

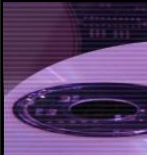
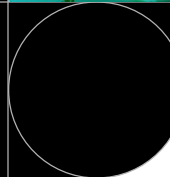
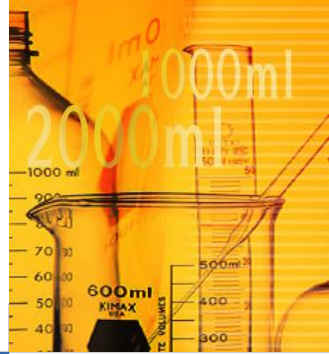
Machine learning

Chapter 7

Model evaluation

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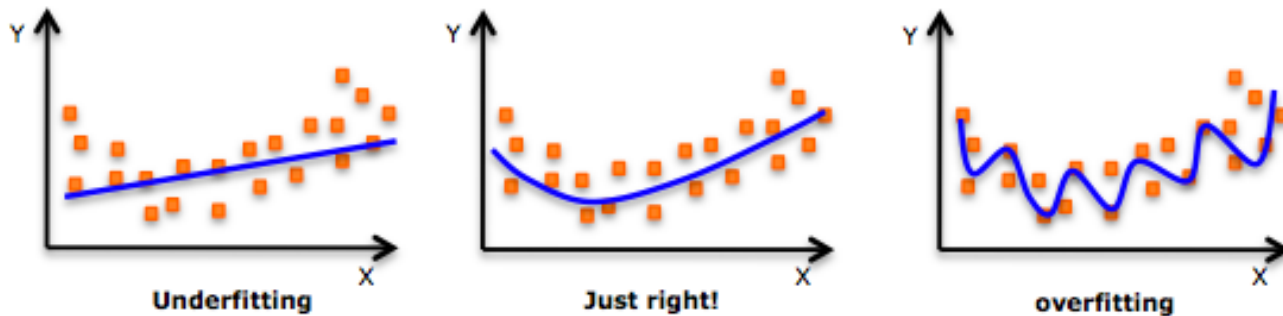
Bio Information Technology Lab.



- Overfitting/underfitting
- error
- K-fold validation
- 모델 개발 절차 정리

Overfitting

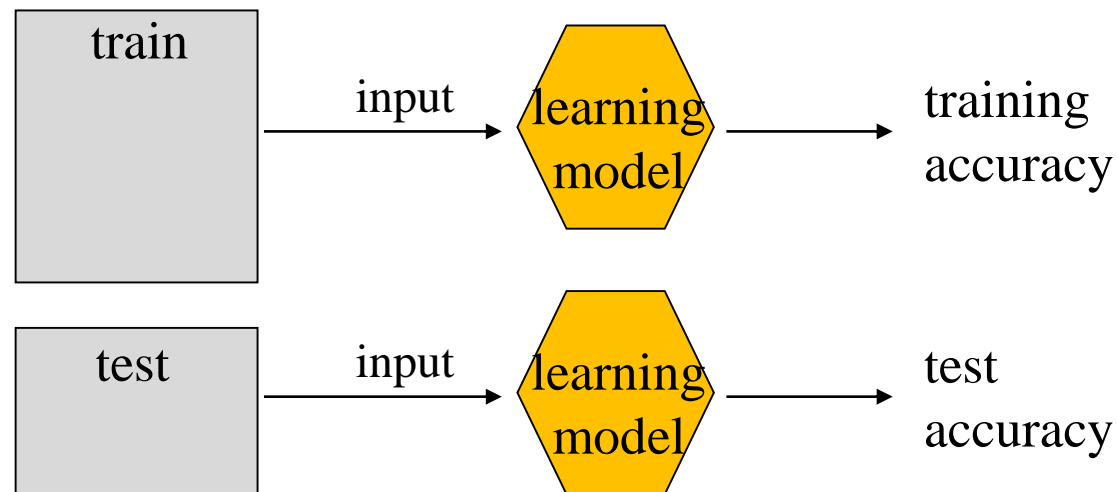
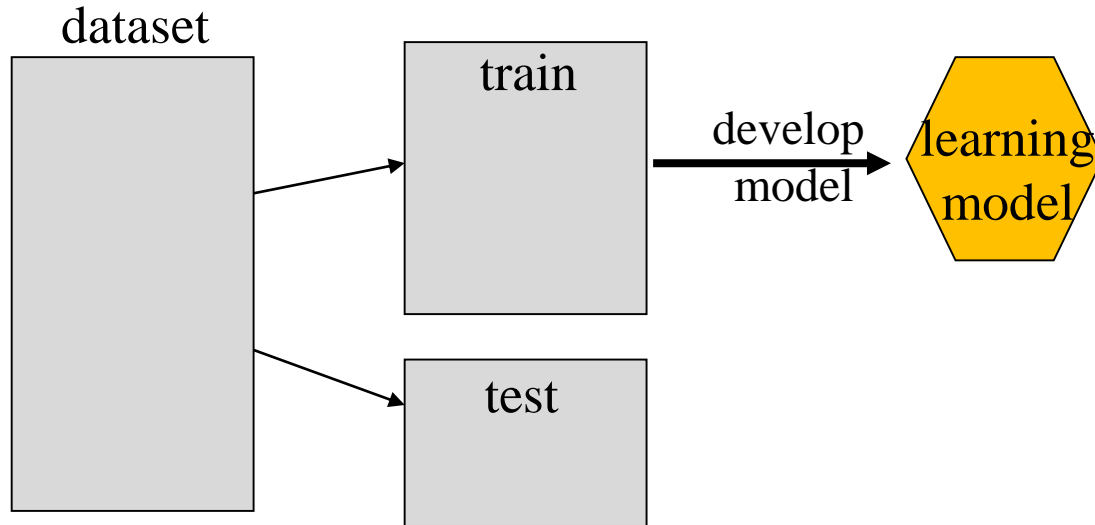
- Overfitting이란 문자 그대로 너무 과도하게 데이터에 대해 모델을 learning을 한 경우를 의미
- 주어진 훈련데이터에 꼭 맞는 모델 생성



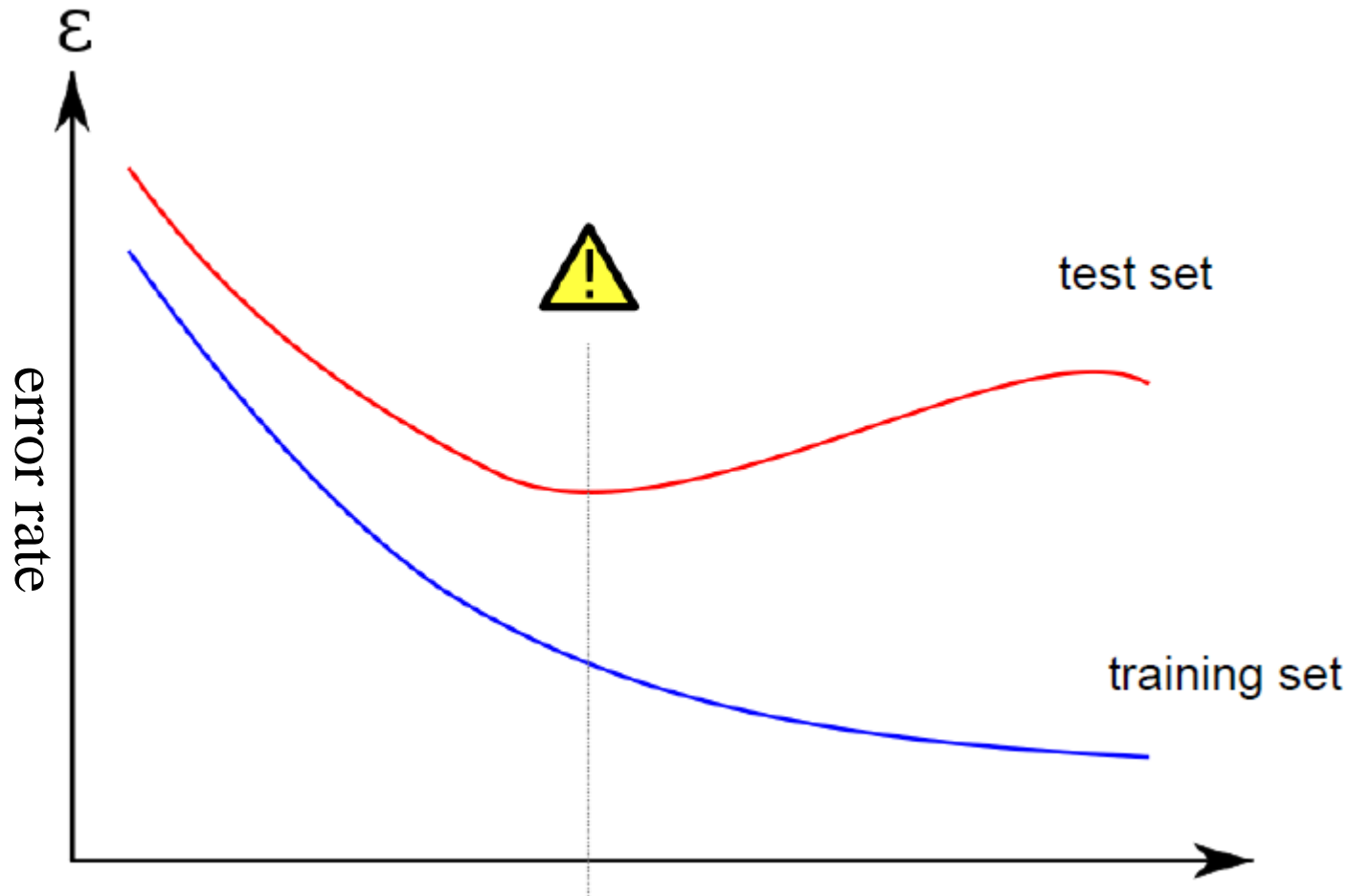
(<http://sanghyukchun.github.io/59/>)

Low error on training data
and high error on test data !

Overfitting



Overfitting



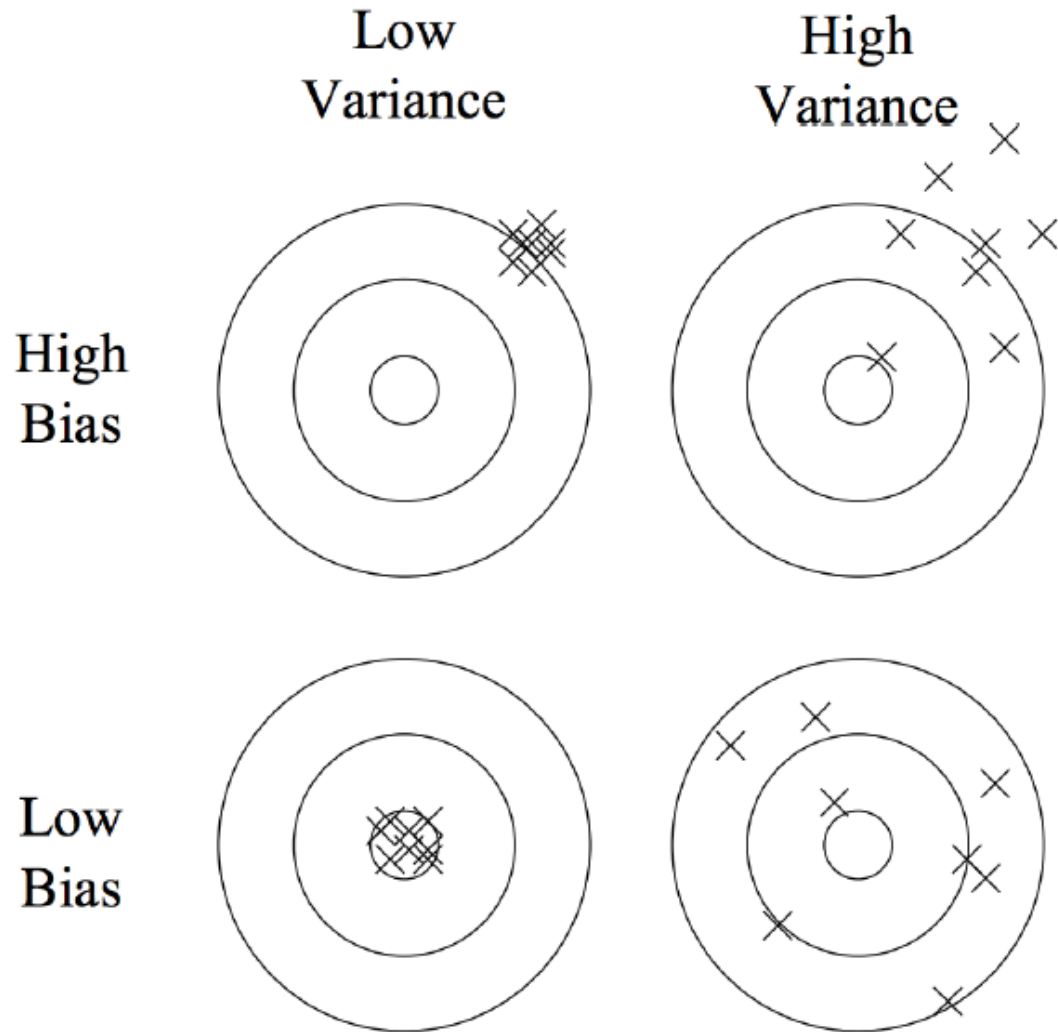
Overfitting

- Variance & Bias : Model 의 error 를 일으키는 요소
- Variance of model : 훈련자료가 바뀌었을 때 모형이 바뀌는 정도 (훈련자료에 대한 모형 변동성)
- Bias of model : 개발된 모형과 실제 모형간의 차이
- Bias-Variance tradeoff
 - 모형에 대한 가정이 약할수록 편향은 작아지고 분산이 커지는 반면, 모형에 대한 가정이 강할수록 편향은 커지고 분산은 줄어든다
- 분산과 편향을 조절하여 최적의 성능을 가지는 모델을 만드는 것이 machine learning 의 과제

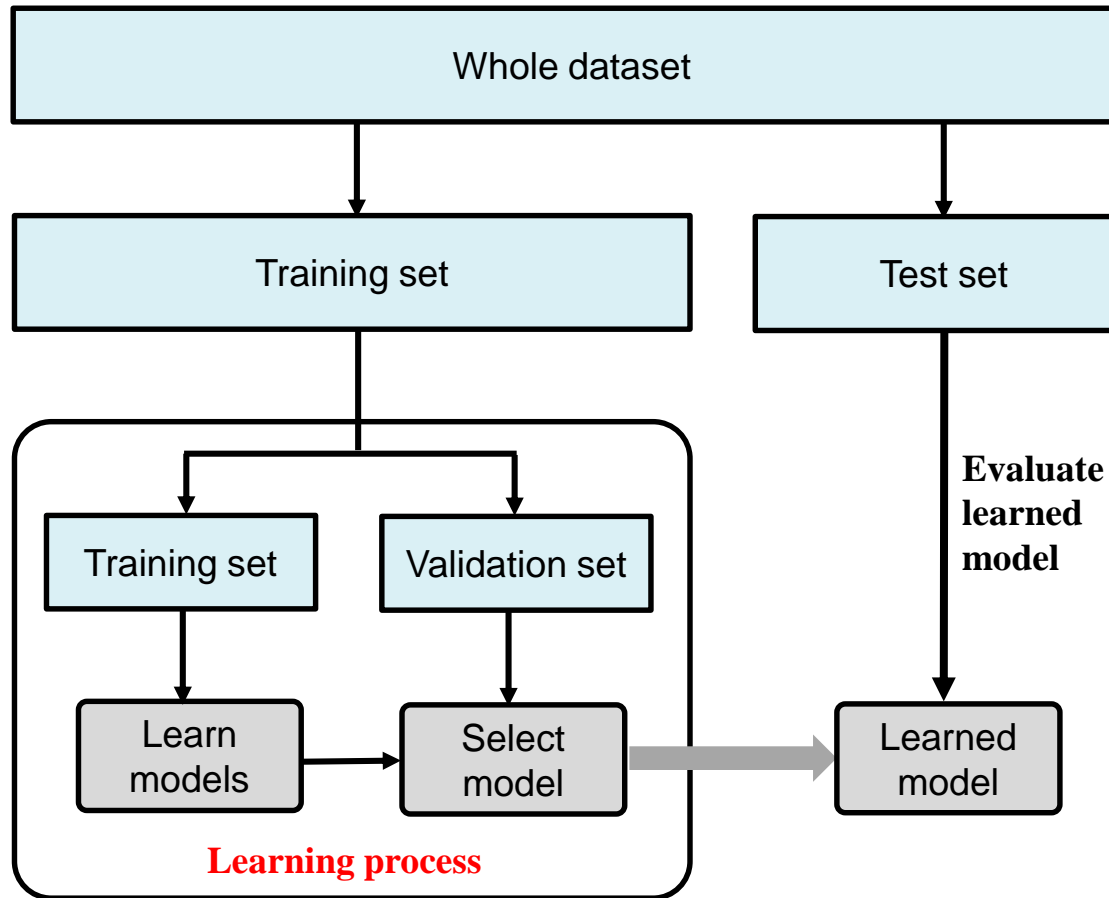
Overfitting

Underfitting:
High Bias
Low Variance

Overfitting:
Low Bias
High Variance



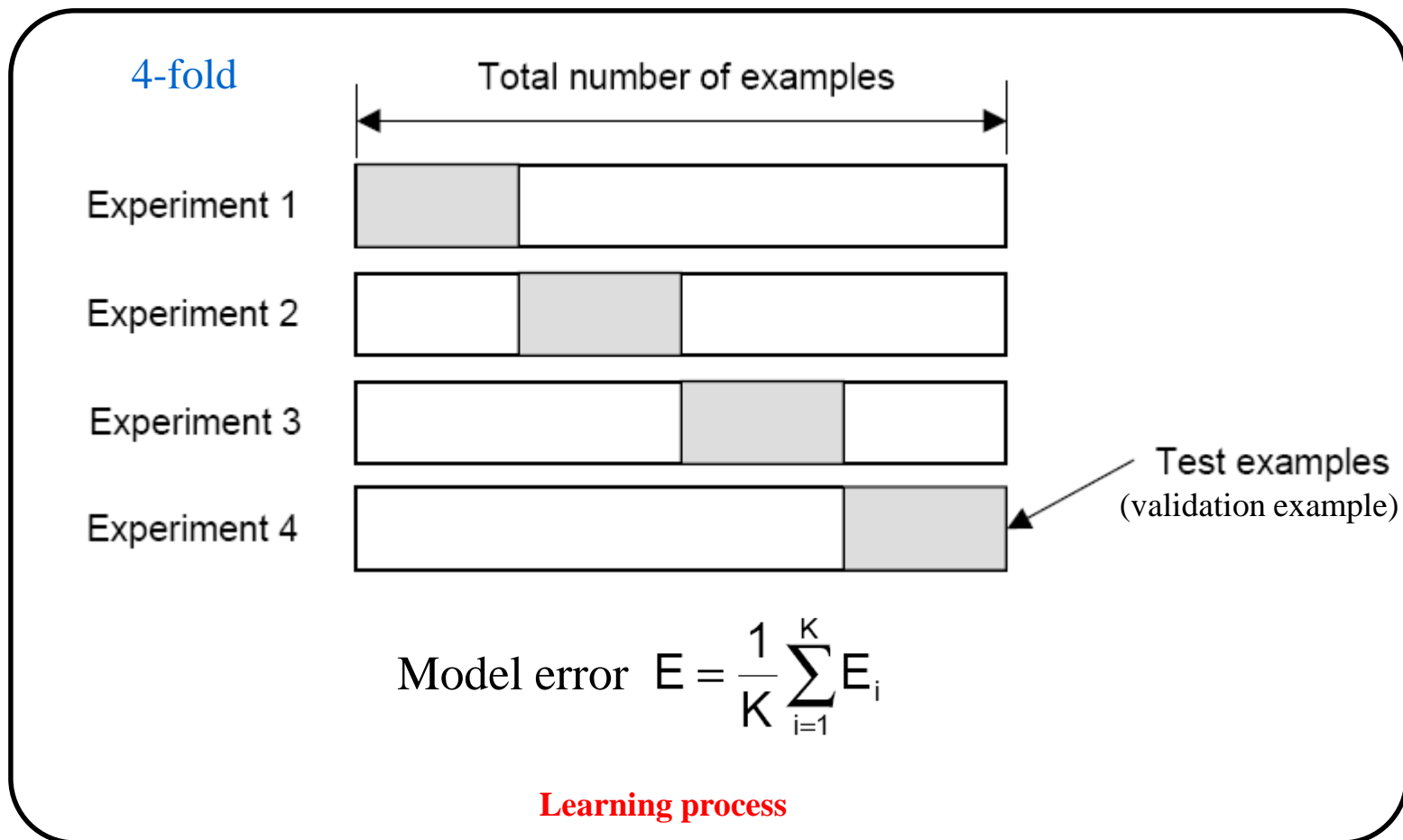
Practical model learning



- Learning process
 - Choose learning algorithm (svm, NN, RF, C5.0, ...)
 - Parameter tuning

Practical model learning

- K-fold cross validation



E 를 가장 작게 만드는 model parameter 를 찾는 것이 learning

- LOOCV (Leave-one-out cross-validation)
 - For each training example (x_i, y_i)
 - Train a classifier with all training data except (x_i, y_i)
 - Test the classifier's accuracy on (x_i, y_i)
 - LOOCV accuracy = average of all n accuracies
 - LOOCV = N -fold cross-validation where N is # of examples

Example

- liver.csv 데이터셋에 대해 SVM learning model 을 만들고 평가
 - SVM 모델의 parameter 중 최적 kernel 과 gamma 값을 결정
 - Use 5-fold cross validation

1. define kfold test function

```
kfold.svm <- function (ds,cl, ker, gam=NULL, fold=5) {  
  library(caret)           # for createFolds  
  library("e1071")         # for SVM  
  
  set.seed(100)  
  k.fold <- createFolds(as.vector(cl),k=fold)  
  cl = factor(cl)  
  acc = c()                # classification result  
  for (i in 1:fold) {  
    this.fold = k.fold[[i]]  
    train.ds = ds[-c(this.fold),]  
    train.cl = cl[-c(this.fold)]  
    test.ds  = ds[c(this.fold),]  
    test.cl  = cl[c(this.fold)]  
    model = NULL  
    if (is.null(gam)) {  
      model = svm(train.ds,train.cl, kernel=ker)  
    } else {  
      model = svm(train.ds,train.cl, kernel=ker, gamma=gam)  
    }  
  
    result = predict(model, test.ds)  
    acc[i] = mean(result==test.cl)  
  
  }  
  print(mean(acc))  
  return(mean(acc))  # average accuracy of k-fold test  
}
```

2. Read dataset

```
setwd("D:/work")  
whole.ds = read.csv("liver.csv")  
str(whole.ds)
```

3. divide train/test dataset

```
tsidx = sample(1:nrow(whole.ds), 100, replace=F)  
train.ds = whole.ds[-tsidx,]  
test.ds  = whole.ds[tsidx,]
```

4. setup candidate kernel and gamma

```
ker = c("linear", "polynomial", "radial", "sigmoid")  
gam = c(1/6, 1/4, 1/8)
```

```
## 5. find best kernel, gamma
```

```
max.acc = 0
```

```
max.ker = 0
```

```
max.gam = 0
```

```
for (k in 1:4) {    # kernel
```

```
  if (k==1) {      # linear kernel
```

```
    acc = kfold.svm(train.ds[, -1], factor(train.ds[, 1]),  
                    ker=ker[k])
```

```
    if (acc > max.acc) {
```

```
      max.acc = acc; max.ker=k; max.gam=0;
```

```
    }
```

```
  next
```

```
}
```

```
for (g in 1:3) {    # gamma
```

```
  acc = kfold.svm(train.ds[, -1], factor(train.ds[, 1]),  
                  ker=ker[k], gam=gam[g])
```

```
  if (acc > max.acc) {
```

```
    max.acc = acc; max.ker=k; max.gam=g;
```

```
  }
```

```
}
```

```
}
```

```
print(max.acc)
print(max.ker)    # 3
print(max.gam)    # 3

## 6. build final model using all train data
model2 = svm(train.ds[,-1],factor(train.ds[,1]),
              kernel=ker[max.ker],gamma=gam[max.gam])

## 7. Evaluate final model
result = predict(model2, test.ds[,-1])
acc= mean(result==test.ds[,1])    # accuracy
acc

# Analysis of prediction result
library(gmodels)
CrossTable(test.ds[,1], result,
            prop.chisq = FALSE, prop.c = FALSE, prop.r = FALSE,
            dnn = c('actual default', 'predicted default'))
```