

STA414 Assignment 3

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1. Fitting a linear model

The direct summary of simple linear model can be shown as:

Call:

```
lm(formula = train1y ~ V1 + V2 + V3 + V4 + V5 + V6 + V7 + V8,  
    data = data.frame(train1x))
```

Residuals:

Min	1Q	Median	3Q	Max
-1.40576	-0.31558	-0.03542	0.26756	1.95052

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	5.09323	0.44713	11.391	< 2e-16 ***
V1	0.21757	0.02145	10.142	< 2e-16 ***
V2	1.58882	0.71488	2.222	0.02718 *
V3	2.56441	0.60984	4.205	3.68e-05 ***
V4	1.90180	0.44280	4.295	2.53e-05 ***
V5	-0.65827	0.23777	-2.769	0.00607 **
V6	0.30995	0.29234	1.060	0.29008
V7	0.26580	0.05045	5.268	3.05e-07 ***
V8	-0.46711	0.11209	-4.167	4.30e-05 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5391 on 241 degrees of freedom

Multiple R-squared: 0.594, Adjusted R-squared: 0.5805

F-statistic: 44.07 on 8 and 241 DF, p-value: < 2.2e-16

- By observation, the Adjusted R-squared value is 0.5805, not a good sign.
- The $\Pr(>|t|)$ for V6 is comparatively high, probably we can ignore it when fitting a linear model, so the re-do of fitting is below:

Call:

```
lm(formula = train1y ~ V1 + V2 + V3 + V4 + V5 + V7 + V8, data = data.frame(train1x))
```

Residuals:

Min	1Q	Median	3Q	Max
-1.33637	-0.30870	-0.04837	0.27276	2.00091

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	4.99873	0.43826	11.406	< 2e-16 ***
V1	0.22210	0.02103	10.563	< 2e-16 ***
V2	1.60312	0.71494	2.242	0.0258 *
V3	2.61755	0.60793	4.306	2.42e-05 ***
V4	1.98178	0.43644	4.541	8.84e-06 ***
V5	-0.70383	0.23391	-3.009	0.0029 **
V7	0.27002	0.05031	5.368	1.87e-07 ***
V8	-0.43856	0.10883	-4.030	7.48e-05 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5392 on 242 degrees of freedom

Multiple R-squared: 0.5921, Adjusted R-squared: 0.5803

F-statistic: 50.18 on 7 and 242 DF, p-value: < 2.2e-16

- Therefore,

The MSE in terms of 8 covariates is 0.2801569

The MSE in terms of 7 covariates is 0.2814637

- And the prediction is `y_predict`.

2. Fitting a Gaussian process model with linear covariance

- The calculated MSE of fitting a Gaussian process model with linear covariance is 0.443493.

3. Fitting Gaussian process model without/with rescaling

- Set the `res` and `res2` matrix as two 3 by 400 matrices, considering the step, starting and ending values of hyperparameters.
- The two generated text files, `output1.txt` and `output2.txt` are hyperparameters candidates for non-scaling

GP and re-scaling GP respectively. The second line and third line of such files are values of `gamma` and `rho`.

- *output1.txt* and *output2.txt* are included in appendices.
- The minimizer hyperparameters `gamma` and `rho` for MSE are acquired by calling `index` and `index2` in console after running our code, then call `res[,index]` and `res2[,index2]` respectively.

```
> res[,index]
[1] 60.76519  9.60000  0.16000
> res2[,index2]
[1] 68.40608  5.10000  0.96000
```

- For non-scaling, `gamma == 9.6`, `rho == 0.16`
- For rescaling, `gamma == 5.1`, `rho == 0.96`
- The MSE for non-scaling Gaussian process model is `0.2934913`.
- The MSE for rescaling Gaussian process model is `0.2403158`.

4. Runtime comparison

- By using `proc.time()` we can get runtime for each model fitting.

```
simple linear:
  user  system elapsed
 0.022   0.002   0.025

gaussian process with linear covariance:
  user  system elapsed
18.144   0.036  18.181

gaussian process non-scaling:
  user  system elapsed
2425.194   7.831 2434.902

gaussian process scaling:
  user  system elapsed
2505.971   6.253 2515.121
```

5. Summary

Using 5-fold cross-validation

model	simple linear	GP with linear cov	GP with hyperpar	GP with hyper (rescaling)
MSE	0.2801569	0.443493	0.2934913	0.2403158
runtime	0.022	18.144	2425.194	2505.971

- Since Gaussian process with hyperparameters (re-scaling) has the smallest MSE among all, it is the best model fitting for our data. Simple linear model has a larger MSE, and Gaussian process with hyperparameters (non-scaling) has an MSE slightly larger than the previous one. In general, all of three MSEs are quite close to each other.
- However, Gaussian process with linear covariance has a rather outlying MSE, probably because its parameters are not carefully selected to minimize the MSE.
- The runtime of simple linear model and GP with linear covariance are tolerable. But GP with hyperparameters takes much longer time (approx. 40 minutes) to run due to the existence of nested for-loop inside code.

Using 10-fold cross-validation

model	GP with hyperpar	GP with hyper (rescaling)
MSE	0.2935	0.2406

- During a previous pilot run, I change the required 5-fold cross-validation to 10-fold, which is widely used in practice. It turns out that the MSE for linear and GP with linear covariance don't change (of course they don't, they don't have hyperparameters!). What I actually want to say is that the MSE with/without rescaling are only tiny little bit higher than 5-fold. So the number of folds does not have great influence on MSE here.
- And runtime of 5-fold and 10-fold are similar.

6. Appendices

- `a3.r`

```
# set up!
train1x <- as.matrix(read.table("./train1x", header=F))
train1y <- as.matrix(read.table("./train1y", header=F))
testx <- as.matrix(read.table("./testx", header=F))
testy <- as.matrix(read.table("./testy", header=F))
```

```

# divide!
section <- function(train1x, train1y, i) {
  x_test <- train1x[((i-1)*50+1):(i*50),]
  x_train <- train1x[-(((i-1)*50+1):(i*50)),]
  y_test <- as.matrix(train1y[((i-1)*50+1):(i*50)])
  y_train <- as.matrix(train1y[-(((i-1)*50+1):(i*50))])
  return(list(x_test,x_train,y_test,y_train))
}

# covariance functions!
K1 <- function(i,j) {
  return(100^2*(i%*%j))
}

K2 <- function(gamma,rho,x,y) {
  return(100^2+gamma^2*exp(-(rho^2)*sum((x-y)^2)))
}

# cross-validation!
cv <- function(gamma, rho, train1x, train1y) {
  MSE <- matrix(0,1,5)
  for (k in 1:5) {
    x_test <- section(train1x,train1y,k)[1][[1]]
    x_train <- section(train1x,train1y,k)[2][[1]]
    y_test <- section(train1x,train1y,k)[3][[1]]
    y_train <- section(train1x,train1y,k)[4][[1]]
    C <- matrix(0,200,200)
    for (i in 1:200) {
      for (j in 1:200) {
        C[i,j] <- K2(gamma,rho,x_train[i,],x_train[j,])
      }
    }
    C <- C + diag(200)
    predict <- matrix(0,1,50)
    for (i in 1:50) {
      t <- matrix(0,1,200)
      for (j in 1:200) {
        t[j] <- K2(gamma,rho,x_train[j,],x_test[i,])
      }
      predict[i] <- t%%solve(C)%*%y_train
    }
    MSE[k] <- sum((t(y_test) - predict)^2)
  }
  return(sum(MSE))
}

```

```
}
```

- `script.r`

```
source("a3.r")

##### simple linear model #####
t1 <- proc.time()

mse <- function(m) {
  mse <- mean(m$residuals^2)
  return(mse)
}

m1 <- lm(train1y~V1+V2+V3+V4+V5+V6+V7+V8, data=data.frame(train1x))
summary(m1)
mse(m1)

## what if we drop V6?
m2 <- lm(train1y~V1+V2+V3+V4+V5+V7+V8, data=data.frame(train1x))
summary(m2)
mse(m2)

cat(" The MSE in terms of 8 covariates is ", mse(m1), "\n",
    "The MSE in terms of 7 covariates is ", mse(m2), "\n")

## prediction
y_predict <- predict(m2,newdata=data.frame(testx),interval='prediction')

t2 <- proc.time()
print(t2-t1)

##### Gaussian process with linear covariance #####
t1 <- proc.time()
C <- matrix(0,250,250)
for (i in 1:250) {
  for (j in 1:250) {
    C[i, j] <- K1(train1x[i,],train1x[j,])
  }
}

C <- C + diag(250)

predict <- matrix(0,1,2500)
```

```

for (i in 1:nrow(testy)) {
  t <- matrix(0,1,250)
  for (j in 1:250) {
    t[j] <- K1(train1x[j,],testx[i,])
  }
  predict[i] <- t%%solve(C,train1y)
}

MSE2 <- sum((t(testy) - predict)^2)/2500
print(MSE2)
t2 <- proc.time()
print(t2-t1)

##### Gaussian process with hyperparameters (non-scaling) #####
t1 <- proc.time()
res <- matrix(0,3,400)
num <- 1
for (gamma in seq(0.1,10,0.5)) {
  for (rho in seq(0.01,1,0.05)) {
    res[1,num] <- cv(gamma,rho,train1x,train1y)
    res[2,num] <- gamma
    res[3,num] <- rho
    num <- num + 1
    # it's more like a progress tracking feature, not really need this
    cat(num, res[1,num-1],res[2,num-1],res[3,num-1],"\n")
  }
}

write.table(res, "./output1.txt", sep="\t")

index <- which(res[1,] == min(res[1,]))
gamma <- res[2,index]
rho <- res[3,index]

C <- matrix(0,250,250)
for (i in 1:250) {
  for (j in 1:250) {
    C[i, j] <- K2(gamma,rho,train1x[i,],train1x[j,])
  }
}

C <- C + diag(250)

predict <- matrix(0,1,2500)
for (i in 1:nrow(testy)) {

```

```

t <- matrix(0,1,250)
for (j in 1:250) {
  t[j] <- K2(gamma,rho,train1x[j,],testx[i,])
}
predict[i] <- t%%solve(C,train1y)
}

MSE3 <- sum((t(testy) - predict)^2)/2500
print(MSE3)
t2 <- proc.time()
print(t2-t1)

##### Gaussian process with hyperparameters (re-scaling) #####

t1 <- proc.time()

trainxx <- train1x
testxx <- testx
trainxx[,1] <- trainxx[,1]/10
trainxx[,7] <- trainxx[,7]/10
testxx[,1] <- testxx[,1]/10
testxx[,7] <- testxx[,7]/10

res2 <- matrix(0,3,400)
num2 <- 1
for (gamma in seq(0.1,10,0.5)) {
  for (rho in seq(0.01,1,0.05)) {
    res2[1,num2] <- cv(gamma,rho,trainxx,train1y)
    res2[2,num2] <- gamma
    res2[3,num2] <- rho
    num2 <- num2 + 1
    cat(num2, res2[1,num2-1],res2[2,num2-1],res2[3,num2-1],"\n")
  }
}

write.table(res2, "./output2.txt", sep="\t")

index2 <- which(res2[1,] == min(res2[1,]))
gamma <- res2[,index2][2]
rho <- res2[,index2][3]

C <- matrix(0,250,250)
for (i in 1:250) {
  for (j in 1:250) {
    C[i, j] <- K2(gamma,rho,trainxx[i,],trainxx[j,])
  }
}

```



```

    }
  }

  C <- C + diag(250)

  predict2 <- matrix(0,1,2500)
  for (i in 1:nrow(testy)) {
    t <- matrix(0,1,250)
    for (j in 1:250) {
      t[j] <- K2(gamma,rho,trainxx[j,],testxx[i,])
    }
    predict2[i] <- t%%solve(C,train1y)
  }

  MSE4 <- sum((t(testy) - predict2)^2)/2500
  print(MSE4)
  t2 <- proc.time()
  print(t2-t1)

```

- `output1.txt`
- `output2.txt`

"V1 "	"V2 "	"V3 "	"V4 "	"V5 "	"V6 "	"V7 "	"V8 "	"V9 "
"V10 "	"V11 "	"V12 "	"V13 "	"V14 "	"V15 "	"V16 "	"V17 "	"V18 "
"V19 "	"V20 "	"V21 "	"V22 "	"V23 "	"V24 "	"V25 "	"V26 "	"V27 "
"V28 "	"V29 "	"V30 "	"V31 "	"V32 "	"V33 "	"V34 "	"V35 "	"V36 "
"V37 "	"V38 "	"V39 "	"V40 "	"V41 "	"V42 "	"V43 "	"V44 "	"V45 "
"V46 "	"V47 "	"V48 "	"V49 "	"V50 "	"V51 "	"V52 "	"V53 "	"V54 "
"V55 "	"V56 "	"V57 "	"V58 "	"V59 "	"V60 "	"V61 "	"V62 "	"V63 "
"V64 "	"V65 "	"V66 "	"V67 "	"V68 "	"V69 "	"V70 "	"V71 "	"V72 "
"V73 "	"V74 "	"V75 "	"V76 "	"V77 "	"V78 "	"V79 "	"V80 "	"V81 "
"V82 "	"V83 "	"V84 "	"V85 "	"V86 "	"V87 "	"V88 "	"V89 "	"V90 "
"V91 "	"V92 "	"V93 "	"V94 "	"V95 "	"V96 "	"V97 "	"V98 "	"V99 "
"V100 "	"V101 "	"V102 "	"V103 "	"V104 "	"V105 "	"V106 "	"V107 "	"V108 "
"V109 "	"V110 "	"V111 "	"V112 "	"V113 "	"V114 "	"V115 "	"V116 "	"V117 "
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"V127 "	"V128 "	"V129 "	"V130 "	"V131 "	"V132 "	"V133 "	"V134 "	"V135 "
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"V379 "	"V380 "	"V381 "	"V382 "	"V383 "	"V384 "	"V385 "	"V386 "	"V387 "
"V388 "	"V389 "	"V390 "	"V391 "	"V392 "	"V393 "	"V394 "	"V395 "	"V396 "
"V397 "	"V398 "	"V399 "	"V400 "					
"1 "	174.520883789647			170.201585517756			162.454479587056	
154.838828584857			149.094746492124			145.456100713123		
143.5350942038	142.841314505976			142.968512746336				
143.624522192522		144.611260604651			145.797203369065			
147.094968276245		148.445939930721			149.810491926912			

151.161852638846	152.482132085303	153.759627120006
154.986934921175	156.159626826466	170.023033923731
122.10115204717	107.411536755318	100.31698679248
91.8812355576204	89.5243784263575	95.352745549002
87.3109914780852	86.9976999316556	88.0747208334191
87.064862917945	87.2891668655801	86.952218700934
88.6405633155912	89.341388574246	87.619665521091
91.0933313859508	92.119648197333	88.0670244426856
107.679739979985	97.1333165530281	90.1627957854049
82.7387927424703	79.4029292734537	160.983264731851
77.1668387334297	76.9206115443786	88.6479959079192
76.5774840838766	76.4014485845361	77.800038380411
76.3192593350162	76.5213714291251	76.7552526724422
77.4478160805544	78.1318364931547	76.2923673440082
79.8419411271962	150.503784847495	76.9032223866394
90.5145030292758	80.6401043497518	78.9348509260599
73.2898771522493	72.7264831330135	101.66781658322
72.5445784470465	72.381620744106	75.366632056999
72.0105219494104	71.9436417843116	72.6373098996116
72.3804428277971	72.8900306143082	72.1851121487278
74.3341924679065	75.2213287800834	72.0586403683416
140.847457310096	97.8603839797681	73.5514807603492
74.9933357563152	70.9652915385365	76.2072212730146
70.0359065378306	70.1643968509362	85.0717043962651
70.1593455853466	70.1296682288439	69.9834393936187
70.2003674370404	70.4995177692692	70.1739786475152
71.7168436059389	72.5403453464856	70.108141933239
74.4719364061423	75.5808533574202	71.019539571486
94.9609704403852	80.4719157049163	73.4605749768036
68.2079423090687	67.998051718064	132.915753191886
68.7019891364644	68.9128964217399	71.0351375675412
69.3458557154596	69.483419957009	68.4178394734311
70.2408344803987	70.9688046736581	69.1605807542255
72.8309822120671	73.8877691261311	69.7418818414177
76.2777267767858	126.72470703478	71.851757116974
76.6190610604814	68.2384237634496	75.03139031881
66.733279813832	67.4158521114613	92.5254812101538
68.3736709145316	68.913969798602	66.3880258843477
69.5517515564044	69.9716300465595	67.8817101535418
71.5990168558314	72.6500183819577	69.2858239420234
74.9631844129624	76.2451120724949	70.6727262140717
121.952762063138	90.3588251631566	73.7721288191769
66.2293070016386	65.1415919808575	77.6373112427655
66.8206476106412	67.5038410209594	73.4342188544779
69.1323938509792	69.6428902931928	65.9163196724132
70.5959588422249	71.4958939910849	68.3164887590808
73.8040497909432	75.0614213827603	70.0128389410808
77.8154777107837	79.3578508399333	72.6029440787581
88.3662367539919	70.8288196605147	76.3888992143116
64.2717488860956	65.4018946461949	118.240292295595
		64.7598775214353
		66.5106919914616

67.4370335812833	68.5830010591469	69.63916751835
70.2449438120701	70.7092017339274	71.4613460720118
72.5511123573492	73.8194575913297	75.1578782817577
76.5489369649092	78.0175200259867	79.5935456283572
81.2860226411304	115.29381194333	86.5002215194956
68.7117565778265	63.6692696722866	63.6630876616469
65.1019007499194	66.4054114962362	67.5906415462469
69.0685258085419	70.3262027515258	70.9956998534047
71.5565119674127	72.4826137295058	73.7484779360354
75.1605989441719	76.6295717259077	78.1566797891491
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9.6	9.6	9.6	9.6	9.6			
"3"	0.01	0.06	0.11	0.16	0.21	0.26	0.31
0.41	0.46	0.51	0.56	0.61	0.66	0.71	0.76
0.86	0.91	0.96	0.01	0.06	0.11	0.16	0.21
0.31	0.36	0.41	0.46	0.51	0.56	0.61	0.66
0.76	0.81	0.86	0.91	0.96	0.01	0.06	0.11
0.21	0.26	0.31	0.36	0.41	0.46	0.51	0.56
0.66	0.71	0.76	0.81	0.86	0.91	0.96	0.01
0.11	0.16	0.21	0.26	0.31	0.36	0.41	0.46
0.56	0.61	0.66	0.71	0.76	0.81	0.86	0.91
0.01	0.06	0.11	0.16	0.21	0.26	0.31	0.36
0.46	0.51	0.56	0.61	0.66	0.71	0.76	0.81
0.91	0.96	0.01	0.06	0.11	0.16	0.21	0.26
0.36	0.41	0.46	0.51	0.56	0.61	0.66	0.71
0.81	0.86	0.91	0.96	0.01	0.06	0.11	0.16
0.26	0.31	0.36	0.41	0.46	0.51	0.56	0.61
0.71	0.76	0.81	0.86	0.91	0.96	0.01	0.06
0.16	0.21	0.26	0.31	0.36	0.41	0.46	0.51
0.61	0.66	0.71	0.76	0.81	0.86	0.91	0.96
0.06	0.11	0.16	0.21	0.26	0.31	0.36	0.41
0.51	0.56	0.61	0.66	0.71	0.76	0.81	0.86
0.96	0.01	0.06	0.11	0.16	0.21	0.26	0.31
0.41	0.46	0.51	0.56	0.61	0.66	0.71	0.76
0.86	0.91	0.96	0.01	0.06	0.11	0.16	0.21
0.31	0.36	0.41	0.46	0.51	0.56	0.61	0.66
0.76	0.81	0.86	0.91	0.96	0.01	0.06	0.11
0.21	0.26	0.31	0.36	0.41	0.46	0.51	0.56
0.66	0.71	0.76	0.81	0.86	0.91	0.96	0.01
0.11	0.16	0.21	0.26	0.31	0.36	0.41	0.46
0.56	0.61	0.66	0.71	0.76	0.81	0.86	0.91

0.01	0.06	0.11	0.16	0.21	0.26	0.31	0.36	0.41
0.46	0.51	0.56	0.61	0.66	0.71	0.76	0.81	0.86
0.91	0.96	0.01	0.06	0.11	0.16	0.21	0.26	0.31
0.36	0.41	0.46	0.51	0.56	0.61	0.66	0.71	0.76
0.81	0.86	0.91	0.96	0.01	0.06	0.11	0.16	0.21
0.26	0.31	0.36	0.41	0.46	0.51	0.56	0.61	0.66
0.71	0.76	0.81	0.86	0.91	0.96	0.01	0.06	0.11
0.16	0.21	0.26	0.31	0.36	0.41	0.46	0.51	0.56
0.61	0.66	0.71	0.76	0.81	0.86	0.91	0.96	0.01
0.06	0.11	0.16	0.21	0.26	0.31	0.36	0.41	0.46
0.51	0.56	0.61	0.66	0.71	0.76	0.81	0.86	0.91
0.96	0.01	0.06	0.11	0.16	0.21	0.26	0.31	0.36
0.41	0.46	0.51	0.56	0.61	0.66	0.71	0.76	0.81
0.86	0.91	0.96	0.01	0.06	0.11	0.16	0.21	0.26
0.31	0.36	0.41	0.46	0.51	0.56	0.61	0.66	0.71
0.76	0.81	0.86	0.91	0.96				

"V1 "	"V2 "	"V3 "	"V4 "	"V5 "	"V6 "	"V7 "	"V8 "	"V9 "
"V10 "	"V11 "	"V12 "	"V13 "	"V14 "	"V15 "	"V16 "	"V17 "	"V18 "
"V19 "	"V20 "	"V21 "	"V22 "	"V23 "	"V24 "	"V25 "	"V26 "	"V27 "
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"V64 "	"V65 "	"V66 "	"V67 "	"V68 "	"V69 "	"V70 "	"V71 "	"V72 "
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"V82 "	"V83 "	"V84 "	"V85 "	"V86 "	"V87 "	"V88 "	"V89 "	"V90 "
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[illegible]

0.56	0.61	0.66	0.71	0.76	0.81	0.86	0.91	0.96
0.01	0.06	0.11	0.16	0.21	0.26	0.31	0.36	0.41
0.46	0.51	0.56	0.61	0.66	0.71	0.76	0.81	0.86
0.91	0.96	0.01	0.06	0.11	0.16	0.21	0.26	0.31
0.36	0.41	0.46	0.51	0.56	0.61	0.66	0.71	0.76
0.81	0.86	0.91	0.96	0.01	0.06	0.11	0.16	0.21
0.26	0.31	0.36	0.41	0.46	0.51	0.56	0.61	0.66
0.71	0.76	0.81	0.86	0.91	0.96	0.01	0.06	0.11
0.16	0.21	0.26	0.31	0.36	0.41	0.46	0.51	0.56
0.61	0.66	0.71	0.76	0.81	0.86	0.91	0.96	0.01
0.06	0.11	0.16	0.21	0.26	0.31	0.36	0.41	0.46
0.51	0.56	0.61	0.66	0.71	0.76	0.81	0.86	0.91
0.96	0.01	0.06	0.11	0.16	0.21	0.26	0.31	0.36
0.41	0.46	0.51	0.56	0.61	0.66	0.71	0.76	0.81
0.86	0.91	0.96	0.01	0.06	0.11	0.16	0.21	0.26
0.31	0.36	0.41	0.46	0.51	0.56	0.61	0.66	0.71
0.76	0.81	0.86	0.91	0.96				