# TU: K-Nearest Neighbors

Industrial AI & Automation by Y.K.Kim

Author: Jin Kwak/21900031

Mod: 2024.09.19

## Introduction

Classification with kNN

## Example: Classification Using Nearest Neighbors

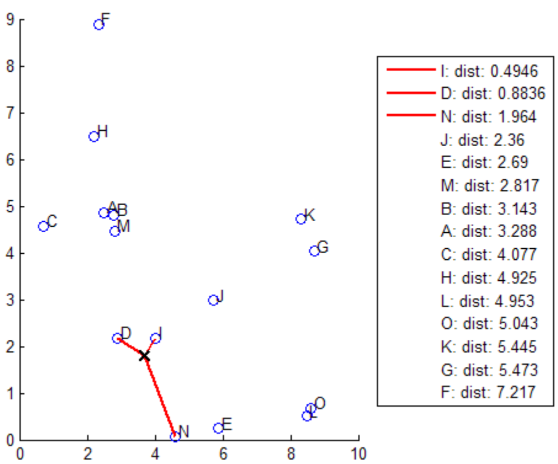
### Distance Metrics

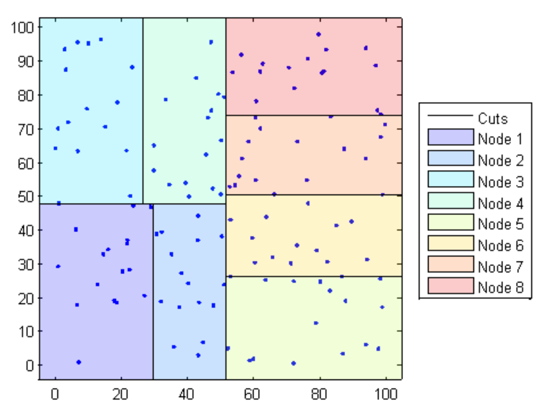
Use `pdist2` to find the distance between a set of data and query points.

- Euclidean distance
- Standardized Euclidean distance
- Mahalanobis distance
- Cosine distance

### *k*-Nearest Neighbor Search and Radius Search

- **Exhaustive Search(default)**
- **Kd-Tree (feature <10)**




Randomly generate normally distributed data into two matrices. The number of rows can vary, but the number of columns must be equal. This example uses 2-D data for plotting.

```
rng(1) % For reproducibility
```

```
% Input Data
X = randn(50,2);

% Query
Y = randn(4,2);

h = zeros(3,1);
figure
h(1) = plot(X(:,1),X(:,2),'bx');
hold on
h(2) = plot(Y(:,1),Y(:,2),'rs','MarkerSize',10);
title('Heterogeneous Data')
```

**Mahalanobis distance**

Find the indices of the three nearest observations in `X` to each observation in `Y`.

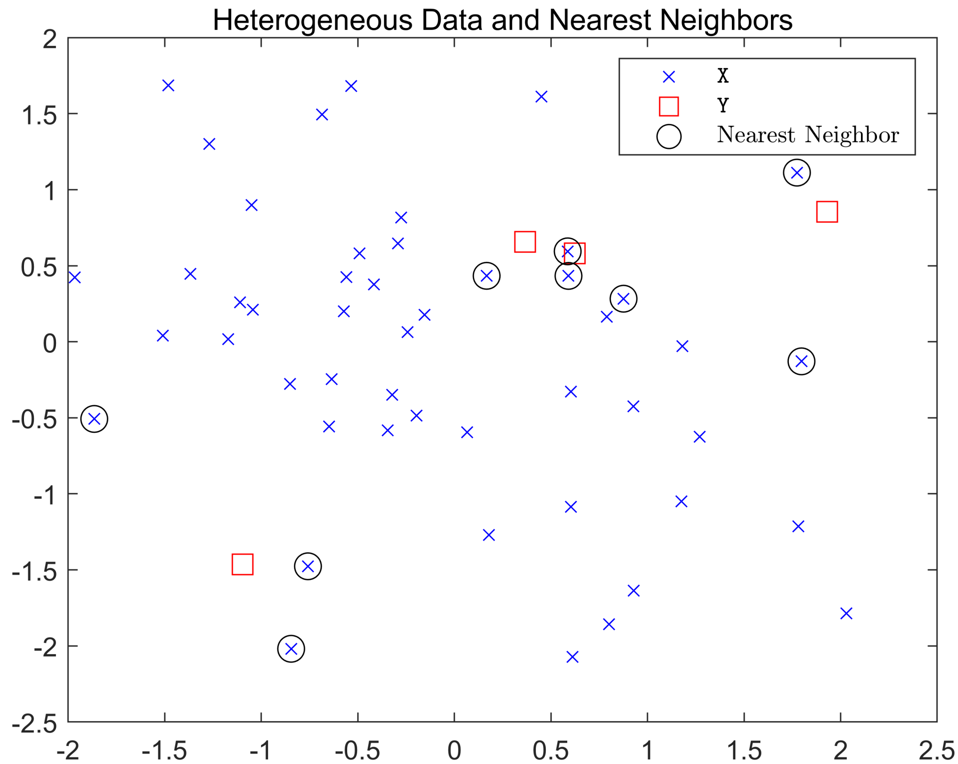
```
k = 3;
[Idx,D] = knnsearch(X,Y,'Distance','mahalanobis','k',k);
```

`idx` and `D` are 4-by-3 matrices.

- `idx(j,1)` is the row index of the closest observation in `X` to observation *j* of `Y`, and `D(j,1)` is their distance.
- `idx(j,2)` is the row index of the next closest observation in `X` to observation *j* of `Y`, and `D(j,2)` is their distance.
- And so on.

Identify the nearest observations in the plot.

```
for j = 1:k
    h(3) = plot(X(Idx(:,j),1),X(Idx(:,j),2),'ko','MarkerSize',10);
end
legend(h,{'\texttt{X}','\texttt{Y}','Nearest Neighbor'},'Interpreter','latex')
title('Heterogeneous Data and Nearest Neighbors')
hold off
```




# Exercise

## Exercise : K-NN Classification with CWRU

### Dataset :  CWRU dataset features

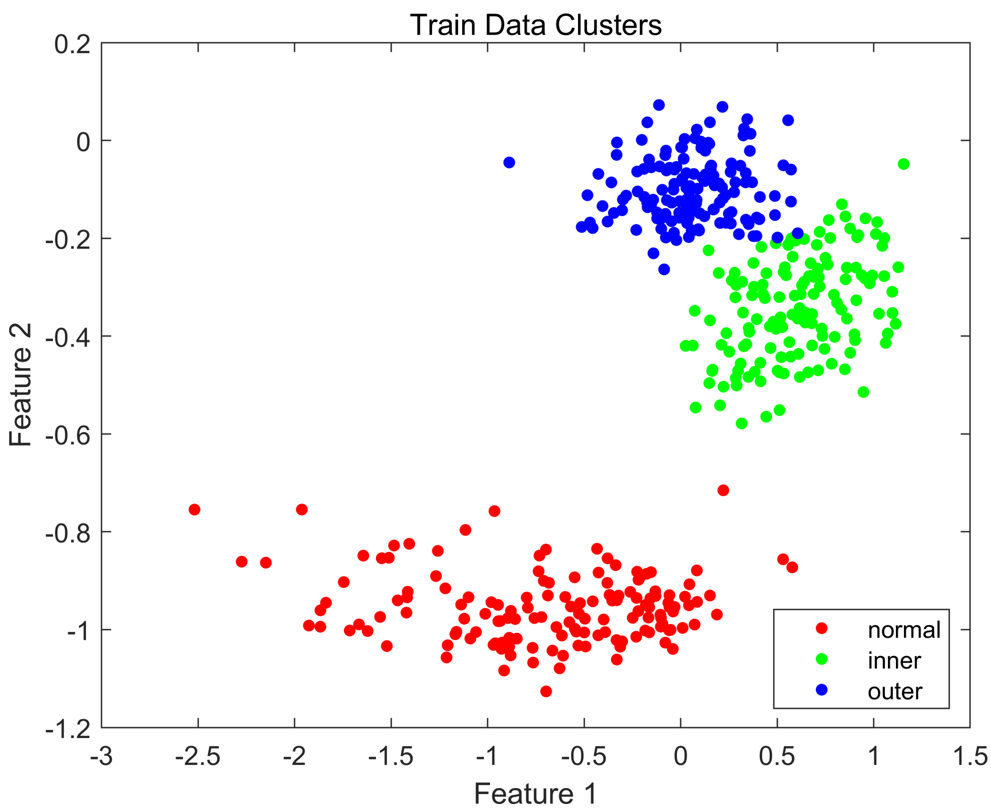
- Given dataset contains many features extracted from CWRU dataset
- We will select 2~3 features for exercise
- Normal,  Outer and Inner Race Fault

```
clear

%% Train
load("../../Dataset/CWRU_selected_Dataset/Feature_data/sample_train.mat");

feature1 = "sv";                    % skewness value of time data
feature2 = "ipf";                   % impulse factor
X(:, 1) = table2array(glob_all_train(:, feature1));
X(:, 2) = table2array(glob_all_train(:, feature2));
Y = class_cwru_train;        % fault class
N = size(X,1);
tbl=table(X(:, 1),X(:, 2),Y);
```

```
%% Test
load("../../Dataset/CWRU_selected_dataset/Feature_data/sample_test.mat");

Xtest(:, 1) = table2array(glob_all_test(:, feature1));
Xtest(:, 2) = table2array(glob_all_test(:, feature2));
Ytest = class_cwru_test;
Ntest=size(Xtest,1);
tblTest=table(Xtest(:, 1),Xtest(:, 2),Ytest);
```

### Plot Test Data

```
figure
gscatter(X(:,1),X(:,2),Y)
title('Train Data Clusters')
xlabel('Feature 1')
ylabel('Feature 2')
```




### KNN Train

Construct the classifier using `fitcknn`.

```
rng(10); % For reproducibility
```

```
Mdl = fitcknn(X, Y)
```

```
Mdl = 
  ClassificationKNN
           ResponseName: 'Y'
  CategoricalPredictors: []
             ClassNames: {'inner'  'normal'  'outer'}
         ScoreTransform: 'none'
        NumObservations: 432
               Distance: 'euclidean'
           NumNeighbors: 1


  Properties, Methods
```

### Training loss (all train set)

Examine the resubstitution loss, which, by default, is the fraction of misclassifications from the predictions of `Mdl`. (For nondefault cost, weights, or priors, see loss.).

```
loss_train = loss(Mdl, X, Y)
```

```
loss_train = 0
```

The classifier predicts incorrectly for 4% of the training data.

### Cross-validation (k-fold)

Construct a cross-validated classifier from the model.

```
cv = cvpartition(Y,'KFold',10)
```

```
cv = 
K-겹 교차 검증 분할
   NumObservations: 432
       NumTestSets: 10
         TrainSize: 389  388  388  389  389  389  389  389  389  389
          TestSize: 43  44  44  43  43  43  43  43  43  43
```

Examine the cross-validation loss, which is the average loss of each cross-validation model when predicting on data that is not used for training.

```
cv_val = crossval(Mdl,'CVPartition',cv);
error  = kfoldLoss(cv_val);
```

The cross-validated classification accuracy resembles the resubstitution accuracy.

Therefore, you can expect `Mdl` to misclassify approximately 4% of new data, assuming that the new data has about the same distribution as the training data.

### Predict test data

Predict the classification of test data

```
predictClass = predict(Mdl, Xtest)
```

```
predictClass = 108×1 cell
'normal'
'normal'
'normal'
'normal'
'normal'
'normal'
'normal'
'normal'
'normal'
'normal'
     ⋮
```

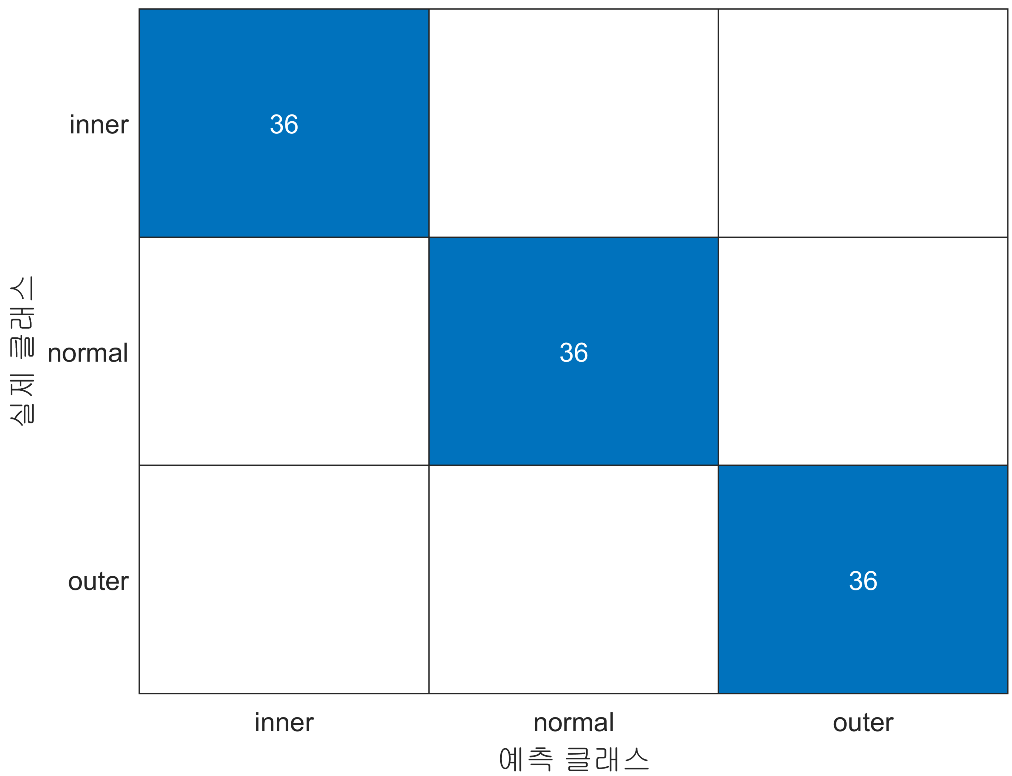
### Calculate the loss  of Test

```
%%% YOUR CODE GOES HERE
loss_test=loss(Mdl, Xtest, Ytest)
```

```
loss_test = 0
```

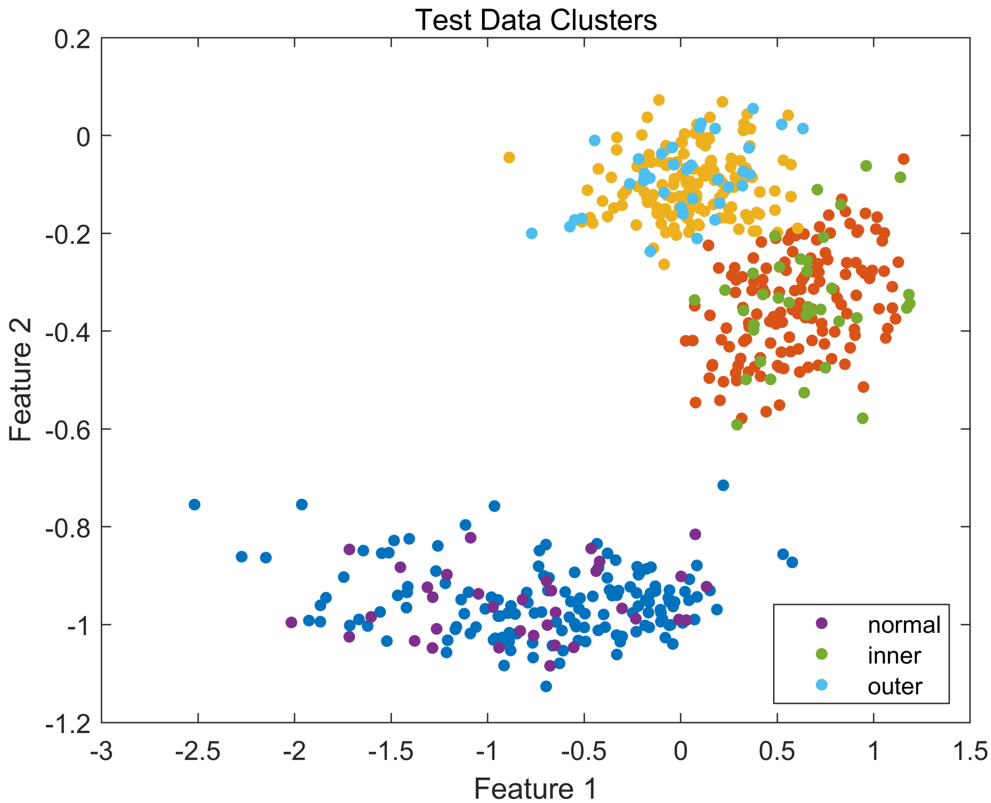
### Plot  Confusion matrix of Test data

```
%%% YOUR CODE GOES HERE
conf_mat = confusionchart(Ytest, predictClass);
```




**Plot Test Results and Misclassified Test data**

```
%%% YOUR CODE GOES HERE
bad = ~strcmp(predictClass,Ytest);
color = lines(6);                % Generate color values
figure
gscatter(X(:,1),X(:,2),Y, color(1:3,:))
hold on
gscatter(Xtest(:,1),Xtest(:,2),Ytest, color(4:6,:))
hold on;
plot(Xtest(bad,1), Xtest(bad,2), 'kx');
hold off;
title('Test Data Clusters')
xlabel('Feature 1')
ylabel('Feature 2')
```

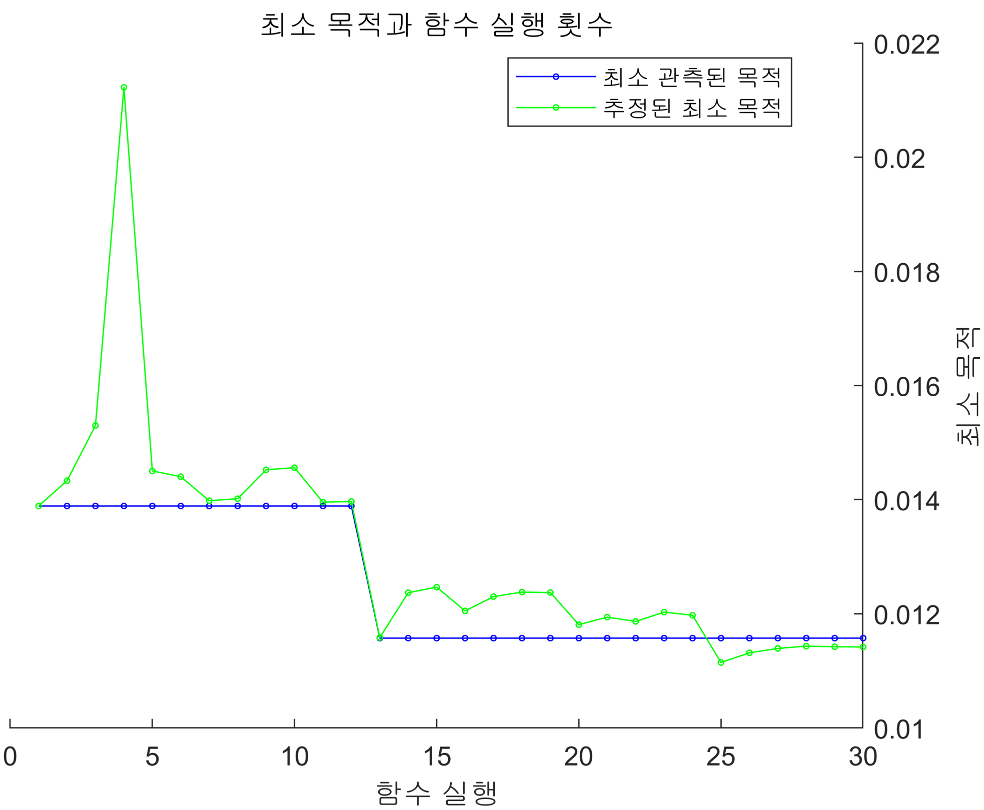


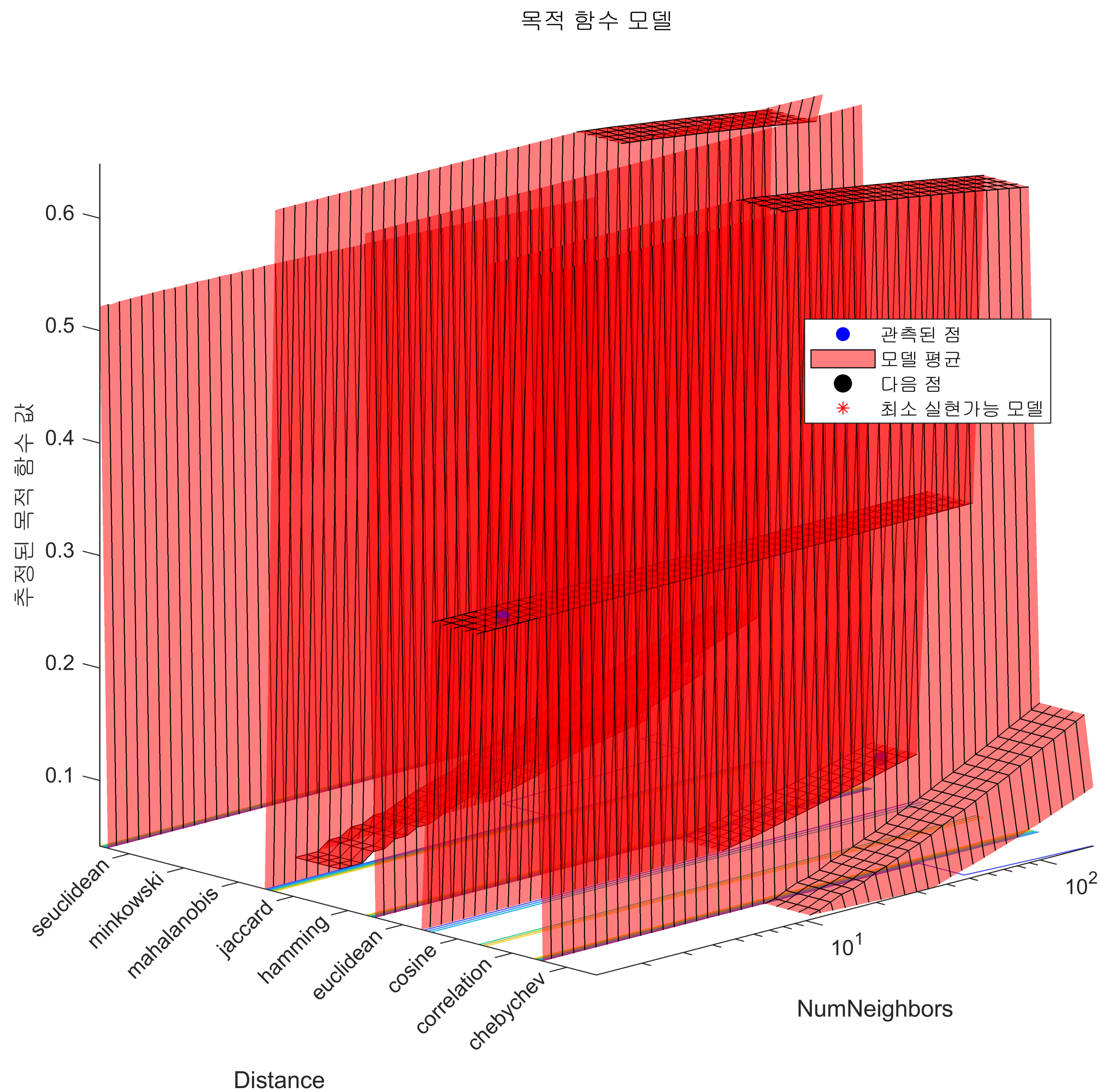

### Optimization of Fitted KNN

```
Mdl = fitcknn(X,Y,'OptimizeHyperparameters','auto',...
    'HyperparameterOptimizationOptions',...
    struct('AcquisitionFunctionName','expected-improvement-plus'))
```

| Iter | Eval result | Objective | Objective runtime | BestSoFar (observed) | BestSoFar (estim.) | NumNeighbors | Distance |
|---|---|---|---|---|---|---|---|
| 1 | Best | 0.013889 | 0.14524 | 0.013889 | 0.013889 | 3 | minkowski |
| 2 | Accept | 0.018519 | 0.064981 | 0.013889 | 0.014332 | 18 | cityblock |
| 3 | Accept | 0.078704 | 0.039656 | 0.013889 | 0.0153 | 141 | euclidean |
| 4 | Accept | 0.31713 | 0.08292 | 0.013889 | 0.021225 | 2 | cosine |
| 5 | Accept | 0.018519 | 0.035891 | 0.013889 | 0.014504 | 2 | minkowski |
| 6 | Accept | 0.05787 | 0.080052 | 0.013889 | 0.014402 | 215 | seuclidean |
| 7 | Accept | 0.11574 | 0.033154 | 0.013889 | 0.013982 | 215 | minkowski |
| 8 | Accept | 0.016204 | 0.036409 | 0.013889 | 0.014017 | 1 | cityblock |
| 9 | Accept | 0.016204 | 0.029888 | 0.013889 | 0.014523 | 1 | seuclidean |
| 10 | Accept | 0.016204 | 0.029157 | 0.013889 | 0.01456 | 3 | chebychev |
| 11 | Accept | 0.16898 | 0.042738 | 0.013889 | 0.013956 | 215 | chebychev |
| 12 | Accept | 0.016204 | 0.030166 | 0.013889 | 0.013967 | 1 | chebychev |
| 13 | Best | 0.011574 | 0.030669 | 0.011574 | 0.011584 | 7 | seuclidean |
| 14 | Accept | 0.66667 | 0.04511 | 0.011574 | 0.01237 | 2 | spearman |
| 15 | Accept | 0.016204 | 0.068493 | 0.011574 | 0.012467 | 1 | mahalanobis |
| 16 | Accept | 0.17824 | 0.03283 | 0.011574 | 0.012051 | 216 | mahalanobis |
| 17 | Accept | 0.66667 | 0.031116 | 0.011574 | 0.012301 | 1 | jaccard |
| 18 | Accept | 0.66667 | 0.034893 | 0.011574 | 0.012381 | 1 | correlation |

```
|   19 | Accept |     0.66667 |    0.033241 |    0.011574 |    0.012373 |          216 |      hamming |
|   20 | Accept |    0.016204 |    0.024817 |    0.011574 |     0.01181 |            1 |    euclidean |
|=====================================================================================================|
| Iter | Eval   | Objective   | Objective   | BestSoFar   | BestSoFar   | NumNeighbors |     Distance |
|      | result |             | runtime     | (observed)  | (estim.)    |              |              |
|=====================================================================================================|
|   21 | Accept |    0.016204 |    0.029917 |    0.011574 |    0.011942 |            1 |    minkowski |
|   22 | Accept |    0.085648 |    0.035829 |    0.011574 |    0.011866 |          215 |    cityblock |
|   23 | Accept |    0.013889 |    0.030008 |    0.011574 |     0.01203 |            4 |    cityblock |
|   24 | Accept |    0.018519 |    0.029724 |    0.011574 |    0.011975 |            4 |    euclidean |
|   25 | Accept |    0.011574 |    0.042631 |    0.011574 |    0.011147 |            4 |   seuclidean |
|   26 | Accept |    0.011574 |    0.031941 |    0.011574 |    0.011317 |            4 |   seuclidean |
|   27 | Accept |    0.011574 |    0.027652 |    0.011574 |    0.011394 |            4 |   seuclidean |
|   28 | Accept |    0.011574 |     0.03311 |    0.011574 |    0.011434 |            4 |   seuclidean |
|   29 | Accept |     0.66667 |    0.027086 |    0.011574 |    0.011423 |            1 |      hamming |
|   30 | Accept |      0.6088 |    0.038803 |    0.011574 |    0.011418 |          216 |  correlation |
```






```
________________________________________________________________
최적화가 완료되었습니다.
MaxObjectiveEvaluations 30회에 도달했습니다.
총 함수 실행 횟수: 30
총 경과 시간: 14.838초
총 목적 함수 실행 시간: 1.2781

최선의 관측된 실현가능점:
    NumNeighbors      Distance
    ____________    __________

         7          seuclidean

관측된 목적 함수 값 = 0.011574
추정된 목적 함수 값 = 0.012228
함수 실행 시간 = 0.030669
```

```
최선의 추정된 실현가능점(모델에 따라 다름):
    NumNeighbors     Distance  
    ____________    __________

         4          seuclidean

추정된 목적 함수 값 = 0.011418
추정된 함수 실행 시간 = 0.03375
Mdl = 
  ClassificationKNN
                         ResponseName: 'Y'
                CategoricalPredictors: []
                           ClassNames: {'inner'  'normal'  'outer'}
                       ScoreTransform: 'none'
                      NumObservations: 432
    HyperparameterOptimizationResults: [1×1 BayesianOptimization]
                             Distance: 'seuclidean'
                         NumNeighbors: 4


  Properties, Methods
```

Compare performance of KNN with other classification methods

KNN: good for low-dimension data (curse of dimensionality)

Training: Lazy Learning Algorithm

Easy to understand but slow for prediction

Depends on number of neighbors or distance