Lab Assignment 2

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Question 1: Optimizing parameters

1

Finding a0, a1, a2 that minimizes squared error between the selected function and interpolate function using optim()

```
parabolic_inter = function(a,x){
  a0 = a[1]
  a1 = a[2]
  a2 = a[3]
  res = a0 + a1*x + a2*(x^2)
  return(res)
}
sum_square_error = function(a,x,func){
  x0 = x[1]
  x1 = x[2]
  x2 = x[3]
  res = sum((func(x0)-parabolic_inter(a,x0))^2,(func(x1)-parabolic_inter(a,x1))^2,
            (func(x2)-parabolic_inter(a,x2))^2)
  return(res)
}
opt = function(x,func){
  a = c(0,0,0)
  res = optim(a,sum_square_error,x = x,func = func)
  res = res$par
  return(res)
}
```

2

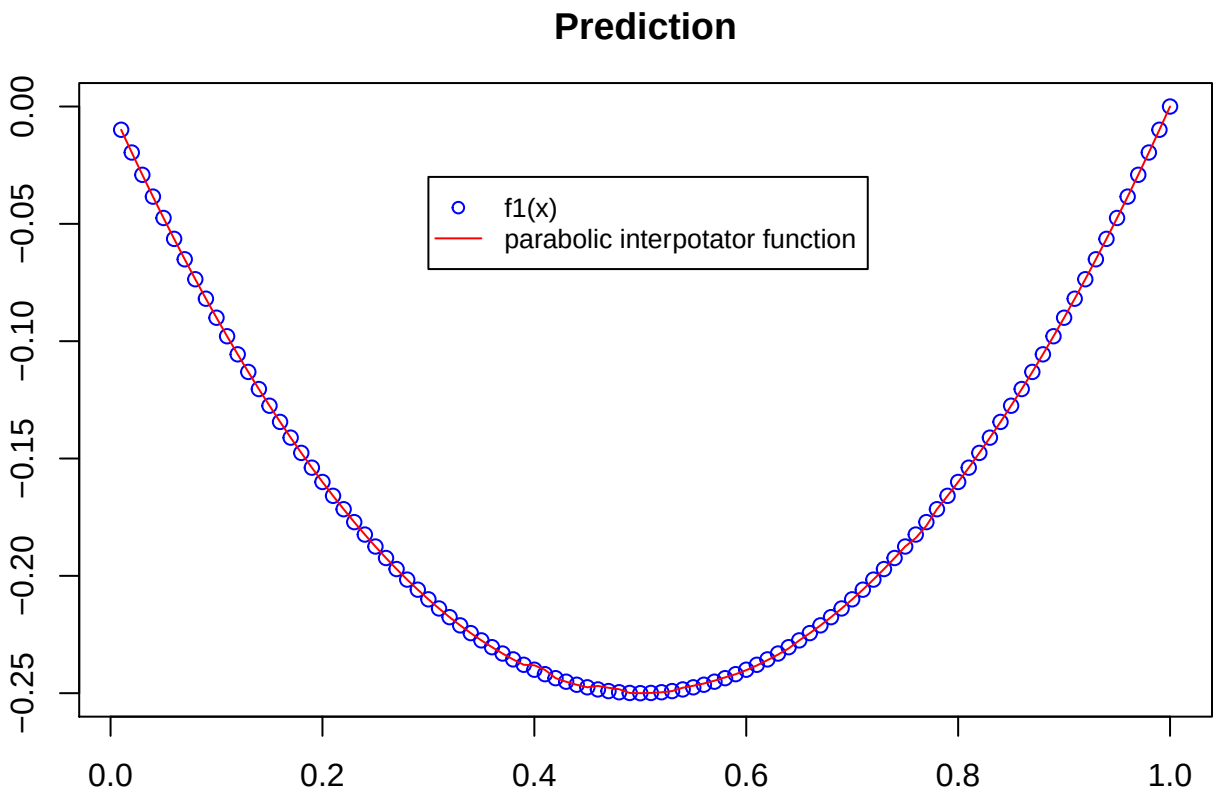
Approximate function

```
approx = function(n,func){
 interval = 1/n
 midpoint = 1/(2*n)
 res = data.frame()
 for(i in 1:n){
   end_point = i/n
```

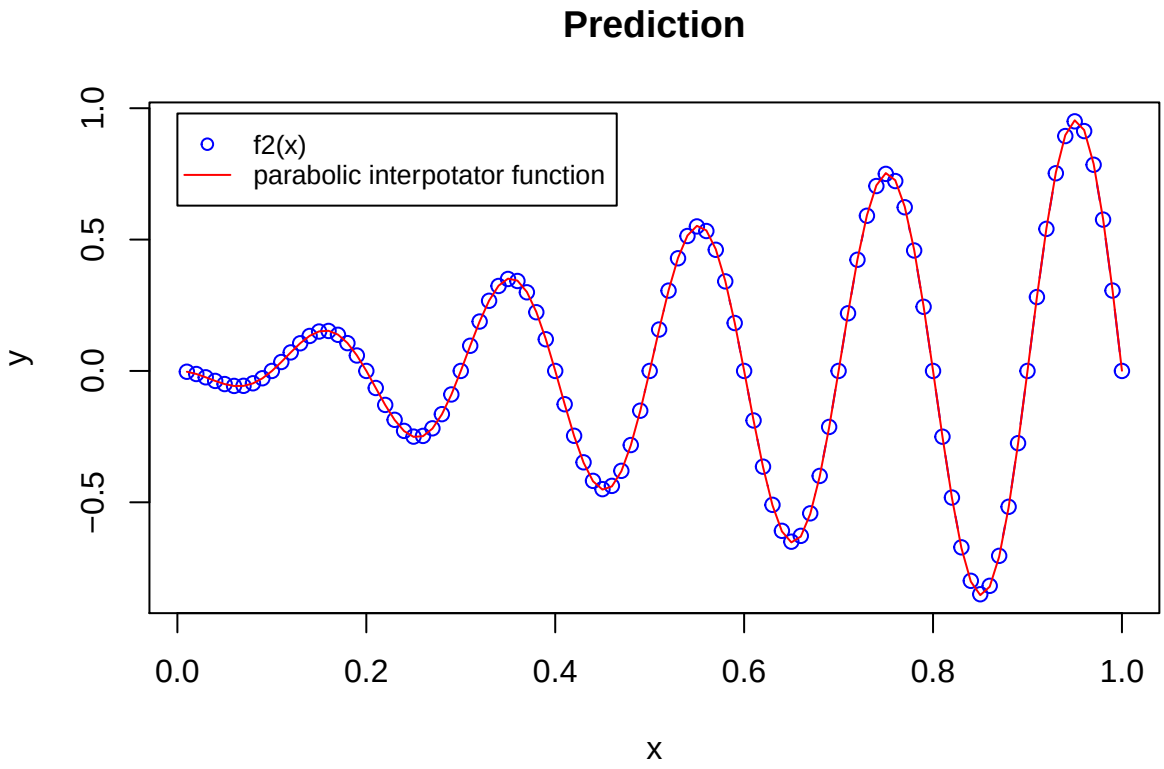
```
   x = c((end_point - interval),(end_point - midpoint),end_point)
   res = append(res,as.data.frame(opt(x,func)))
 }
 return(res)
}
```

3

Comparing the result from f1(x) and parabolic interpolator function for 100 subintervals.



Comparing the result from f2(x) and piecewise parabolic interpolator function for 100 subintervals.



Observing the above two plots , we can say that the prediction from piecewise parabolic interpolater was fair as the predictions has very low errors.

Question 2: Maximizing likelihood

1. Load the data to R environment.

```
load("data.RData")
```

2. A sample from normal distribution with some parameters μ, σ.

The probability density function of normal distribution is:

$$f(y) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

We have the following n = 100 i.i.d observations:

$$x_1, x_2, ..., x_n$$

The likelihood function:

$$f(x_1, x_2, ..., x_n|\sigma, \mu) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}} = (\frac{1}{\sigma\sqrt{2\pi}})^n e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2}$$

The log likelihood function:

$$log(f(x_1, x_2, ..., x_n|\sigma, \mu)) = log((\frac{1}{\sigma\sqrt{2\pi}})^n e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2})$$

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

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

Let's call

$$log(f(x_1, x_2, ..., x_n|\sigma, \mu))$$

as L and derivation of the log-likelihood by μ by setting partial derivatives to zero

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

Solve this equation, we get

$$\frac{1}{2\sigma^2}\sum_{i=1}^{n}(2\hat{\mu} - 2x_i) = 0$$

Because σ^2 should be larger than 0, Mean of the sample

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

Similarly, derivation of the log-likelihood by σ

$$\frac{\partial L}{\partial \sigma} = -\frac{n}{\sigma} + \sum_{i=1}^{n}(x_i-\mu)^2\sigma^{-3} = 0$$

Variance of the sample

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

Standard Deviation of the sample

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

```
mu_hat =  sum(data)/length(data)
# formula for sigma
sigma_hat = sqrt(sum((data - mu_hat)^2)/length(data))
cat(paste("Mean of data", mu_hat))
```

```
Mean of data 1.27552760103638
```

```
cat(paste("Standard Deviation of data", sigma_hat))
```

```
Standard Deviation of data 2.00597647210603
```

3. Minus log–likelihood function with initial parameters μ = 0, = 1.

```
minusloglikenormal <- function(theta){
  mu = theta[1]
  sigma = theta[2]
  n = length(data)
  ans =  ((n/2) * log(2*pi * (sigma^2))) + (sum((data - mu)^2)) / (2 * sigma^2)
  return(ans)
}
```

Gradient method

```
gradient <- function(theta){
  mu = theta[1]
  sigma = theta[2]
  n = length(data)
  dMu = sum(mu - data)/(sigma^2)
  dSigma = (n/sigma) - (sum((data-mu)^2)/(sigma^3))
  gr = c(dMu,dSigma)
  return(gr)
}
# Conjugate Gradient method without gradient method:
opt_cg <- optim(par = c(0, 1), fn = minusloglikenormal, method = "CG")

# Conjugate Gradient method without gradient method:
opt_cg_gr <- optim(par = c(0, 1), fn = minusloglikenormal, gr = gradient,  method = "CG")

# BGFS method without gradient method:
opt_bfgs <- optim(par = c(0, 1), fn = minusloglikenormal, method = "BFGS")

# BGFS method with gradient method:
opt_bfgs_gr <- optim(par = c(0, 1), fn = minusloglikenormal, gr = gradient, method = "BFGS")
```

It is more convenient to maximize the log of the likelihood function. Because the logarithm is monotonically increasing function of its argument, maximization of the log of a function is equivalent to maximization of the function itself. Taking the log not only simplifies the subsequent mathematical analysis, but it also helps numerically because the product of a large number of small probabilities can easily underflow the numerical precision of the computer, and this is resolved by computing instead the sum of the log probabilities.

4. Algorithms converge

```
cg1 = c(opt_cg$convergence, opt_cg$par, opt_cg$value, opt_cg$counts[1],
        opt_cg$counts[2])
cg2 = c(opt_cg_gr$convergence, opt_cg_gr$par, opt_cg_gr$value,
        opt_cg_gr$counts[1], opt_cg_gr$counts[2])
bfgs1 = c(opt_bfgs$convergence, opt_bfgs$par, opt_bfgs$value,
          opt_bfgs$counts[1], opt_bfgs$counts[2])
bfgs2 = c(opt_bfgs_gr$convergence, opt_bfgs_gr$par, opt_bfgs_gr$value,
          opt_bfgs_gr$counts[1], opt_bfgs_gr$counts[2])
df <- as.data.frame(matrix(c(cg1, cg2, bfgs1, bfgs2), nrow=6))
rownames(df) <- c("Convergence", "Mean", "Standard Deviation", "minusloglikelihood",
                  "function evaluation", "gradient evaluation")
colnames(df) <- c("CG", "CG with gradient", "BFGS", "BFGS with gradient")
knitr::kable(x = df, caption = "Comparison table of the different algorithms")
```

Table 1: Comparison table of the different algorithms

	CG	CG with gradient	BFGS	BFGS with gradient
Convergence	0.000000	0.000000	0.000000	0.000000
Mean	1.275528	1.275528	1.275528	1.275528
Standard Deviation	2.005977	2.005977	2.005977	2.005977
minusloglikelihood	211.506949	211.506949	211.506949	211.506949
function evaluation	208.000000	53.000000	41.000000	39.000000
gradient evaluation	35.000000	17.000000	15.000000	15.000000

The algorithms converged to the true value of μ and σ in above mentioned all cases because it is generated from the normal distribution, where the log likelihood function is a continuous differentiable function that has only one global maximum. The results for different algorithms are same except for number of function and gradient evaluation. We need to choose algorithm with minimum runs of function evaluations. CG algorithm (with or without gradient) is not a best option because no of function evaluations are high. So it is better to avoid it as it makes algorithm slow and expensive in terms of computational resources. Hence BFGS with gradient is the best option.

Appendix

```
knitr::opts_chunk$set(echo = TRUE, comment = NA)
parabolic_inter = function(a,x){
  a0 = a[1]
  a1 = a[2]
  a2 = a[3]
  res = a0 + a1*x + a2*(x^2)
  return(res)
}
sum_square_error = function(a,x,func){
  x0 = x[1]
  x1 = x[2]
  x2 = x[3]
  res = sum((func(x0)-parabolic_inter(a,x0))^2,(func(x1)-parabolic_inter(a,x1))^2,
            (func(x2)-parabolic_inter(a,x2))^2)
  return(res)
}
opt = function(x,func){
  a = c(0,0,0)
  res = optim(a,sum_square_error,x = x,func = func)
  res = res$par
  return(res)
}
approx = function(n,func){
 interval = 1/n
 midpoint = 1/(2*n)
 res = data.frame()
 for(i in 1:n){
   end_point = i/n
   x = c((end_point - interval),(end_point - midpoint),end_point)
   res = append(res,as.data.frame(opt(x,func)))
 }
 return(res)
}
f1 = function(x){
  res = -x *(1-x)
  return(res)
}
f2 = function(x){
  res = -x * sin(10*pi*x)
  return(res)
}
```

```r
x = c()
for(i in 1:100){x[i] = i/100}

approx1 = approx(100,f1)
interpolate_result1 = c()
for(i in 1:length(approx1)){
  a = as.vector(approx1[[i]])
  interpolate_result1 = append(interpolate_result1,parabolic_inter(a,x[i]))
}
par(mar = c(3,3,3,0))
plot(x,f1(x),xlab = "x",ylab = "y",col = "blue", type = "b")
lines(x,interpolate_result1,col = "red")
title("Prediction")
legend(0.3, -0.03, legend=c("f1(x)", "parabolic interpotator function"),
       col=c("blue", "red"), pch=c(1,NA),lty=c(0,1), cex=0.8)

approx2 = approx(100,f2)
interpolate_result2 = c()
for(i in 1:length(x)){
  a = as.vector(approx2[[i]])
  interpolate_result2 = append(interpolate_result2,parabolic_inter(a,x[i]))
}
plot(x,f2(x),xlab = "x",ylab = "y",col = "blue", type = "b")
lines(x,interpolate_result2,col = "red")
title("Prediction")
legend(0, 0.98, legend=c("f2(x)", "parabolic interpotator function"),
       col=c("blue", "red"), pch=c(1,NA),lty=c(0,1), cex=0.8)
load("data.RData")
mu_hat =  sum(data)/length(data)
# formula for sigma
sigma_hat = sqrt(sum((data - mu_hat)^2)/length(data))
cat(paste("Mean of data", mu_hat))
cat(paste("Standard Deviation of data", sigma_hat))
minusloglikenormal <- function(theta){
  mu = theta[1]
  sigma = theta[2]
  n = length(data)
  ans =  ((n/2) * log(2*pi * (sigma^2))) + (sum((data - mu)^2)) / (2 * sigma^2)
  return(ans)
}
gradient <- function(theta){
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  n = length(data)
  dMu = sum(mu - data)/(sigma^2)
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  gr = c(dMu,dSigma)
  return(gr)
}
# Conjugate Gradient method without gradient method:
opt_cg <- optim(par = c(0, 1), fn = minusloglikenormal, method = "CG")

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```r
opt_cg_gr <- optim(par = c(0, 1), fn = minusloglikenormal, gr = gradient,  method = "CG")

# BGFS method without gradient method:
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cg2 = c(opt_cg_gr$convergence, opt_cg_gr$par, opt_cg_gr$value,
        opt_cg_gr$counts[1], opt_cg_gr$counts[2])
bfgs1 = c(opt_bfgs$convergence, opt_bfgs$par, opt_bfgs$value,
          opt_bfgs$counts[1], opt_bfgs$counts[2])
bfgs2 = c(opt_bfgs_gr$convergence, opt_bfgs_gr$par, opt_bfgs_gr$value,
          opt_bfgs_gr$counts[1], opt_bfgs_gr$counts[2])
df <- as.data.frame(matrix(c(cg1, cg2, bfgs1, bfgs2), nrow=6))
rownames(df) <- c("Convergence", "Mean", "Standard Deviation", "minusloglikelihood",
                  "function evaluation", "gradient evaluation")
colnames(df) <- c("CG", "CG with gradient", "BFGS", "BFGS with gradient")
knitr::kable(x = df, caption = "Comparison table of the different algorithms")
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