq(0,40,length.out = 100)
b1.1 = seq(0.001,0.03,length.out=100)
b1.2 = seq(0.1,10,length.out=100)

nll.grid = expand.grid(a1,b1.1)
nll.grid$NLL = NA
no = 0
# Construct first contour
for (i in 1:length(a1)){
  for (j in 1:length(b1.1)){
    no = no + 1
    nll.grid[no,1] = a1[i]
    nll.grid[no,2] = b1.1[j]
    nll.grid[no,3] = nll.mle(a=a1[i],b=b1.1[j],sd=2.06)
  }
}
library(reshape2)
z1.1 = as.matrix(dcast(nll.grid,Var1~Var2)[,-1])
```

```
## Using NLL as value column: use value.var to override.
```

```r
# Construct second contour
no = 0
for (i in 1:length(a1)){
  for (j in 1:length(b1.2)){
    no = no + 1
    nll.grid[no,1] = a1[i]
    nll.grid[no,2] = b1.2[j]
    nll.grid[no,3] = nll.mle(a=a1[i],b=b1.2[j],sd=2.06)
  }
}
z1.2 = as.matrix(dcast(nll.grid,Var1~Var2)[,-1])
```

```
## Using NLL as value column: use value.var to override.
```

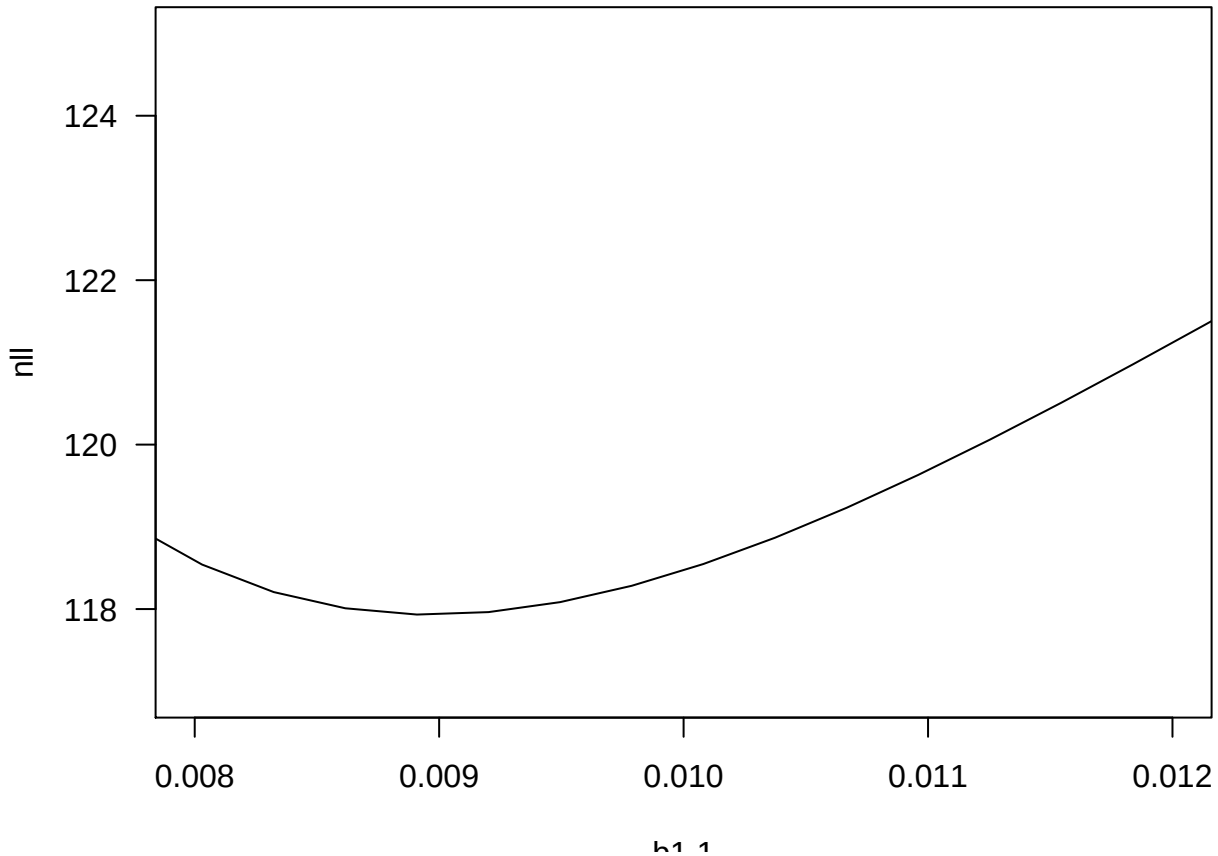
```r
# Plot the two contours
par(mfrow = c(2,1), mar = c(0,4,1,1), las = 1)
contour(a1,b1.2,z1.2,nlevels = 20, xaxt = "n", yaxt = "n", ylim = c(0,9))
axis(2, seq(1,9,2))
points(start_a[4],start_b[4],pch=4, col = 4, lwd = 2)
points(coef(mle2.1[[1]])[1],coef(mle2.1[[1]])[2],pch=19, col = 2)
points(coef(mle2.1[[2]])[1],coef(mle2.1[[2]])[2],pch=19, col = 3)
points(coef(mle2.1[[4]])[1],coef(mle2.1[[4]])[2],pch=19, col = 4)
contour(a1,b1.2,z1.2,levels=120,col=2,add=T)

par(mar = c(3.5,4,0.5,1))
contour(a1,b1.1,z1.1,nlevels = 20)
points(coef(best_mle2.1)[1],coef(best_mle2.1)[2],pch=19)
points(start_a[1],start_b[1],pch=4, col = 2, lwd = 2)
points(start_a[2],start_b[2],pch=4, col = 3, lwd = 2)
points(start_a[3],start_b[3],pch=4, col = 1, lwd = 2)
contour(a1,b1.1,z1.1,levels=120,col=2,add=T)
```




```
# profile
nll.mle1 = function(a,sd){
  # this calculates the mean y for a given value of x: the deterministic function
  mu = a*(1-exp(-b*x))
  # this calculates the likelihood of the function given the probability
  # distribution, the data and mu and sd
  nll = -sum(dnorm(y,mean=mu,sd=sd,log=T))
  return(nll)
}

nll = numeric(length(b1.1))
for (i in 1:length(b1.1)){
  b = b1.1[i]
  mle.21 = mle2(nll.mle1,start=list(a=25,sd=7.96),data=data.frame(x=shapes1$x,y=shapes1$y),method="Neld
  nll[i] = -logLik(mle.21)
}
```

```
## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(y, mean = mu, sd = sd, log = T): NaNs produced
```

```
par(mfrow = c(1,1))
plot(nll~ b1.1,type="l",xlim=c(0.008,0.012), ylim = c(117,125))
```




```
which.min(nll)
```

```
## [1] 28
```

```
# cutoff
-logLik(best_mle2.1) + qchisq(0.95, 1)/2
```

```
## 'log Lik.' 119.852 (df=3)
```

```
which(nll < 119.852)
```

```
##  [1] 23 24 25 26 27 28 29 30 31 32 33 34 35
```

```
b1.1[c(23,35)]
```

```
## [1] 0.007444444 0.010959596
```

```
plot(nll~ b1.1,type="l",xlim=c(0.0070,0.012),ylim=c(116,125))
abline(v=c(0.00744,0.01096),lty=2)
abline(v=0.008968,lty=1,lwd=2)
abline(v=c(0.00738,0.01103),lty=2,col="red")

se.mu = sqrt(diag(solve(best_mle2.1@details$hessian))[2])
b + c(-1,1)*qnorm(0.975) * se.mu
```

```
## [1] 0.02820818 0.03179182
```

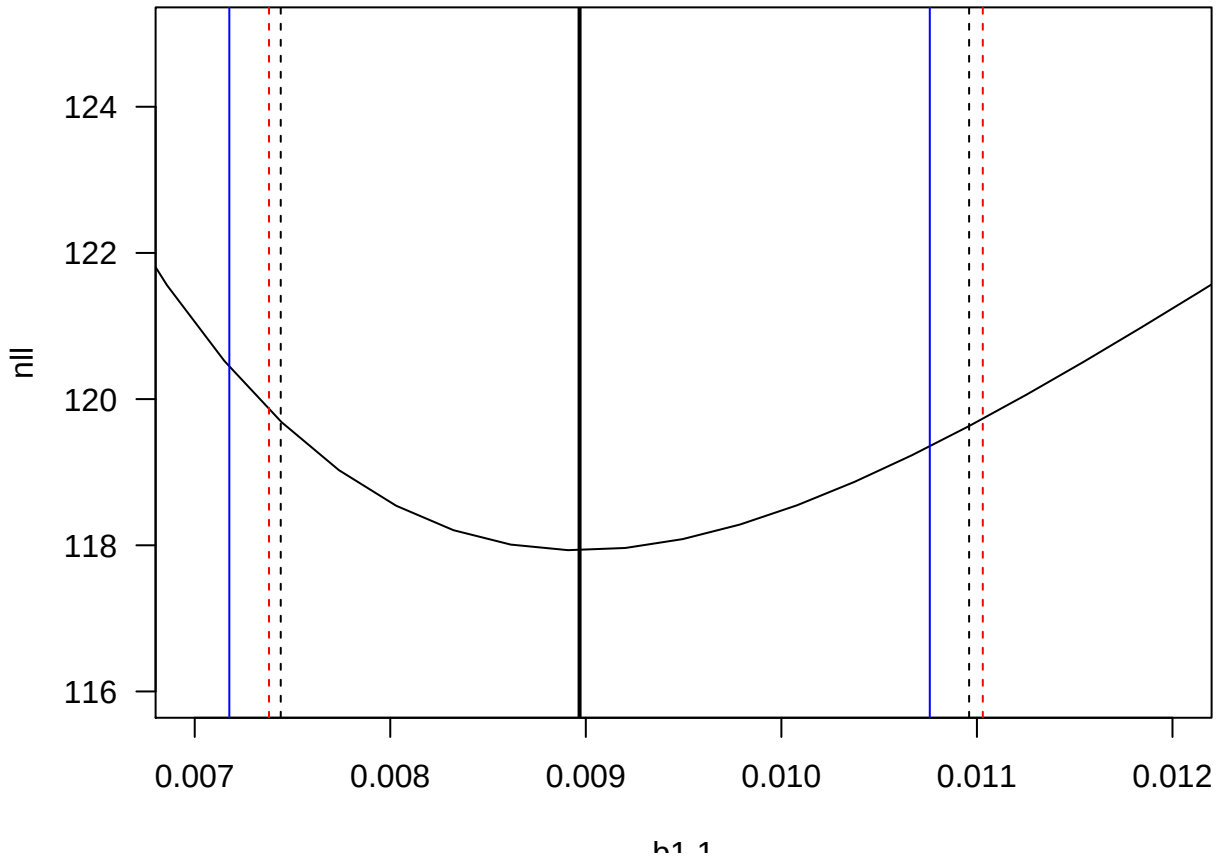
```
confint(best_mle2.1)
```

```
## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced
```

```
## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced

## Warning in dnorm(shapes1$y, mean = mu, sd = sd, log = T): NaNs produced
```

```
##           2.5 %      97.5 %
## a  22.103944203 23.62291394
## b   0.007380444  0.01111312
## sd  1.732265956  2.52072547
```

```
abline(v=c(0.007177,0.0107589),col="blue")
```



Hints for choosing deterministic functions and stochastic functions

1. Deterministic functions

   dataset 1 light response curve. There are a number of options of functions to choose from, depending on the level of sophistication: $\frac{ax}{(b+x)}$, $a(1-e^{(-bx)})$, $\frac{1}{2\theta}(\alpha I + p_{max} - \sqrt{(\alpha I + p_{max})^2 - 4\theta I p_{max}})$ see page 98. A parameter `d` can be added in all cases to shift the curve up or down. The y represents net photosynthesis $\mu molCO_2/m^2 s$

   dataset 2 The dataset describes a functional responses. Bolker mentions four of those $min(ax, s)$ $\frac{ax}{(b+x)}$, $\frac{ax^2}{(b^2+x^2)}$, $\frac{ax^2}{(b+cx+x^2)}$ The y is measured in grams prey eaten per unit time.

   dataset 3 Allometric relationships generally have the form ax^b. The y represent the total number of cones produced.

   dataset 4 This could be logistic growth $n(t) = \frac{K}{1+(\frac{K}{n_0})e^{-rt}}$ or the gompertz function $f(x) = e^{-ae^{-bx}}$. The y represent the population size (numbers).

   dataset 5 What about a negative exponential? $ae{-}bx$ or a power function ax^b. The y represent a number per unit area.

   dataset 6 Species reponse curves are curves that describe the probability of presence as a function of some factor. A good candidate good be a unimodel response curve. You could take the equation of the normal distribution without the scaling constant: e.g. $ae^{\frac{-(x-\mu)^2}{2\sigma^2}}$. The y represent presence or absence of the species (no units).

2. Stochastic functions/Probability distributions

   dataset 1 y represents real numbers and both positive and negative numbers occur. This implies that we should choose a continuous probability distribution. In addition, the numbers seems unbound. Within the family of continuous probability distributions, the normal seems a good candidate distribution because this one runs from -inf to +inf. In contrast the Gamma and the Lognormal only can take positive numbers, so these distributions cannot handle the negative numbers. In addition, the beta distribution is not a good candidate because it runs from 0-1.

   dataset 2 y represents real numbers and only positive numbers occur. The data represents a functional response (intake rate of the predator), and it is likely that you can only measure positive numbers (number of prey items per unit of time). This implies that we should choose a continuous probability distribution. Within the family of continuous probability distributions, the Gamma and the Lognormal could be taken as candidate distributions because they can only take positive numbers (beware that the Gamma cannot take 0). However, you could try to use a normal as well.

   dataset 3 y seems represents counts (this is the cone dataset that is introduced in ch. 6.). Given that it contains counts we can pick a distribution from the family of discrete distributions. The Poisson and the Negative Binomial could be good candidates to describe this type of data.

   dataset 4 y represents population size over time. From looking at the data, they seems to represent counts. Given that it contains counts we can pick a distribution from the family of discrete distributions. The Poisson and the Negative Binomial could be good candidates to describe this type of data.

   dataset 5 No information is given on y. The data clearly seems to represent counts. Thus the same reasoning applies here as to the two previous datasets.

   dataset 6 The data (y) represents species occurences (presence/absence). The binomial model would be a good model to predict the probability of presence.