Lab 2 - Computational Statistics

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Assignment 1

File mortality_rate.csv contains information about mortaily rates of the fruit flies during a certain period.

1. Import this file to R and add one more variable LMR to the data which is the natural logarithm of Rate. Afterwards, divide the data into training and test sets by using the following code:

1.2. Write your own function myMSE that for given parameters lambda and list *pars* containing vectors X, Y, Xtest, Ytest fits a LOESS model with response Y and predictor X using loess() function with penalty lambda (parameter enp.target in loess()) and then predicts the model for Xtest. The function should compute the predictive MSE, print it and return as a result.

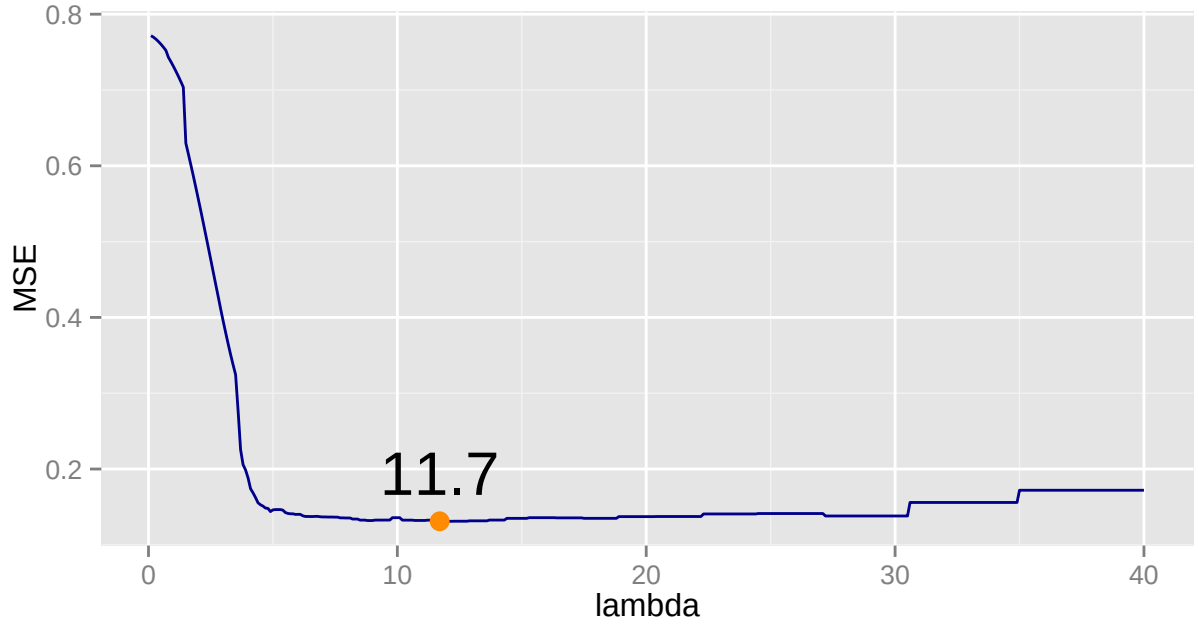
Data is imported and splitted into a training set and a test set with each set containing 50 % of the original set.

Thereafter, the function *myMSE* is written. It takes the arguments *pars* (a list including *X*, *Y*, *XTest* and *YTest*) and the argument *lambda*. The latter parameter specifies the penalty parameter *enp.target* in *loess*. The *myMSE* function then uses *loess* to make a model which is evaluated on the test set. Returned by *myMSE* is the predictive MSE.

```
myMSE <- function(lambda, pars){
  model <- loess(pars$Y~pars$X, data=pars[1:2], enp.target = lambda)
  Pred <- predict(model, newdata=pars$Xtest)
  MSE <- (1/length(pars$Y)) * sum((Pred-pars$Ytest)^2)
  print(MSE)
  return(MSE)
}
```

1.3

A plot of the predictive MSE values against the respective *lambda* values in the range 0.1 to 40 by steps of 0.1 is shown below.



The lowest predictive MSE value, 0.131047, is obtained when *lambda* is equal to 11.7, so that is the optimal *lambda* value. Since the predictive MSE has been calculated for all values from 0.1 to 40 by steps of 0.1, 400 evaluations of *myMSE* were required to find the optimal value for *lambda*.

1.4. Use optimize() function for the same purpose, specify range for search [0.1, 40] and the accuracy 0.01. Have the function managed to find the optimal MSE value? How many myMSE function evaluations were required? Compare to step 3.

The function *optimize* is a faster approach for finding the optimal MSE value. It uses a combination of golden section search and successive parabolic interpolation as the optimizing method. The output given by the function is shown below and when comparing to the values given in *1.3* it is noted that the function not managed to find the optimal MSE value. However, the difference between both the optimal MSE value and the *lambda* value is small compared to optimal values obtained in *1.3*.
By counting the prints it is concluded that 18 *myMSE* evaluations where needed to find the value thought to optimal. That is just 4.5 % of the evaluations required for the simple approach method applied in *1.3*

```
## [1] 0.1358018
## [1] 0.1412809
## [1] 0.1326581
## [1] 0.1401702
## [1] 0.1325391
## [1] 0.1321441
## [1] 0.1325542
## [1] 0.1321441
## [1] 0.1325391
## [1] 0.1321441
## [1] 0.1321441
## [1] 0.1321441
## [1] 0.1321441
## [1] 0.1321441
```

```
## [1] 0.1321441
## [1] 0.1321441
## [1] 0.1321441
## [1] 0.1321441
```

```
## $minimum
## [1] 10.69361
##
## $objective
## [1] 0.1321441
```

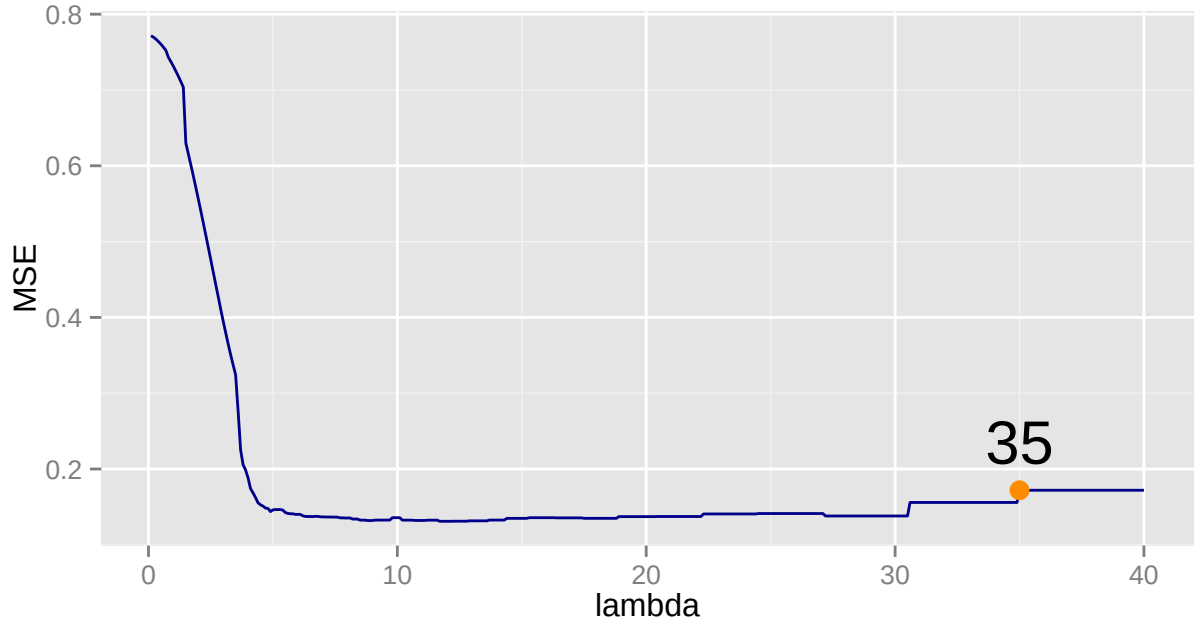
1.5. Use optim() function and BFGS method with starting point lambda=35 to find the optimal lambda value. How many myMSE function evaluations were required? Compare the results you obtained with the results from step 4 and make conclusions.

The output below gives that three evaluations of *myMSE* were conducted before it was concluded that the optimal *lambda* value was found. Although, it has to be noted that chosen value for *lambda* is exactly the same as the starting value, which is quite far from the optimal values chosen by the simple approach and the golden section search. Also the MSE value is quite far from the optimal MSE value obtained in *1.4*.

```
## [1] 0.1719996
## [1] 0.1719996
## [1] 0.1719996
```

```
## $par
## [1] 35
##
## $value
## [1] 0.1719996
##
## $counts
## function gradient
##        1        1
##
## $convergence
## [1] 0
##
## $message
## NULL
```

The given results can be explained by a look of the plot over the MSE values for all *lambda* values in the range 0.1 to 40.



At the chosen starting point is the slope of the curve for the predictive MSE values zero, so the point is a local minimum. The implications of starting at a local minimum when using the *BFSG* method is that it not will keep on iterate and look if there is a better solution. Instead it will just investigate the MSE values closest to the starting point and discover that it already is at a local minima and as a result of this stay at *lambda* equal to 35.
A comparsion between the methods tested in *1.4* and *1.5* then gives that the golden section search conducted in *1.4* performs better for this specific dataset. The performance is measured by the respective methods closeness to the optimal values of *lambda* and the predictive MSE.

Assignment 2

File data.RData contains a sample from normal distribution with some parameters μ, σ.

2.1. Load the data to R environment.

2.2. Write down the log-likelihood function for 100 observations and derive maximum likelihood estimators for μ, σ analytically by setting partial derivatives to zero. Use formulas derived to obtain parameter estimates for the data loaded.

The probability density function for the normal distribution:

$$f(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} exp(-\frac{(x-\mu)^2}{2\sigma^2})$$

For a sample of n observations that are independent and identically distributed the likelihood is:

$$\prod f(x_i|\mu,\sigma) = (\frac{1}{\sqrt{2\pi\sigma^2}})^n exp(-\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2})$$

Then, the log likelihood is:

$$log(L(\mu,\sigma)) = nlog(\frac{1}{\sqrt{2\pi\sigma^2}}) + (-\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2})$$

The derivatives of the log likelihood is computed to obtain the maximum likelihood estimators for μ and σ. First the ML estimator for μ:

$$\frac{\partial log(L(\mu,\sigma))}{\partial \mu} = 0 + \frac{2\sum_{i=1}^{n}(x_i-\mu)}{2\sigma^2}$$

$$\hat{\mu} = \overline{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

This is equal to the sample mean.

Then, finally, the ML estimator for σ:

$$\frac{\partial log(L(\mu,\sigma))}{\partial \sigma} = -\frac{n}{\sigma} + \frac{1}{\sigma^3} * (\sum_{i=1}^{n}(x_i-\mu)^2)$$

$$\hat{\sigma} = \sqrt{\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{n}}$$

This is equal to the square root of the unadjusted sample variance.

The parameter estimates obtained for μ and σ when the formulas above are used on the data set is 1.2755276 for the mean and 2.0059765 for the standard deviation.

2.3. Now you are assumed to derive maximum likelihood estimates numerically. Why it is a bad idea to maximize likelihood rather than maximizing log-likelihood?

The result would be the same either if we use the loglikelihood or the likelihood. Therefore the simple one would be more convenient to work with. ln general the loglikehood is the convenient one, since it make the function easier to work with.

2.4. Optimize the minus log-likelihood function with initial parameters $\mu = 0, \sigma = 1$. Try both Conjugate Gradient method and BFGS algorithm with gradient specified and without.

2.5. Did algorithms converge in all cases? What were the optimal values of parameters and how many function and gradient evaluations it required for algorithms to converge? Which settings would you recommend?

In the table below can a summary of the respective algorithms conducted in *2.4* be viewed. It is concluded that in all of the cases did the algorithms converge. A conjugate gradient optimizer without gradient specified required the highest amount of both function and gradient evaluations and the conjugate gradient with gradient specified the second highest number of function and gradient evaluations. The BFGS algorithms with and without specified gradient required the same amount of gradient evaluations and the algorithm with specified gradient required two function evaluations less.

method	specified gradient	converge	optimal value (mu, sigma)	function evalutaion	gradient evalutaion
BFGS	no	yes	1.275528, 2.005977	40	15
BFGS	yes	yes	1.275528, 2.005977	38	15
CG	no	yes	1.275528, 2.005977	169	31
CG	yes	yes	1.275528, 2.005976	56	17

The choosen setting then is the BFGS with specified gradient since it requires the lowest number of evaluations.

Appendix

```
mort_rate<-read.csv2("C:\\Users\\Gustav\\Documents\\Computational-Statistics\\Lab2\\mortality_rate.csv"
mort_rate$LMR <- log(mort_rate$Rate)

n=dim(mort_rate)[1]
set.seed(123456)
id=sample(1:n, floor(n*0.5))
train=mort_rate[id,]
test=mort_rate[-id,]
myMSE <- function(lambda, pars){
  model <- loess(pars$Y~pars$X, data=pars[1:2], enp.target = lambda)
  Pred <- predict(model, newdata=pars$Xtest)
  MSE <- (1/length(pars$Y)) * sum((Pred-pars$Ytest)^2)
  print(MSE)
  return(MSE)
}
Data <- list(X=train$Day, Y=train$LMR, Xtest=test$Day, Ytest=test$LMR)
# 1.3
Lambda <-  seq(0.1,40, by=0.1)
modelMSE <- 0
j <- 0
for(i in Lambda){
  j <- j+1
  modelMSE[j] <- myMSE(Lambda[j], Data)
}
library(ggplot2)
MSEdata <- data.frame(MSE=modelMSE, lambda=Lambda)
ggplot(MSEdata, aes(x=lambda, y=MSE, label=lambda)) + geom_line(col="darkblue")+
  geom_text(data=subset(MSEdata, MSE <= min(MSEdata$MSE))[1,],vjust=-0.6, size=8) +
  geom_point(data=subset(MSEdata, MSE <= min(MSEdata$MSE))[1,], size=3.5, col="darkorange")
Optim <- optimize(f=myMSE, interval = c(0.1, 40), tol=0.01, pars=Data)
Optim
optim(par=35, fn=myMSE, method = "BFGS", pars=Data)
ggplot(MSEdata, aes(x=lambda, y=MSE, label=lambda)) + geom_line(col="darkblue")+
  geom_text(data=subset(MSEdata,  MSEdata$lambda == 35),vjust=-0.6, size=8) +
  geom_point(data=subset(MSEdata,  MSEdata$lambda == 35), size=3.5, col="darkorange")
# 2.1
load("C:\\Users\\Gustav\\Documents\\Computational-Statistics\\Lab2\\data.RData")
Data2 <- data
# Maximum likelihood estimates
# my
MeanEst <- sum(Data2) / length(Data2)
# sigma
sigmaEst <- sqrt((1/length(Data2)) * sum((Data2-MeanEst)^2))

# 2.4
# minus log-like function
loglikef <- function(par,...){
  my <- par[1]
  sigma <- par[2]
  n <- length(data)
  loglike <- -(n*log(1/(sqrt(2*pi*sigma^2))) - (sum((data-my)^2)/(2*sigma^2)))
```

```
  return(loglike)
}

gradientf <- function(par,...){
  n <- length(data)
  my <- par[1]
  sigma <- par[2]
  myML <-  - (sum(data-my)) / (sigma^2)
  mySigma <- -(  (-n/sigma) + (1/(sigma^3)) * sum((data-my)^2))
  return(c(myML, mySigma))
}
optim(par = c(0,1), fn=loglikef, method = "CG", data=Data2)
optim(par = c(0,1), fn=loglikef, gr=gradientf,  method = "CG", data=Data2)
optim(par = c(0,1), fn=loglikef , method = "BFGS", data=Data2)
optim(par = c(0,1), fn=loglikef, gr=gradientf,  method = "BFGS", data=Data2)
## NA
```