TP Krigeage - Challenge

```
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```

Dans ce compte rendu, nous présentons les différentes méthodes testées. On teste chaque méthode par la crosse validation afin d'évaluer la performance de la manière la plus pertinante possible puisqu'on a remarqué que le changement de la décomposition train/test peut changer largement les résultats trouvés. La méthode retenue est celle de la partie 8.

Les prédiction

1. Dévision en ensemble d'apprentissage et ensemble test

On commence d'abord par déviser notre base de données à une base d'apprentissage et une base test afin de voir le meilleur modèle en calculant RMSE sur les données test.

Notre base de données contient 700 observations avec 7 variables. La base d'apprentissage contiendra 550 observations et la base de test contiendra 150. Cela nous permet d'avoir les paramètres optimaux de chaque modèle tout en évitant le surpprentissage puisque le RMSE sera calculé sur l'ensemble de test.

```
set.seed(12345)
Observations = read.csv("defi_observations.csv", header = TRUE)
p < -7
n<-700
X=Observations[,1:p]
Y=Observations[,(p+1)]
n_app<-550
n_{\text{test}} < -150
y_app<-Observations[1:n_app,8]</pre>
X_app<-Observations[1:n_app,1:p]</pre>
y test<-Observations[(n app+1):n,8]</pre>
X_test<-Observations[(n_app+1):n,1:p]</pre>
mu.y<-mean(y_app)</pre>
# prédiction de Y par sa moyenne sur les données d'apprentissage
RMSE.ref<-sqrt(sum((y_test-mu.y)^2)/n_test)</pre>
print(RMSE.ref)
```

```
## [1] 6.556478
```

On remarque que La valeur RMSE en utilisant la moyenne est très élevée.

1.a Dévision en ensemble d'apprentissage et ensemble test et moyenne avec Cross Validation

```
#mélanger les données aléatoirement
Observations(sample(nrow(Observations)),]
#Creation de 10 plis de taille egale
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)</pre>
1R < -seq(1,5)
# 10 plis validation croisée
for(i in 1:5){
  testIndexes <- which(folds==i,arr.ind=TRUE)</pre>
  y_app_cv<-Observations[-testIndexes,8]</pre>
  X_app_cv<-Observations[-testIndexes,1:p]</pre>
  y_test_cv<-Observations[testIndexes,8]</pre>
  X_test_cv<-Observations[testIndexes,1:p]</pre>
  mucv.y<-mean(y_app_cv)</pre>
  # prédiction de Y par sa moyenne sur les données d'apprentissage
  RMSE.ref<-sqrt(sum((y_test_cv-mucv.y)^2)/n_test)</pre>
  1R[i] <- RMSE.ref</pre>
  #print(RMSE.ref)
print(mean(1R))
```

[1] 6.085994

2. La fonction pour calculer RMSE

On implémente une fonction qui calcule la valeur de RMSE et qui en même temps trace le graphe des résidus et le graphe des observations en fonction des prédictions.

```
rmse<-function(y, ypred, trace=FALSE){

rmse=y-ypred

if( trace){
 plot( ypred, y, xlab="Ypred", ylab="Ytrue")
  abline(a=0,b=1, col="blue")
  title(" Valeurs observées en fonctions des prédictions")

plot(rmse, main="Résidus")
}

return( sqrt( mean( rmse**2) ) )
}</pre>
```

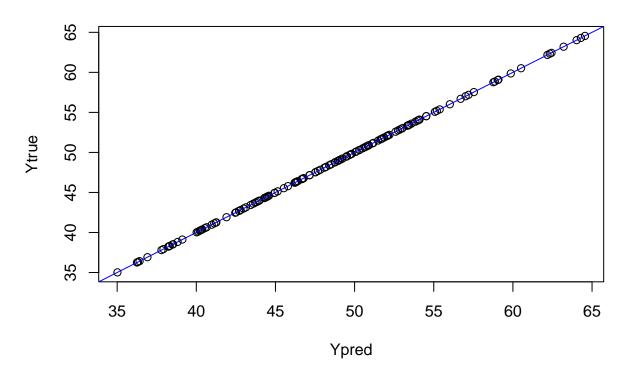
3. Krigeage Simple

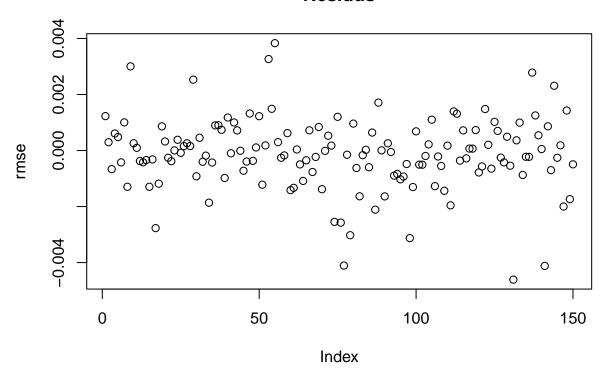
Nous commençant par la méthode de krigeage simple, et on varie la valeur de theta afin d'avoir la valeur RMSE la plus petite.

library(DiceKriging)

```
## Warning: package 'DiceKriging' was built under R version 4.3.2
```

```
theta=rep(9.4,7)
Msimple<-km(formula=~1,design=X_app,response=y_app,coef.trend=0,coef.cov=theta,coef.var = 1)
predsimple<-predict(object =Msimple,newdata=X_test,type="SK",ckeckNames=False )
Meansimple<-predsimple$mean
rmse(y_test, Meansimple, trace=TRUE)</pre>
```





[1] 0.001278394

3.a Krigeage Simple avec CrossValidation

```
#Randomly shuffle the data
Observations<-Observations[sample(nrow(Observations)),]</pre>
#Create 10 equally size folds
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)</pre>
1R < -seq(1,5)
#Perform 10 fold cross validation
for(i in 1:5){
  #Segement your data by fold using the which() function
  testIndexes <- which(folds==i,arr.ind=TRUE)</pre>
  y_app_cv<-Observations[-testIndexes,8]</pre>
  X_app_cv<-Observations[-testIndexes,1:p]</pre>
  y_test_cv<-Observations[testIndexes,8]</pre>
  X_test_cv<-Observations[testIndexes,1:p]</pre>
  Msimplecv<-km(formula=~1,design=X_app_cv,response=y_app_cv,coef.trend=0,coef.cov=theta,coef.var = 1)</pre>
  predsimplecv<-predict(object =Msimplecv,newdata=X_test_cv,type="SK",ckeckNames=False )</pre>
  Meansimplecv<-predsimplecv$mean
  lR[i] <- rmse(y test cv, Meansimplecv)</pre>
  #print(rmse(y_test_cv, Meansimplecv))
```

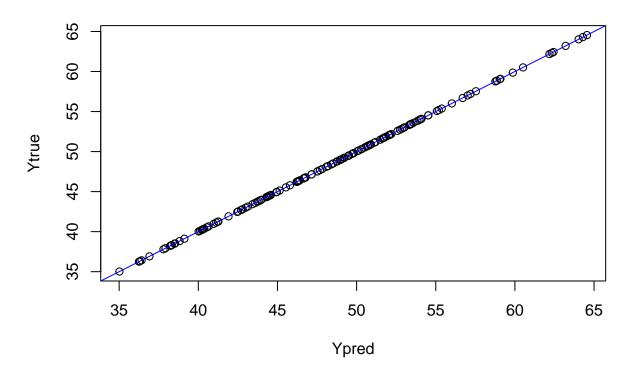
```
print(mean(1R))
```

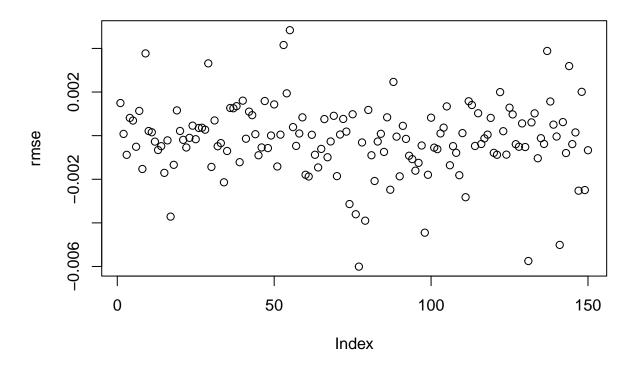
[1] 0.001203203

4. Krigeage Ordinaire

On teste après la méthode de krigeage ordinaire

```
theta=rep(8,7)
Mordinaire<-km(formula=~1,design=X_app,response=y_app,coef.trend=NULL,coef.cov=theta,coef.var = 1)
predordinaire<-predict(object =Mordinaire,newdata=X_test,type="UK",ckeckNames=False )
Meanordinaire<-predordinaire*mean
rmse(y_test, Meanordinaire, trace=TRUE)</pre>
```





[1] 0.001659609

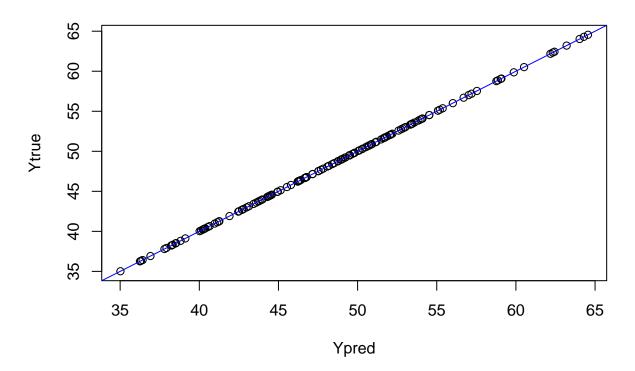
4. Krigeage Ordinaire avec CrossValidation

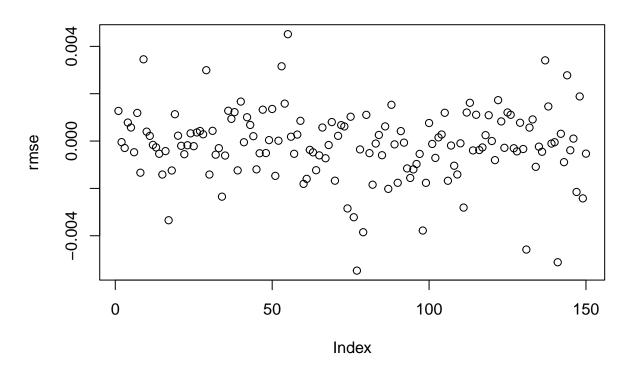
```
Observations(sample(nrow(Observations)),]
#Create 10 equally size folds
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)</pre>
1R < -seq(1,5)
#Perform 10 fold cross validation
for(i in 1:5){
  #Segement your data by fold using the which() function
  testIndexes <- which(folds==i,arr.ind=TRUE)</pre>
  y_app_cv<-Observations[-testIndexes,8]</pre>
  X_app_cv<-Observations[-testIndexes,1:p]</pre>
  y_test_cv<-Observations[testIndexes,8]</pre>
  X_test_cv<-Observations[testIndexes,1:p]</pre>
  Mordinaire < -km (formula = ~1, design = X_app_cv, response = y_app_cv, coef.trend = NULL, coef.cov = theta, coef.var =
  predordinaire<-predict(object =Mordinaire,newdata=X_test_cv,type="UK",ckeckNames=False )</pre>
  Meanordinaire <- predordinaire $mean
  1R[i] <- rmse(y_test_cv, Meanordinaire)</pre>
print(mean(1R))
```

5. Krigeage universal

Pour la mèthode de krigeage universel, on teste les deux formule " $y\sim1+X$ " et " $y\sim1+X+X^2$ " qui nous donne presque le même résultat

```
theta=rep(8.4,7)
Muniversel <- km(formula = ~y_app~1+.+.^2, coef.trend = NULL, design = X_app, response = y_app,coef.cov
preduniversel <- predict(object = Muniversel, newdata = X_test, type = "UK")
meanuniversel <- preduniversel$mean
rmse(y_test, meanuniversel, trace=TRUE)</pre>
```





[1] 0.001505418

5.a Krigeage universal avec CrossValidation

```
Observations<-Observations[sample(nrow(Observations)),]</pre>
#Create 10 equally size folds
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)</pre>
1R < -seq(1,5)
#Perform 10 fold cross validation
for(i in 1:5){
  #Segement your data by fold using the which() function
  testIndexes <- which(folds==i,arr.ind=TRUE)</pre>
  y_app_cv<-Observations[-testIndexes,8]</pre>
  X_app_cv<-Observations[-testIndexes,1:p]</pre>
  y_test_cv<-Observations[testIndexes,8]</pre>
  X_test_cv<-Observations[testIndexes,1:p]</pre>
  Muniversel <- km(formula = ~y_app_cv~1+.+.^2, coef.trend = NULL, design = X_app_cv, response = y_app_
  preduniversel <- predict(object = Muniversel, newdata = X_test_cv, type = "UK")</pre>
  meanuniversel <- preduniversel$mean</pre>
  1R[i] <- rmse(y_test_cv, meanuniversel)</pre>
```

```
print(mean(1R))
```

[1] 0.001265007

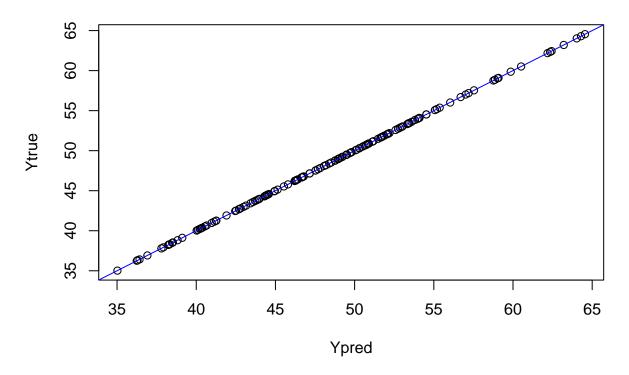
6. Optimisation par LOO

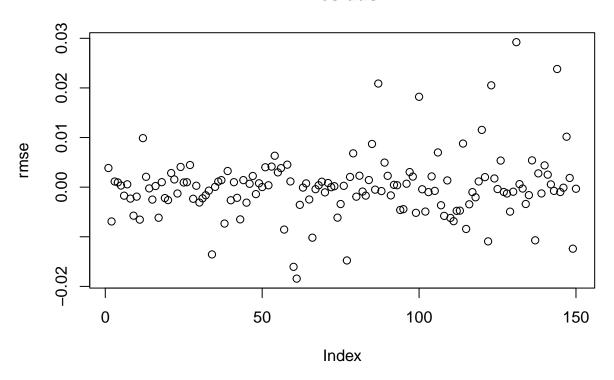
Dans les dernières méthodes, l'optimisation de la portée n'est pas simple puisque on parle d'un vecteur de 7 composantes et pas d'un simple réel, pour cette raison on utilise la méthode de leave-one-out et la méthode du maximum de vraisemblance.

Dans l'implémentation de ces deux méthodes, on varie à chaque fois la structure de covariance "covtype" entre "gauss", "matern5_2", "matern3_2", "exp" ou "powexp" et dans tous les cas la covariance gaussienne nous donne les meilleur résultats.

```
famille="matern5_2"
Mloo<-km(formula=~.^2,design=X_app,response=y_app,covtype="gauss",coef.trend=NULL,estim.method = "L00")
##
## optimisation start
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
  * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
##
       X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
       X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
       X6:X7
##
## * covariance model :
##
     - type : gauss
##
     - nugget : NO
##
     - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
     - parameters upper bounds : 1.99172 1.998102 1.987558 1.997227 1.996341 1.992466 1.993762
##
##
     - best initial criterion value(s): 0.002371201
##
## N = 7, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                                                    0.022418
## At iterate
                  0 f=
                           0.0023712
                                      |proj g|=
                                       |proj g|=
## At iterate
                  1 f =
                            0.0019121
                                                      0.015991
                  2 f =
                            0.0012673
                                       |proj g|=
                                                     0.0067028
## At iterate
## At iterate
                  3 f =
                            0.0010391
                                       |proj g|=
                                                     0.0037562
## At iterate
                  4 f =
                           0.00085974
                                       |proj g|=
                                                     0.0021381
## At iterate
                  5 f =
                           0.00067381
                                       |proj g|=
                                                     0.0014966
## At iterate
                  6 f =
                           0.00050924
                                       |proj g|=
                                                      0.002225
## At iterate
                  7
                    f =
                           0.00039184
                                       |proj g|=
                                                    0.00075765
## At iterate
                  8 f =
                           0.00031826
                                       |proj g|=
                                                    0.00045745
## At iterate
                  9 f =
                           0.00021033
                                       |proj g|=
                                                    0.00084691
## At iterate
                 10 f =
                            0.0001872
                                       |proj g|=
                                                    0.00037111
## At iterate
                 11 f =
                           0.00011452
                                                    0.00020296
                                       |proj g|=
## At iterate
                12 f =
                           7.4145e-05
                                       |proj g|=
                                                    8.6717e-05
## At iterate
                                                    6.8228e-05
                13 f =
                            5.619e-05
                                       |proj g|=
```

```
## At iterate 14 f = 4.0166e-05 |proj g|=
                                                  9.8244e-05
                          3.8851e-05 |proj g|=
## At iterate 15 f =
                                                  5.5958e-05
                          3.8519e-05 |proj g|=
## At iterate 16 f =
                                                  1.6897e-05
## At iterate 17 f = 
## At iterate 18 f =
                          3.8423e-05
                                      |proj g|=
                                                  1.6904e-05
                          3.7277e-05
                                     |proj g|=
                                                  1.7874e-05
## At iterate 19 f =
                          3.5767e-05 |proj g|=
                                                  2.0386e-05
## At iterate 20 f =
                          3.5586e-05
                                     |proj g|=
                                                  1.0585e-05
## At iterate 21 f =
                          3.5505e-05 |proj g|=
                                                  1.1551e-06
                          3.5505e-05 |proj g|=
## At iterate 22 f =
                                                  3.0987e-06
##
## iterations 22
## function evaluations 24
## segments explored during Cauchy searches 23
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 3.09875e-06
## final function value 3.55045e-05
##
## F = 3.55045e-05
## final value 0.000036
## converged
bestThetaLOO = coef(Mloo, "range")
sd2L00 = coef(Mloo, "sd2")
predLOO<-predict(object=Mloo,newdata=X_test,type="UK",ckeckNames=FALSE )</pre>
MeanLOO<-predLOO$mean
rmse(y_test, MeanLOO, trace=TRUE)
```





```
## [1] 0.006303565
```

```
message("DiceKriging: par optimisation MLE, theta= ", bestThetaL00)
```

DiceKriging: par optimisation MLE, theta= 0.3938690598057541.998102292418481.987557558808481.9972273

6.a Optimisation par LOO CV

```
Observations<-Observations[sample(nrow(Observations)),]
#Create 10 equally size folds
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)
lR<-seq(1,5)
#Perform 10 fold cross validation
for(i in 1:5){
    #Segement your data by fold using the which() function
    testIndexes <- which(folds==i,arr.ind=TRUE)
    y_app_cv<-Observations[-testIndexes,8]
    X_app_cv<-Observations[-testIndexes,1:p]
    y_test_cv<-Observations[testIndexes,8]
    X_test_cv<-Observations[testIndexes,1:p]

Mloo<-km(formula=-.^2,design=X_app_cv,response=y_app_cv,covtype="gauss",coef.trend=NULL,estim.method</pre>
```

```
bestThetaLOO = coef(Mloo, "range")
 sd2L00 = coef(Mloo, "sd2")
 predLOO<-predict(object=Mloo,newdata=X_test_cv,type="UK",ckeckNames=FALSE )</pre>
 MeanLOO<-predLOO$mean
 1R[i] <- rmse(y_test_cv, MeanLOO)</pre>
}
##
## optimisation start
## -----
## * estimation method
                      : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
##
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
##
    - type : gauss
    - nugget : NO
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
##
    - parameters upper bounds : 1.99172 1.998102 1.982769 1.998337 1.996341 1.996626 1.991921
##
##
    - best initial criterion value(s): 0.001477276
## N = 7, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
             0 f=
                         0.0014773 |proj g|=
                                                0.0067133
                1 f =
## At iterate
                          0.0014247
                                     |proj g|=
                                                  0.0065746
              2 f =
## At iterate
                         0.00092759
                                     |proj g|=
                                                 0.00087924
                                     |proj g|=
## At iterate
             3 f =
                         0.00063567
                                                 0.00087569
## At iterate
             4 f =
                         0.00032165
                                     |proj g|=
                                                  0.0026527
                                     |proj g|=
                                                 0.00074148
## At iterate 5 f =
                         0.00013515
                6 f =
## At iterate
                         0.00010375
                                     |proj g|=
                                                 0.00021058
## At iterate
                7 f =
                         7.5594e-05
                                     |proj g|=
                                                 9.7586e-05
## At iterate 8 f =
                          4.452e-05
                                     |proj g|=
                                                 0.00012336
## At iterate 9 f =
                         4.1504e-05
                                     |proj g|=
                                                 9.1811e-05
## At iterate 10 f =
                                     |proj g|=
                         3.8098e-05
                                                 4.3778e-05
3.7297e-05
                                                 2.4199e-05
                                     |proj g|=
## At iterate 12 f =
                         3.6409e-05
                                                 1.8073e-05
                                     |proj g|=
                         3.4204e-05
## At iterate 13 f =
                                     |proj g|=
                                                 1.6962e-05
## At iterate 14 f =
                          3.231e-05
                                     |proj g|=
                                                 1.5142e-05
## At iterate 15 f =
                         3.1108e-05
                                     |proj g|=
                                                 3.4583e-05
## At iterate 16 f =
                         3.0946e-05
                                     |proj g|=
                                                 1.0029e-05
## At iterate 17 f =
                         3.0917e-05
                                     |proj g|=
                                                 9.4372e-07
## At iterate
                18 f =
                         3.0916e-05
                                     |proj g|=
                                                 8.7536e-07
##
## iterations 18
## function evaluations 21
## segments explored during Cauchy searches 19
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
```

norm of the final projected gradient 8.75356e-07

```
## final function value 3.09157e-05
##
## F = 3.09157e-05
## final value 0.000031
## converged
##
## optimisation start
## -----
## * estimation method
                        : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
       X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
##
    - type : gauss
     - nugget : NO
##
     - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
##
     - parameters upper bounds : 1.988234 1.998102 1.987558 1.990277 1.994731 1.996244 1.987477
##
##
     - best initial criterion value(s) : 0.002717226
##
## N = 7, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                          0.0027172 |proj g|=
## At iterate
                 0 f=
                                                  0.0097358
## At iterate
                 1 f =
                           0.0025977
                                      |proj g|=
                                                    0.0093399
## At iterate
                 2 f =
                          0.00099668
                                      |proj g|=
                                                   0.00099835
                 3 f =
## At iterate
                          0.00088434
                                      |proj g|=
                                                   0.00079969
## At iterate
                 4 f =
                          0.00063578
                                       |proj g|=
                                                    0.0010631
                                       |proj g|=
## At iterate
              5 f =
                          0.00020537
                                                     0.001024
## At iterate
                 6 f =
                          0.00016776
                                       |proj g|=
                                                    0.0023293
## At iterate
                 7 f =
                          7.3289e-05
                                      |proj g|=
                                                   0.00069068
## At iterate
                 8 f =
                          5.7825e-05
                                       |proj g|=
                                                   0.00044391
## At iterate
                 9 f =
                          4.3061e-05
                                      |proj g|=
                                                   0.00020573
## At iterate
                10 f =
                          3.7082e-05
                                      |proj g|=
                                                   5.5601e-05
              11 f =
## At iterate
                          3.5016e-05
                                      |proj g|=
                                                   5.7728e-05
## At iterate
              12 f =
                           3.207e-05
                                      |proj g|=
                                                   4.0215e-05
## At iterate
              13 f =
                          2.9838e-05
                                      |proj g|=
                                                    1.622e-05
## At iterate
                14 f =
                          2.9261e-05
                                      |proj g|=
                                                   1.4073e-05
              15 f =
## At iterate
                                      |proj g|=
                          2.8969e-05
                                                   1.0117e-05
## At iterate
              16 f =
                          2.7701e-05
                                      |proj g|=
                                                   9.1691e-06
## At iterate
                17 f =
                                      |proj g|=
                                                    6.594e-06
                          2.7645e-05
## At iterate
                18 f =
                          2.7627e-05
                                      |proj g|=
                                                   7.0306e-06
## At iterate
                19 f =
                          2.7617e-05
                                      |proj g|=
                                                   2.2449e-07
## At iterate
                20 f =
                          2.7617e-05
                                      |proj g|=
                                                   1.3267e-09
##
## iterations 20
## function evaluations 21
## segments explored during Cauchy searches 20
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 1.32671e-09
## final function value 2.76173e-05
##
```

```
## F = 2.76173e-05
## final value 0.000028
## converged
##
## optimisation start
## -----
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
       X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
       X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
##
       X6:X7
## * covariance model :
##
     - type : gauss
##
     - nugget : NO
##
     - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
##
     - parameters upper bounds : 1.99172 1.998102 1.987558 1.998337 1.996341 1.996626 1.993762
##
     - best initial criterion value(s): 0.00535388
##
## N = 7, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f=
                          0.0053539
                                      |proj g|=
                                                   0.034338
                 1 f =
## At iterate
                           0.0038921
                                      |proj g|=
                                                     0.016898
## At iterate
                 2 f =
                           0.0030867
                                      |proj g|=
                                                      0.01077
## At iterate
                 3 f =
                           0.0023486
                                      |proj g|=
                                                    0.0063883
## At iterate
                 4 f =
                           0.0016151
                                       |proj g|=
                                                     0.003315
                 5 f =
## At iterate
                          0.00098939
                                       |proj g|=
                                                    0.0017544
## At iterate
                 6 f =
                          0.00026112
                                       |proj g|=
                                                   0.00050641
                                       |proj g|=
## At iterate
                7 f =
                          0.00016384
                                                   0.00090227
## At iterate
                 8 f =
                          0.00010298
                                       |proj g|=
                                                   0.00015131
## At iterate
                 9 f =
                          8.8119e-05
                                       |proj g|=
                                                   0.00014444
## At iterate
              10 f =
                          7.7097e-05
                                       |proj g|=
                                                   6.5739e-05
              11 f =
## At iterate
                           5.416e-05
                                      |proj g|=
                                                   0.00015439
## At iterate
                12 f =
                          5.0826e-05
                                       |proj g|=
                                                   0.00012659
              13 f =
## At iterate
                                                   4.5259e-05
                           4.682e-05
                                      |proj g|=
## At iterate
              14 f =
                             3.9e-05
                                      |proj g|=
                                                   0.00012641
## At iterate
              15 f =
                          3.8034e-05
                                      |proj g|=
                                                    6.219e-05
## At iterate
                16 f =
                           3.702e-05
                                      |proj g|=
                                                   2.2132e-05
## At iterate
              17 f =
                                      |proj g|=
                          3.6411e-05
                                                   5.8173e-05
## At iterate
              18 f =
                            3.55e-05
                                      |proj g|=
                                                   7.1271e-05
## At iterate
              19 f =
                          3.4913e-05
                                      |proj g|=
                                                   4.6208e-05
## At iterate
                20 f =
                          3.3567e-05
                                      |proj g|=
                                                   5.4087e-05
## At iterate
                21 f =
                                      |proj g|=
                          3.3124e-05
                                                   6.7728e-05
## At iterate
                22 f =
                          3.2137e-05
                                       |proj g|=
                                                   4.5975e-05
                23 f =
## At iterate
                          3.1906e-05
                                       |proj g|=
                                                   8.0565e-06
                                       |proj g|=
## At iterate
                24 f =
                          3.1885e-05
                                                   5.3058e-06
## At iterate
                25 f =
                          3.1872e-05
                                       |proj g|=
                                                   7.3458e-06
## At iterate
                26 f =
                          3.1853e-05
                                      |proj g|=
                                                   5.5428e-06
## At iterate
                27 f =
                           3.185e-05
                                       |proj g|=
                                                   4.3748e-07
## At iterate
                28 f =
                           3.185e-05
                                      |proj g|=
                                                    1.933e-08
##
## iterations 28
## function evaluations 29
```

```
## segments explored during Cauchy searches 28
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 1.93303e-08
## final function value 3.18495e-05
##
## F = 3.18495e-05
## final value 0.000032
## converged
##
## optimisation start
## -----
## * estimation method
                       : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
##
       X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
       X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
##
    - type : gauss
##
     - nugget : NO
     - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
##
     - parameters upper bounds : 1.985485 1.981771 1.987558 1.997227 1.996341 1.996626 1.993762
##
##
     - best initial criterion value(s): 0.03737871
## N = 7, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                 0 f=
                                                     0.2983
## At iterate
                           0.037379 |proj g|=
## At iterate
                 1 f =
                           0.0020855
                                      |proj g|=
                                                     0.012149
## At iterate
                 2 f =
                           0.0019141
                                       |proj g|=
                                                     0.010752
## At iterate
                 3 f =
                          0.00099103
                                       |proj g|=
                                                    0.0042901
## At iterate
                 4 f =
                          0.00066222
                                       |proj g|=
                                                    0.0022559
## At iterate
                 5 f =
                           0.0004514
                                       |proj g|=
                                                    0.0011128
## At iterate
                 6 f =
                          0.00031571
                                       |proj g|=
                                                   0.00062885
## At iterate
                 7 f =
                                                    0.0003432
                           0.0002214
                                       |proj g|=
## At iterate
                 8 f =
                          0.00014568
                                       |proj g|=
                                                   0.00017238
## At iterate
               9 f =
                          9.7456e-05
                                       |proj g|=
                                                   0.00038298
## At iterate
                10 f =
                          6.2446e-05
                                       |proj g|=
                                                   4.5998e-05
## At iterate
              11 f =
                          4.3912e-05
                                                   2.2325e-05
                                       |proj g|=
## At iterate
              12 f =
                          3.8424e-05
                                       |proj g|=
                                                   3.8351e-05
## At iterate
              13 f =
                          3.5815e-05
                                       |proj g|=
                                                   1.5359e-05
## At iterate
                14 f =
                          3.5597e-05
                                       |proj g|=
                                                   4.1006e-06
## At iterate
              15 f =
                          3.5593e-05
                                       |proj g|=
                                                   3.6111e-06
## At iterate
              16 f =
                          3.5578e-05
                                       |proj g|=
                                                   1.3142e-06
## At iterate
                17 f =
                          3.5578e-05
                                       |proj g|=
                                                   3.6571e-07
## iterations 17
## function evaluations 18
## segments explored during Cauchy searches 18
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 3.6571e-07
## final function value 3.55782e-05
```

```
##
## F = 3.55782e-05
## final value 0.000036
## converged
## optimisation start
## -----
## * estimation method
                       : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
##
      X6:X7
## * covariance model :
##
    - type : gauss
##
    - nugget : NO
##
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
##
    - parameters upper bounds : 1.99172 1.998102 1.978714 1.998337 1.994373 1.992466 1.993762
##
    - best initial criterion value(s): 0.01244225
##
## N = 7, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f=
                           0.012442 |proj g|=
                                                   0.096037
                 1 f =
## At iterate
                                      |proj g|=
                           0.0055617
                                                     0.041115
## At iterate
                 2 f =
                           0.0031205
                                      |proj g|=
                                                     0.020799
                 3 f =
## At iterate
                           0.0019552
                                      |proj g|=
                                                    0.0079473
                 4 f =
## At iterate
                           0.0015773
                                      |proj g|=
                                                    0.0035791
              5 f =
## At iterate
                            0.001268
                                      |proj g|=
                                                    0.0019252
                                      |proj g|=
## At iterate
              6 f =
                          0.00086485
                                                     0.001247
                7 f =
## At iterate
                          0.00050465
                                      |proj g|=
                                                    0.0012969
## At iterate
                 8 f =
                          0.00029607
                                      |proj g|=
                                                    0.0011661
              9 f =
## At iterate
                          0.00020414
                                      |proj g|=
                                                   0.00038552
## At iterate
              10 f =
                          0.00013932
                                      |proj g|=
                                                   0.00051184
## At iterate
                11 f =
                          8.9135e-05
                                      |proj g|=
                                                   9.3122e-05
## At iterate 12 f =
                          6.5885e-05
                                      |proj g|=
                                                   4.9652e-05
## At iterate 13 f =
                          5.0252e-05
                                      |proj g|=
                                                    4.085e-05
## At iterate 14 f =
                          4.2698e-05
                                      |proj g|=
                                                   2.5909e-05
## At iterate
              15 f =
                          3.9141e-05
                                                   2.2724e-05
                                      |proj g|=
## At iterate 16 f =
                                      |proj g|=
                          3.8106e-05
                                                   0.00010037
## At iterate
              17 f =
                          3.6527e-05
                                      |proj g|=
                                                   3.2423e-05
## At iterate
              18 f =
                          3.5799e-05
                                      |proj g|=
                                                   1.4282e-05
## At iterate
                19 f =
                          3.4377e-05
                                      |proj g|=
                                                    7.375e-06
## At iterate
                20 f =
                          3.4358e-05
                                      |proj g|=
                                                   3.0506e-06
## At iterate
                21 f =
                          3.4344e-05
                                      |proj g|=
                                                   2.6928e-06
## At iterate
                22 f =
                                                   1.5372e-06
                          3.4343e-05
                                      |proj g|=
## iterations 22
## function evaluations 24
## segments explored during Cauchy searches 23
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 1.53719e-06
## final function value 3.4343e-05
```

```
##
## F = 3.4343e-05
## final value 0.000034
## converged

print(mean(1R))
## [1] 0.005742813
```

7. Optimisation par MLE

At iterate

16 f =

```
MMLE <- km(formula = ~.^2, design = X_app, response = y_app, covtype = "gauss", coef.trend = NULL, est
##
## optimisation start
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
##
    - type : gauss
##
    - nugget : 1e-13
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
    - parameters upper bounds : 1.99172 1.998102 1.987558 1.997227 1.996341 1.992466 1.993762
##
    - variance bounds : 0.06301832 6.547727
##
    - best initial criterion value(s): -488.6816
## N = 8, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                                                    5.6976
## At iterate
                 0 f=
                             488.68 | proj g|=
## At iterate
                 1 f =
                             476.86 |proj g|=
                                                      1.9379
## At iterate
                 2 f =
                             474.24
                                     |proj g|=
                                                      1.9347
## At iterate
                3 f =
                             464.16
                                     |proj g|=
                                                      1.8939
## At iterate 4 f =
                             446.51
                                     |proj g|=
                                                      1.9486
## At iterate 5 f =
                             444.57
                                     |proj g|=
                                                      1.9699
              6 f =
## At iterate
                             439.15
                                     |proj g|=
                                                      1.9917
## At iterate
                7 f =
                             438.93
                                     |proj g|=
                                                      1.9917
## At iterate
             8 f =
                             438.73
                                                      1.9917
                                     |proj g|=
              9 f =
## At iterate
                             438.18
                                     |proj g|=
                                                      1.9917
## At iterate 10 f =
                             437.99
                                     |proj g|=
                                                      1.9917
## At iterate 11 f =
                             437.83
                                     |proj g|=
                                                      1.9917
## At iterate 12 f =
                              437.5
                                     |proj g|=
                                                      1.9916
## At iterate 13 f =
                                     |proj g|=
                             436.45
                                                      1.9908
## At iterate 14 f =
                             434.53
                                     |proj g|=
                                                      1.9884
## At iterate 15 f =
                              432.9
                                     |proj g|=
                                                      6.0438
```

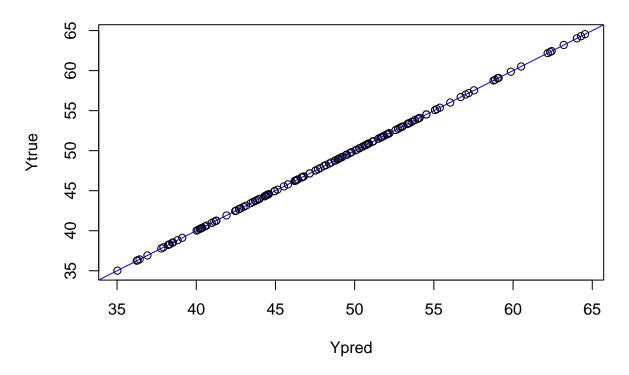
6.0642

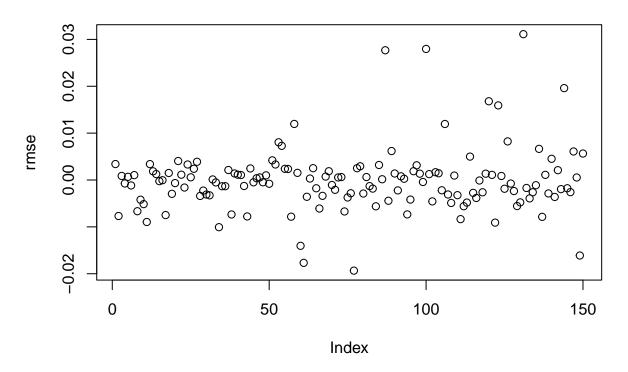
|proj g|=

432.49

	Αt	iterate	17	f	=	432.39	lproj g	_	6.0725
##	Αt	iterate	18	_	=	432.25	proj 8		6.0788
##	Αt	iterate	19	f	=	432.03	proj g		6.0824
##	Αt	iterate	20	f	=	431.86	proj g		6.0803
##	Αt	iterate	21	f	=	431	proj 8		6.0739
##	Αt	iterate	22	f	=	428.83	proj 8	g =	1.9622
##	At	iterate	23	f	=	428.35	proj 8	g =	6.0683
##	At	iterate	24	f	=	425.83	proj g	g =	1.966
##	At	iterate	25	f	=	425.44	proj g	g =	6.0413
##	Αt	iterate	26	f	=	425.21	proj g	τ =	6.0343
##	Αt	iterate	27	f	=	425.09	proj g		4.4456
##	Αt	iterate	28	f	=	425.01	proj g	τ =	1.9084
##	Αt	iterate	29	f	=	424.97	proj g	τ =	1.9024
##	Αt	iterate	30	f	=	424.94	proj g	_	1.92
##	Αt	iterate	31	f	=	424.92	proj g	_	1.9654
##	At	iterate	32	f	=	424.82	proj g	_	1.9652
##	Αt	iterate	33	f	=	424.64	proj g	_	1.9651
##	At	iterate	34	f	=	424.42	proj	_	1.9651
##	At	iterate	35	f	=	424.21	lproj g		6.0045
##	At	iterate	36	f	=	423.95	proj	_	6.0048
##	At	iterate	37	f	=	423.67	proj 8		4.5255
##	At	iterate	38	f	=	423.25	proj 8	-	6.0143
##		iterate	39	f	=	422.75	proj 8	-	6.0106
		iterate	40	_	=	422.58	proj 8	_	6.0062
		iterate	41	_	=	422.17	proj 8	_	5.9956
##		iterate	42	_	=	421.72	proj 8	_	4.6187
##	At	iterate	43	f		421	proj 8		1.6038
##	At	iterate	44	f		420.41	proj 8	_	1.4714
##	At	iterate	45	f		420.28	proj 8	_	1.4664
##	At	iterate	46	f		419.41	proj 8	_	1.3983
##	At	iterate	47	f		418.2	proj 8	_	1.952
##	At	iterate	48	f		416.84	proj 8	_	1.9528
##	At	iterate	49	f		413.44	proj 8	_	1.3192
##	At	iterate	50	f	=	406.55	proj 8	_	6.0079
##	At		51	f	=	403.89	proj 8	_	1.8647
##	At	iterate	52	f	=	402.34		g =	4.8798
		iterate	53	f		400.49	proj 8	-	1.9501
		iterate	54	f		398.38	proj 8		1.9558
		iterate	55	f		396.44	proj 8	-	1.963
		iterate	56	f		388.93	proj 8	_	1.9607
##		iterate	57	f		369.14	proj g		1.953
##		iterate	58	f	=	176.4	proj 8	-	1.9545
##		iterate	59	f	=	168.62	proj 8	_	1.9539
##		iterate	60		=	-229.69	proj 8		1.9152
##		iterate	61		=	-342.1	proj 8		1.868
##	At		62		=	-420.94	lproj g		1.8479
##	At		63	f	=	-465.88	proj 8		6.3964
##	At		64	f	_	-669.1	proj 8		6.3389
##	At		65	f	_	-981.33	proj 8		6.3271
##	At		66	f	_	-1109.9	proj 8		6.2025
		iterate	67		_	-1216.1	proj 8		6.1998
		iterate	68	f	=	-1216.1 -1234.2	proj 8		6.1592
		iterate	69	f	=	-1234.2 -1287.6	proj 8		5.9928
		iterate	70	f		-1320.9		-	5.9928
##	ΑL	Tretare	10	т	_	-1320.9	lproj g	51-	5.9211

```
## At iterate 71 f =
                            -1326.9 |proj g|=
                                                     5.8896
## At iterate 72 f =
                            -1330.4 |proj g|=
                                                     5.8384
                            -1333.6 |proj g|=
## At iterate 73 f =
                                                      5.77
## At iterate 74 f =
                             -1336
                                     |proj g|=
                                                     5.7242
## At iterate 75 f =
                            -1336.7
                                     |proj g|=
                                                     5.7156
## At iterate 76 f =
                            -1337.3
                                     |proj g|=
                                                     5.6904
                                     |proj g|=
## At iterate 77 f =
                            -1337.4
                                                     5.6808
## At iterate 78 f =
                            -1337.8
                                     |proj g|=
                                                     1.6116
## At iterate 79 f =
                            -1338.6
                                     |proj g|=
                                                     1.6092
## At iterate 80 f =
                            -1339.4
                                     |proj g|=
                                                     1.6044
## At iterate 81 f =
                            -1339.4
                                     |proj g|=
                                                     1.603
## At iterate 82 f =
                            -1339.5
                                     |proj g|=
                                                     1.6025
                            -1339.6
## At iterate 83 f =
                                     |proj g|=
                                                     1.3802
## At iterate 84 f =
                            -1339.6
                                     |proj g|=
                                                    0.20326
## At iterate 85 f =
                            -1339.6
                                     |proj g|=
                                                   0.013945
## At iterate 86 f =
                            -1339.6 |proj g|=
                                                 0.00034213
##
## iterations 86
## function evaluations 119
## segments explored during Cauchy searches 94
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 0.00034213
## final function value -1339.62
##
## F = -1339.62
## final value -1339.616662
## converged
predMLE <- predict(object = MMLE, newdata = X_test , type="UK" , checkNames=FALSE, se.compute=TRUE)</pre>
MeanMLE<-predMLE$mean</pre>
rmse(y_test, MeanMLE, trace=TRUE)
```





```
## [1] 0.006756957
```

```
bestThetaMLE = coef(MMLE, "range")
sd2MLE = coef(MMLE, "sd2")

message("DiceKriging: par optimisation MLE, theta= ", bestThetaMLE)
```

DiceKriging: par optimisation MLE, theta= 0.3880583424710951.998102292418481.987557558808481.9972273

7.a Optimisation par MLE avec CV

```
Observations<-Observations[sample(nrow(Observations)),]
#Create 10 equally size folds
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)
lR<-seq(1,5)
#Perform 10 fold cross validation
for(i in 1:5){
    #Segement your data by fold using the which() function
    testIndexes <- which(folds==i,arr.ind=TRUE)
    y_app_cv<-Observations[-testIndexes,8]
    X_app_cv<-Observations[-testIndexes,1:p]
    y_test_cv<-Observations[testIndexes,8]</pre>
```

```
X_test_cv<-Observations[testIndexes,1:p]</pre>
  MMLE <- km(formula = ~.^2, design = X_app_cv, response = y_app_cv, covtype = "gauss", coef.trend = NU
  predMLE <- predict(object = MMLE, newdata = X_test_cv , type="UK" , checkNames=FALSE, se.compute=TRUE</pre>
  MeanMLE<-predMLE$mean
 lR[i] <- rmse(y_test_cv, MeanMLE)</pre>
  #print(rmse(y_test_cv, Meanordinaire))
}
##
## optimisation start
## -----
## * estimation method
                       : MLE
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
##
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6 · X7
## * covariance model :
##
    - type : gauss
##
     - nugget : 1e-13
##
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
     - parameters upper bounds : 1.99172 1.988534 1.987558 1.998337 1.996341 1.996244 1.991921
##
     - variance bounds : 0.06654336 6.962068
     - best initial criterion value(s): 135.4504
##
##
## N = 8, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f=
                            -135.45 |proj g|=
                                                    6.0087
## At iterate
                1 f =
                             -716.69 | proj g|=
                                                      2.4388
## At iterate
               2 f =
                             -873.48
                                                      2.6765
                                     |proj g|=
                3 f =
## At iterate
                             -896.44
                                     |proj g|=
                                                      2.7661
## At iterate
                4 f =
                             -941.69
                                     |proj g|=
                                                      2.8959
## At iterate 5 f =
                             -1203.2
                                     |proj g|=
                                                      3.6353
## At iterate 6 f =
                              -1219
                                     |proj g|=
                                                      3.6482
                7 f =
## At iterate
                             -1245.8
                                                       3.659
                                     |proj g|=
## At iterate 8 f =
                             -1255.5
                                                        3.63
                                     |proj g|=
## At iterate
              9 f =
                             -1295.9
                                                      3.3884
                                     |proj g|=
              10 f =
## At iterate
                             -1310.8
                                     |proj g|=
                                                      3.3031
## At iterate 11 f =
                             -1320.1
                                     |proj g|=
                                                      3.3047
                             -1325.1
## At iterate 12 f =
                                     |proj g|=
                                                      3.3046
## At iterate 13 f =
                              -1329
                                     |proj g|=
                                                      3.2975
## At iterate 14 f =
                             -1329.3
                                     |proj g|=
                                                      3.2922
## At iterate 15 f =
                             -1329.4
                                     |proj g|=
                                                      3.2872
## At iterate 16 f =
                             -1329.6
                                     |proj g|=
                                                      3.2717
## At iterate 17 f =
                             -1330.3
                                     |proj g|=
                                                       3.229
## At iterate 18 f =
                             -1332.2
                                     |proj g|=
                                                      3.1034
                             -1337.1
## At iterate 19 f =
                                                      2.7682
                                     |proj g|=
## At iterate 20 f =
                             -1347.1
                                     |proj g|=
                                                      1.9581
## At iterate 21 f =
                             -1360.3
                                     |proj g|=
                                                      5.5046
```

6.1232

-1384.9 |proj g|=

At iterate

22 f =

```
-1387.3
## At iterate
                23 f =
                                      |proj g|=
                                                       1.4214
## At iterate
                24 f =
                             -1387.8
                                      |proj g|=
                                                       1.4119
## At iterate 25 f =
                             -1388.2
                                      |proj g|=
                                                       3.6333
                26 f =
## At iterate
                             -1388.3
                                                       1.6096
                                      |proj g|=
## At iterate 27 f =
                             -1388.3
                                      |proj g|=
                                                      0.52043
## At iterate 28 f =
                             -1388.3
                                      |proj g|=
                                                      0.38243
## At iterate 29 f =
                             -1388.3
                                      |proj g|=
                                                      0.17303
## At iterate 30 f =
                                                    0.026205
                             -1388.3
                                      |proj g|=
## At iterate
                31 f =
                             -1388.3
                                      |proj g|=
                                                    0.0030675
##
## iterations 31
## function evaluations 37
## segments explored during Cauchy searches 39
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 0.00306754
## final function value -1388.27
##
## F = -1388.27
## final value -1388.266938
## converged
## optimisation start
## -----
## * estimation method
                       : MLE
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
##
      X6:X7
## * covariance model :
##
    - type : gauss
##
    - nugget : 1e-13
##
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
##
    - parameters upper bounds : 1.985485 1.998102 1.977007 1.998337 1.996341 1.996626 1.992937
##
    - variance bounds : 0.06330323 6.759943
##
    - best initial criterion value(s): 113.7156
## N = 8, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f=
                            -113.72 |proj g|=
                                                    5.8887
                 1 f =
## At iterate
                              -815.6
                                     |proj g|=
                                                       5.2501
                 2 f =
## At iterate
                             -963.16
                                     |proj g|=
                                                       5.2139
                 3 f =
## At iterate
                             -1083.7
                                      |proj g|=
                                                      1.4226
                4 f =
## At iterate
                             -1100.4
                                      |proj g|=
                                                       1.4453
                             -1255.3
## At iterate
                5 f =
                                      |proj g|=
                                                       1.6163
                 6 f =
## At iterate
                             -1313.4
                                      |proj g|=
                                                       1.5239
## At iterate
                 7 f =
                             -1329.5
                                      |proj g|=
                                                       1.4961
                 8 f =
## At iterate
                             -1337.8
                                      |proj g|=
                                                       1.6232
## At iterate
                9 f =
                             -1344.5
                                      |proj g|=
                                                      5.9964
## At iterate 10 f =
                             -1353.8
                                      |proj g|=
                                                       6.024
## At iterate 11 f =
                             -1367.2 |proj g|=
                                                      6.0632
## At iterate
              12 f =
                             -1374.2 |proj g|=
                                                      6.0607
```

```
-1378.5
## At iterate
              13 f =
                                     |proj g|=
                                                      6.052
## At iterate 14 f =
                            -1386.2 |proj g|=
                                                     3.3822
## At iterate 15 f =
                            -1393.7
                                     |proj g|=
                                                     1.6142
## At iterate 16 f =
                            -1394.1
                                     |proj g|=
                                                     5.6183
## At iterate 17 f =
                            -1394.2
                                     |proj g|=
                                                     6.0376
## At iterate 18 f =
                            -1394.2
                                     |proj g|=
                                                     6.0367
## At iterate 19 f =
                            -1394.2
                                     |proj g|=
                                                     6.0355
## At iterate 20 f =
                            -1394.2
                                     |proj g|=
                                                     6.0309
## At iterate 21 f =
                            -1394.3
                                     |proj g|=
                                                     6.0195
## At iterate 22 f =
                            -1394.4
                                     |proj g|=
                                                     5.9918
## At iterate 23 f =
                            -1394.6
                                     |proj g|=
                                                     5.8746
             24 f =
## At iterate
                            -1394.8
                                     |proj g|=
                                                      1.608
                                     |proj g|=
                                                     1.4272
## At iterate 25 f =
                              -1395
## At iterate 26 f =
                              -1395
                                     |proj g|=
                                                     1.4249
## At iterate 27 f =
                              -1395
                                     |proj g|=
                                                     1.0253
             28 f =
## At iterate
                              -1395
                                     |proj g|=
                                                      0.161
## At iterate
                29 f =
                              -1395 |proj g|=
                                                    0.016185
##
## iterations 29
## function evaluations 34
## segments explored during Cauchy searches 36
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 0.0161854
## final function value -1395
## F = -1395
## final value -1394.999973
## converged
##
## optimisation start
## -----
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
    - type : gauss
##
    - nugget : 1e-13
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
    - parameters upper bounds : 1.99172 1.998102 1.987558 1.998337 1.996341 1.992466 1.993762
    - variance bounds : 0.06078994 6.34027
##
    - best initial criterion value(s): -197.2073
## N = 8, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                0 f=
## At iterate
                            197.21 |proj g|=
                                                     1.802
## At iterate
                1 f =
                            -447.95 |proj g|=
                                                     5.7692
             2 f =
## At iterate
                             -517.3 |proj g|=
                                                      5.777
## At iterate 3 f =
                            -584.47 |proj g|=
                                                     5.7779
## At iterate
              4 f =
                            -841.11 |proj g|=
                                                     1.709
```

```
5 f =
## At iterate
                              -1060
                                     |proj g|=
                                                      1.7037
## At iterate
                6 f =
                             -1351.6
                                     |proj g|=
                                                      5.8385
                                                      5.8258
## At iterate
                7 f =
                             -1371.9
                                     |proj g|=
                8 f =
## At iterate
                             -1377.1
                                     |proj g|=
                                                      5.8123
## At iterate
                9 f =
                             -1381.1
                                     |proj g|=
                                                      5.7986
## At iterate 10 f =
                             -1382.1
                                     |proj g|=
                                                     5.7882
## At iterate 11 f =
                             -1383.5
                                     |proj g|=
                                                     5.7679
## At iterate 12 f =
                             -1386.2
                                     |proj g|=
                                                     5.7105
## At iterate 13 f =
                             -1391.1
                                     |proj g|=
                                                      1.4796
## At iterate 14 f =
                            -1395.5
                                     |proj g|=
                                                      1.607
## At iterate
             15 f =
                            -1395.6
                                     |proj g|=
                                                      1.402
              16 f =
## At iterate
                             -1395.6
                                     |proj g|=
                                                      1.6057
                            -1395.7
                                     |proj g|=
## At iterate 17 f =
                                                      1.0774
## At iterate 18 f =
                            -1395.7
                                     |proj g|=
                                                     0.69665
## At iterate 19 f =
                            -1395.7
                                     |proj g|=
                                                     0.18507
## At iterate 20 f =
                             -1395.7
                                     |proj g|=
                                                    0.089515
## At iterate
                21 f =
                            -1395.7
                                                       0.131
                                     |proj g|=
##
## iterations 21
## function evaluations 26
## segments explored during Cauchy searches 29
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 0.131005
## final function value -1395.67
## F = -1395.67
## final value -1395.671838
## converged
##
## optimisation start
## -----
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
##
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
    - type : gauss
##
    - nugget : 1e-13
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
    - parameters upper bounds : 1.989814 1.998102 1.987558 1.983115 1.990315 1.996626 1.993762
    - variance bounds : 0.06330028 6.81084
##
    - best initial criterion value(s): 832.977
## N = 8, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                0 f=
## At iterate
                           -832.98 |proj g|=
                                                    1.8007
## At iterate
                1 f =
                            -1239.9 |proj g|=
                                                      1.6513
             2 f =
## At iterate
                            -1259.9 |proj g|=
                                                      6.3178
                            -1271.7 |proj g|=
## At iterate 3 f =
                                                     6.3122
## At iterate
              4 f =
                            -1274.1 |proj g|=
                                                     6.3113
```

```
5 f =
                                      |proj g|=
## At iterate
                              -1309
                                                      6.2763
## At iterate
                 6 f =
                                                       6.206
                             -1359.2
                                     |proj g|=
## At iterate
                7 f =
                             -1364.7
                                      |proj g|=
                                                      6.1955
                8 f =
## At iterate
                             -1368.1
                                      |proj g|=
                                                      6.1876
## At iterate
                9 f =
                             -1371.6
                                      |proj g|=
                                                      6.1714
## At iterate 10 f =
                             -1375.6
                                     |proj g|=
                                                      1.6252
## At iterate 11 f =
                             -1376.9
                                     |proj g|=
                                                      6.153
## At iterate 12 f =
                              -1378
                                      |proj g|=
                                                      6.1498
## At iterate 13 f =
                             -1378.2
                                     |proj g|=
                                                      6.1487
## At iterate 14 f =
                             -1378.3
                                     |proj g|=
                                                      6.1451
## At iterate 15 f =
                             -1378.7
                                      |proj g|=
                                                      6.1332
              16 f =
## At iterate
                             -1379.7
                                      |proj g|=
                                                      6.0918
                             -1381.8
                                     |proj g|=
## At iterate 17 f =
                                                      5.9895
## At iterate 18 f =
                             -1381.9
                                     |proj g|=
                                                      5.9792
## At iterate 19 f =
                              -1384
                                      |proj g|=
                                                      5.8123
             20 f =
## At iterate
                              -1385
                                      |proj g|=
                                                      5.7269
## At iterate 21 f =
                             -1385.1
                                                      2.2969
                                     |proj g|=
                                                      1.6003
## At iterate 22 f =
                             -1385.1
                                      |proj g|=
## At iterate 23 f =
                             -1385.1
                                                     0.11052
                                     |proj g|=
             24 f =
                                     |proj g|=
## At iterate
                             -1385.1
                                                     0.41142
## At iterate
                25 f =
                             -1385.1
                                     |proj g|=
                                                    0.047925
##
## iterations 25
## function evaluations 31
## segments explored during Cauchy searches 32
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 0.0479251
## final function value -1385.14
##
## F = -1385.14
## final value -1385.141365
## converged
##
## optimisation start
## -----
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X3 + X4 + X5 + X6 + X7 + X1:X2 + X1:X3 + X1:X4 + X1:X5 +
      X1:X6 + X1:X7 + X2:X3 + X2:X4 + X2:X5 + X2:X6 + X2:X7 + X3:X4 +
##
      X3:X5 + X3:X6 + X3:X7 + X4:X5 + X4:X6 + X4:X7 + X5:X6 + X5:X7 +
##
      X6:X7
## * covariance model :
    - type : gauss
##
    - nugget : 1e-13
##
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10 1e-10
    - parameters upper bounds : 1.99172 1.986204 1.98205 1.998337 1.996341 1.996626 1.993762
##
##
    - variance bounds : 0.06527738 6.860711
    - best initial criterion value(s): 30.36991
##
##
## N = 8, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f=
                             -30.37 |proj g|=
                                                    1.8271
```

```
1 f =
## At iterate
                              -636.25
                                        |proj g|=
                                                         6.4848
## At iterate
                    f =
                              -890.98
                                        |proj g|=
                                                          6.451
                  3 f =
                              -977.06
                                        |proj g|=
## At iterate
                                                         6.4451
                  4 f =
                              -1176.9
                                                          6.411
## At iterate
                                        |proj g|=
## At iterate
                  5
                     f =
                              -1316.2
                                        |proj g|=
                                                         6.3328
                  6 f =
                              -1338.4
## At iterate
                                        |proj g|=
                                                         6.3085
                  7 f =
                              -1366.5
## At iterate
                                        |proj g|=
                                                         6.2809
## At iterate
                  8 f =
                              -1368.6
                                        |proj g|=
                                                         6.2739
## At iterate
                 9 f =
                              -1375.9
                                        |proj g|=
                                                         6.2499
                 10 f =
## At iterate
                              -1376.7
                                        |proj g|=
                                                          6.247
## At iterate
                 11 f =
                              -1377.8
                                        |proj g|=
                                                         6.2417
                 12 f =
                              -1378.7
                                                          6.237
## At iterate
                                        |proj g|=
                                        |proj g|=
## At iterate
                 13 f =
                                -1379
                                                         6.2361
                              -1379.2
                                                         6.2327
## At iterate
                14 f =
                                        |proj g|=
## At iterate
                15 f =
                              -1379.5
                                        |proj g|=
                                                         6.2261
## At iterate
                 16
                     f =
                              -1380.2
                                        |proj g|=
                                                         6.1986
                    f =
## At iterate
                 17
                              -1381.7
                                        |proj g|=
                                                         6.1348
## At iterate
                 18
                    f =
                              -1383.6
                                                         5.9608
                                        |proj g|=
                                -1384
## At iterate
                 19 f =
                                        |proj g|=
                                                         1.6218
                                        |proj g|=
## At iterate
                 20
                     f =
                              -1387.3
                                                         3.8472
## At iterate
                 21 f =
                              -1387.9
                                        |proj g|=
                                                         5.8113
## At iterate
                 22
                    f =
                              -1387.9
                                                         1.7441
                                        |proj g|=
## At iterate
                 23 f =
                              -1387.9
                                        |proj g|=
                                                         1.3915
## At iterate
                 24 f =
                              -1387.9
                                                        0.62138
                                        |proj g|=
## At iterate
                 25 f =
                              -1387.9
                                        |proj g|=
                                                       0.021347
## At iterate
                 26 f =
                              -1387.9
                                        |proj g|=
                                                      0.0020919
##
## iterations 26
## function evaluations 31
## segments explored during Cauchy searches 33
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 5
## norm of the final projected gradient 0.00209189
## final function value -1387.94
## F = -1387.94
## final value -1387.936669
## converged
print(mean(1R))
```

```
## [1] 0.006683068
```

Dans toutes les méthodes précedentes, avec ou sans cross validation, on obtient une valeur de RMSE de l'ordre de 10^{-3} qui est déjà une valeur très petite par rapport à la moyenne calculée dans la première partie. Pourtant, on va essayer une autre méthode afin de diminuer de plus la valeur RMSE.

8. Régression linéaire

On fait une régression entre y et les 7 variables par une interaction de deuxième ordre afin de voir les variables les moins significatifs

```
library(caret)
## Loading required package: ggplot2
## Loading required package: lattice
# cross validation
train_control <- trainControl(method = "cv",</pre>
                              number = 5)
rlm=lm(y_app~1+.+.^2, data=X_app,trControl = train_control)
## Warning: In lm.fit(x, y, offset = offset, singular.ok = singular.ok, ...) :
## extra argument 'trControl' will be disregarded
summary(rlm)
##
## Call:
## lm(formula = y_app ~ 1 + . + .^2, data = X_app, trControl = train_control)
##
## Residuals:
##
      Min
                1Q Median
                                ЗQ
                                       Max
## -2.1897 -0.5795 -0.1202 0.5229
##
## Coefficients:
##
                Estimate Std. Error t value Pr(>|t|)
## (Intercept) 54.56261
                            0.50275 108.528 < 2e-16 ***
## X1
                            0.52431 21.462 < 2e-16 ***
               11.25255
                            0.55493 -23.567 < 2e-16 ***
## X2
              -13.07802
## X3
                 0.08913
                            0.54720
                                     0.163
                                             0.8707
## X4
                 0.18531
                            0.51606
                                      0.359
                                              0.7197
## X5
                 5.02738
                            0.53714
                                      9.360 < 2e-16 ***
## X6
              -12.68135
                            0.51783 -24.489 < 2e-16 ***
                                    -0.764
## X7
                -0.44855
                            0.58679
                                              0.4450
                            0.44926 -9.900 < 2e-16 ***
## X1:X2
               -4.44755
## X1:X3
                -0.51295
                            0.43528 - 1.178
                                              0.2392
## X1:X4
                            0.43289 -1.217
                                              0.2241
                -0.52687
## X1:X5
                -0.18644
                            0.44295 -0.421
                                              0.6740
## X1:X6
                -0.02597
                            0.41385 -0.063
                                              0.9500
## X1:X7
                0.41368
                            0.44917
                                    0.921
                                              0.3575
## X2:X3
                0.11868
                            0.43086
                                    0.275
                                              0.7831
## X2:X4
                                    0.877
                                              0.3808
                 0.37899
                            0.43207
## X2:X5
                 0.96356
                            0.45311
                                    2.127
                                              0.0339 *
## X2:X6
                 0.96824
                            0.43251
                                      2.239
                                              0.0256 *
## X2:X7
                            0.45124
                                     1.627
                                              0.1044
                 0.73401
## X3:X4
                            0.42241 -0.363
                -0.15315
                                              0.7171
## X3:X5
                                    0.076
                0.03389
                            0.44756
                                              0.9397
## X3:X6
                0.42932
                            0.42944
                                     1.000
                                              0.3179
## X3:X7
                -0.29994
                            0.44474 -0.674
                                              0.5003
## X4:X5
                0.08462
                            0.43857
                                      0.193
                                              0.8471
```

0.4004

0.42112 -0.842

X4:X6

-0.35441

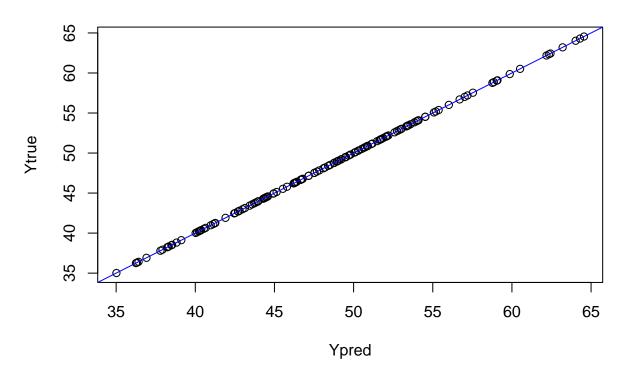
```
## X4:X7
               -0.17403
                          0.44490 -0.391
                                           0.6958
## X5:X6
               -4.03578
                          0.41570 -9.708 < 2e-16 ***
## X5:X7
                          0.43565 -0.423 0.6726
               -0.18418
## X6:X7
                2.48691
                          0.43112 5.768 1.37e-08 ***
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.8149 on 521 degrees of freedom
## Multiple R-squared: 0.9838, Adjusted R-squared: 0.9829
## F-statistic: 1129 on 28 and 521 DF, p-value: < 2.2e-16
```

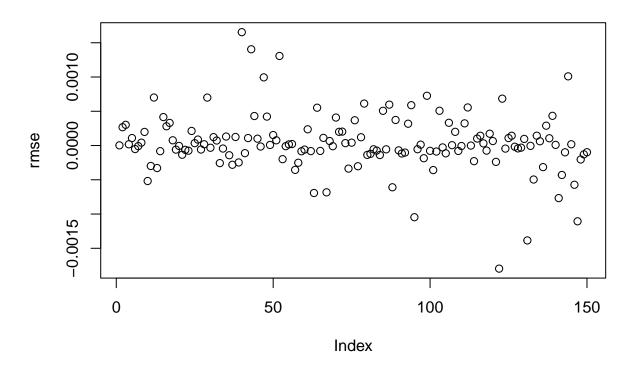
On voit clairement que les variables X3 et X4 sont très peu significatives étant avoir une p_valeur>0.05 et très peu influentes (beta petits par rapport aux autres paramètres). On chosisit du coup d'enlever ces variable et refaire le krigeage avec les 5 autres, en ajoutant les interaction significatifs.

```
X_{app1}=X_{app}[, c(-3, -4)]
X_{\text{test1}}=X_{\text{test}}[, c(-3, -4)]
famille="matern5 2"
 \text{Model} \leftarrow \text{km}(\text{formula} = \text{$^{1+.+.^2+I}(X2^2)+I(X6^2)+I(X5^2)+I(X1^2)-X1:X6-X3:X5-X4:X5-X2:X3-X4:X7, design} = \text{$^{1+.+.^2+I}(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6^2)+I(X6
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!
##
## optimisation start
## -----
## * estimation method
                                                            : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X5 + X6 + X7 + I(X2^2) + I(X6^2) + I(X5^2) + I(X1^2) +
                 X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
##
##
                 X6:X7
## * covariance model :
##
           - type : gauss
##
            - nugget : NO
            - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10
              - parameters upper bounds : 1.99172 1.998102 1.996341 1.992466 1.993762
##
            - best initial criterion value(s): 4.04318e-07
##
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                                            0 f= 4.0432e-07 |proj g|=
                                                                                                                             3.2064e-06
## At iterate
                                             1 f =
                                                                     4.043e-07 | proj g|=
                                                                                                                                  3.2062e-06
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 3.20619e-06
## final function value 4.04304e-07
##
```

```
## F = 4.04304e-07
## final value 0.000000
## converged

pred <- predict(object = Model, newdata = X_test1, type="UK" , checkNames=FALSE, se.compute=TRUE)
Mean<-pred $mean
rmse(y_test,Mean, trace=TRUE)</pre>
```





[1] 0.0004244927

avec Cross Validation

```
Observations(sample(nrow(Observations)),]
#Create 10 equally size folds
folds <- cut(seq(1,nrow(Observations)),breaks=5,labels=FALSE)</pre>
1R < -seq(1,5)
#Perform 10 fold cross validation
for(i in 1:5){
       #Segement your data by fold using the which() function
       testIndexes <- which(folds==i,arr.ind=TRUE)</pre>
       y_app_cv<-Observations[-testIndexes,8]</pre>
       X_app_cv<-Observations[-testIndexes,1:p]</pre>
       y_test_cv<-Observations[testIndexes,8]</pre>
       X_test_cv<-Observations[testIndexes,1:p]</pre>
       X_app1_cv=X_app_cv[, c(-3, -4)]
       X_{\text{test1_cv}} = X_{\text{test_cv}} [, c(-3, -4)]
       famille="matern5_2"
        \label{eq:model} \mbox{Model} <-\mbox{km(formula} = \mbox{$^{-1}$+.+.$^2$+$I(X2^2)$+$I(X6^2)$+$I(X5^2)$+$I(X1^2)$-$X1:X6$-$X3:X5$-$X4:X5$-$X2:X3$-$X4:X7$, design a sign of the context of the context
       pred <- predict(object = Model, newdata = X_test1_cv, type="UK" , checkNames=FALSE, se.compute=TRUE)</pre>
      Mean <- pred $mean
```

```
1R[i] <- rmse(y_test_cv,Mean)</pre>
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!
##
## optimisation start
## -----
## * estimation method
                        : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ^{X1} + ^{X2} + ^{X5} + ^{X6} + ^{X7} + ^{I}(^{X2}^2) + ^{I}(^{X6}^2) + ^{I}(^{X5}^2) + ^{I}(^{X1}^2) +
       X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
##
##
       X6:X7
## * covariance model :
##
    - type : gauss
##
   - nugget : NO
   - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10
     - parameters upper bounds : 1.985485 1.998102 1.996341 1.996244 1.993762
##
     - best initial criterion value(s): 3.372999e-07
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                  0 f=
## At iterate
                           3.373e-07 |proj g|= 7.2838e-06
## At iterate
                  1 f =
                           3.3724e-07 | proj g|=
                                                   7.2828e-06
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 7.28283e-06
## final function value 3.37244e-07
##
## F = 3.37244e-07
## final value 0.000000
## converged
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!
##
## optimisation start
## -----
## * estimation method
                        : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ^{X1} + ^{X2} + ^{X5} + ^{X6} + ^{X7} + ^{I}(^{X2}^2) + ^{I}(^{X6}^2) + ^{I}(^{X5}^2) + ^{I}(^{X1}^2) +
       X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
##
       X6:X7
##
## * covariance model :
```

```
##
    - type : gauss
##
    - nugget : NO
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10
##
     - parameters upper bounds : 1.99172 1.998102 1.996341 1.992466 1.993762
     - best initial criterion value(s): 2.867385e-08
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
               0 f= 2.8674e-08 |proj g|= 1.9465e-07
                 1 f = 2.8673e-08 |proj g|= 1.9466e-07
## At iterate
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 1.9466e-07
## final function value 2.86733e-08
## F = 2.86733e-08
## final value 0.000000
## converged
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!
##
## optimisation start
## * estimation method
                       : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X5 + X6 + X7 + I(X2^2) + I(X6^2) + I(X5^2) + I(X1^2) +
      X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
      X6:X7
##
## * covariance model :
##
   - type : gauss
    - nugget : NO
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10
##
    - parameters upper bounds : 1.99172 1.99367 1.996341 1.996626 1.991921
##
    - best initial criterion value(s): 5.72539e-07
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f = 5.7254e - 07 |proj g| = 8.5069e - 06
                 1 f = 5.7247e-07 |proj g|= 8.5053e-06
## At iterate
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 8.50535e-06
## final function value 5.72469e-07
```

```
##
## F = 5.72469e-07
## final value 0.000001
## converged
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!
## optimisation start
## -----
## * estimation method
                       : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X5 + X6 + X7 + I(X2^2) + I(X6^2) + I(X5^2) + I(X1^2) +
      X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
      X6:X7
##
## * covariance model :
##
   - type : gauss
    - nugget : NO
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10
##
     - parameters upper bounds : 1.989814 1.980276 1.996016 1.996626 1.992937
    - best initial criterion value(s): 4.094824e-08
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
## At iterate
                 0 f= 4.0948e-08 |proj g|=
                                                 7.1621e-07
## At iterate
                 1 f = 4.0947e-08 |proj g|= 7.1619e-07
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 7.16188e-07
## final function value 4.09474e-08
## F = 4.09474e-08
## final value 0.000000
## converged
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!
##
## optimisation start
## * estimation method
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X5 + X6 + X7 + I(X2^2) + I(X6^2) + I(X5^2) + I(X1^2) +
##
      X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
      X6:X7
##
```

```
## * covariance model :
##
     - type : gauss
     - nugget : NO
##
     - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10 1e-10
##
##
     - parameters upper bounds : 1.99172 1.998102 1.993739 1.996626 1.993762
     - best initial criterion value(s): 1.951791e-07
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                                                  2.859e-06
## At iterate
                 0 f= 1.9518e-07 |proj g|=
## At iterate
                 1 f = 1.9517e-07 |proj g|=
                                                   2.8588e-06
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 2.85875e-06
## final function value 1.95171e-07
## F = 1.95171e-07
## final value 0.000000
## converged
print(mean(1R))
```

[1] 0.0004245099

9. Choix de la méthode finale et prédictions

Nous retenons la dernière méthode qui donne un RMSE de l'ordre de 10^{-4} même avec crossValidation.

Pour la prédiction finale, la base d'apprentissage contiendra toute la base de données avec ces 550 observations portant que la base de test contiendra les 150 individus dont on doit prédir leur Y .

```
set.seed(12345)
Observations = read.csv("defi_observations.csv", header = TRUE)
p<-7
n<-550
X_train=Observations[,1:p]
Y_train=Observations[,(p+1)]
X_test2=read.csv("defi_apredire.csv",header=TRUE)
X_t=X_test2[,]
X_train1=X_train[, c(-3, -4)]
X_test2=X_test2[, c(-3, -4)]
famille="matern5_2"
ModelF <- km(formula = ~1+.+.^2+I(X2^2)+I(X6^2)+I(X5^2)+I(X1^2)-X1:X6-X3:X5-X4:X5-X2:X3-X4:X7, design =
## Warning in terms.formula(formula, data = data): 'varlist' has changed (from
## nvar=9) to new 11 after EncodeVars() -- should no longer happen!</pre>
```

```
##
## optimisation start
## -----
## * estimation method
                       : L00
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~X1 + X2 + X5 + X6 + X7 + I(X2^2) + I(X6^2) + I(X5^2) + I(X1^2) +
      X1:X2 + X1:X5 + X1:X7 + X2:X5 + X2:X6 + X2:X7 + X5:X6 + X5:X7 +
##
##
       X6:X7
## * covariance model :
   - type : gauss
##
   - nugget : NO
    - parameters lower bounds : 1e-10 1e-10 1e-10 1e-10
   - parameters upper bounds : 1.99172 1.998102 1.996341 1.996626 1.993762
    - best initial criterion value(s): 5.540233e-08
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At XO, O variables are exactly at the bounds
                                                  3.6147e-07
                 0 f=
                        5.5402e-08 |proj g|=
## At iterate
                 1 f = 5.5402e-08 |proj g|=
## At iterate
                                                   3.6147e-07
##
## iterations 1
## function evaluations 2
## segments explored during Cauchy searches 1
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 0
## norm of the final projected gradient 3.61469e-07
## final function value 5.54016e-08
##
## F = 5.54016e-08
## final value 0.000000
## converged
predF <- predict(object = ModelF, newdata = X_test2, type="UK" , checkNames=FALSE, se.compute=TRUE)</pre>
bestThetaF = coef(ModelF, "range")
sd2F = coef(ModelF, "sd2")
# moyenne krigeage
pred_finale<- predF$mean</pre>
v_Dice <- (predF$sd)^2</pre>
#géneration du la base de prédiction
n_{\text{test}}=150
Predfinale=matrix(0, nrow=n_test, ncol=8)
Predfinale[,1:7]=as.matrix(X_t)
Predfinale[,8] = as.matrix(pred_finale)
Predfinale=as.data.frame(Predfinale)
colnames(Predfinale)=c("X1", "X2", "X3", "X4", "X5", "X6", "X7", "Y")
write.csv(Predfinale, "DefiGroupeSROUR.csv", row.names = FALSE)
#on vérifie que c'est bien lisible
LectureDeMonFichier = read.csv("DefiGroupeSROUR.csv", header = TRUE)
message(ncol(LectureDeMonFichier) == 8, ": bon nombre de colonnes")
```

```
message(nrow(LectureDeMonFichier) == 150, ": bon nombre de lignes")
```

TRUE: bon nombre de lignes

print(LectureDeMonFichier)

```
##
                X1
                            X2
                                        Х3
                                                    X4
                                                                X5
                                                                             X6
## 1
       0.411601309 0.894667082 0.763477052 0.529624839 0.766795721 0.794756301
      0.703325983 \ 0.276269066 \ 0.639110274 \ 0.755133492 \ 0.525654156 \ 0.207658866
##
       0.428880938 0.856445250 0.494293169 0.913113287 0.516348806 0.320523331
##
##
      0.020926437 \ 0.001307846 \ 0.795911017 \ 0.142316077 \ 0.337128106 \ 0.258195351
       0.959199439 0.814550982 0.441762670 0.680214769 0.606672103 0.646589261
##
      0.817537927 0.913834011 0.982690988 0.636652859 0.317443681 0.666416287
##
  6
       0.622883519 0.217458599 0.474901977 0.594381178 0.150970586 0.772329058
##
## 8
      0.134338109 0.515946427 0.294088058 0.965501934 0.510144564 0.628535446
       0.806086040 0.584082038 0.362232656 0.276508078 0.896970342 0.953462048
      0.692783218 0.192636826 0.034217837 0.710073358 0.043380297 0.470089526
## 10
      0.596297865 0.683452528 0.488861019 0.900231653 0.444953818 0.487812820
      0.004953830 0.324407198 0.929781985 0.450156044 0.832097645 0.613418488
      0.709030894 0.664104701 0.897647543 0.509547230 0.166963284 0.428878891
  13
##
      0.519949214 0.144046470 0.019021030 0.121697994 0.202708565 0.374583912
   15
      0.661595809 0.088892540 0.411913071 0.719305859 0.568923868 0.117803665
##
      0.728043630 0.516256936 0.614136651 0.058125504 0.978104395 0.385637579
##
  17
      0.211988267 \ \ 0.369285370 \ \ 0.958712704 \ \ 0.508768995 \ \ 0.482220243 \ \ 0.222000071
##
      0.393297630 0.859088731 0.713796089 0.006810328 0.836232611 0.347318162
      0.099673975 \ 0.902796505 \ 0.364672610 \ 0.932373696 \ 0.214454636 \ 0.072194615
##
  19
##
      0.983029743 0.927529822 0.004050002 0.033721108 0.185642668 0.550041982
      0.748703385 0.417591268 0.353129793 0.047397736 0.216878215 0.253324032
##
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##
  23
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      0.998724761 0.084455822 0.569502471 0.117632811 0.966552276 0.127533981
      ## 25
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      0.350075379 0.160498000 0.049661702 0.413785366 0.675770480 0.148532629
##
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      0.075917175 0.832280834 0.852575900 0.268830310 0.486301845 0.509698773
##
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##
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```
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       0.828923394 \ 0.769049306 \ 0.807887731 \ 0.872223770 \ 0.890707256 \ 0.759304691
       0.645453211 0.302892269 0.616916724 0.194359168 0.773146078 0.020280042
       0.217693194 0.155126530 0.387988219 0.220698333 0.162320791 0.223291317
##
       0.352499263 0.267157064 0.732074833 0.853316235 0.738659525 0.949347803
## 52
       0.201549316 0.933179925 0.150537773 0.989385477 0.642056502 0.386329621
  53
       0.900130307 0.895944321 0.122955907 0.471381604 0.044322344 0.798336108
       0.754018555 \ \ 0.622440270 \ \ 0.230753376 \ \ 0.383924812 \ \ 0.358087872 \ \ 0.627455242
       0.821094877 0.011296893 0.805353787 0.546465619 0.815389625 0.435371363
##
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##
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##
  67
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##
  69
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       0.399392641 0.459283856 0.442235041 0.709771838 0.043106016 0.761138716
       0.459711072 \ 0.997083778 \ 0.722481209 \ 0.425315045 \ 0.241514476 \ 0.609681011
##
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##
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       0.293405992 0.139924661 0.627788353 0.720704145 0.639476709 0.241893880
##
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##
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##
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##
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##
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       0.243596822 0.092823209 0.344732147 0.245568891 0.293250316 0.388979499
       0.029365144 0.226438021 0.506534631 0.069867018 0.523445226 0.814469312
##
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       0.792216022 0.402486092 0.280475911 0.501622726 0.597173909 0.556511827
       0.095025099 0.342687678 0.960758919 0.620007927 0.044998999 0.008262263
##
  86
  87
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       0.253485191 \ 0.733076191 \ 0.460245023 \ 0.054184451 \ 0.293739498 \ 0.849145855
  88
  89
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       0.840303617 \ 0.351478350 \ 0.008984613 \ 0.317251203 \ 0.470077059 \ 0.884161928
##
  90
  91
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##
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##
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```

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## 105 0.584666816 0.590475518 0.733259299 0.878279839 0.471574047 0.673762366
## 106 0.750016854 0.551254706 0.178138885 0.717924527 0.758644631 0.585893066
## 107 0.083689540 0.796656078 0.363375221 0.310102579 0.872793498 0.120634135
## 108 0.734986994 0.524868857 0.483972848 0.905208289 0.921692217 0.073551780
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## 150 0.409642222 0.407943380 0.341650677 0.447098853 0.530168588 0.551152195
##
              Х7
                         Υ
## 1 0.11577590 38.66005
```

```
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```

```
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```

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