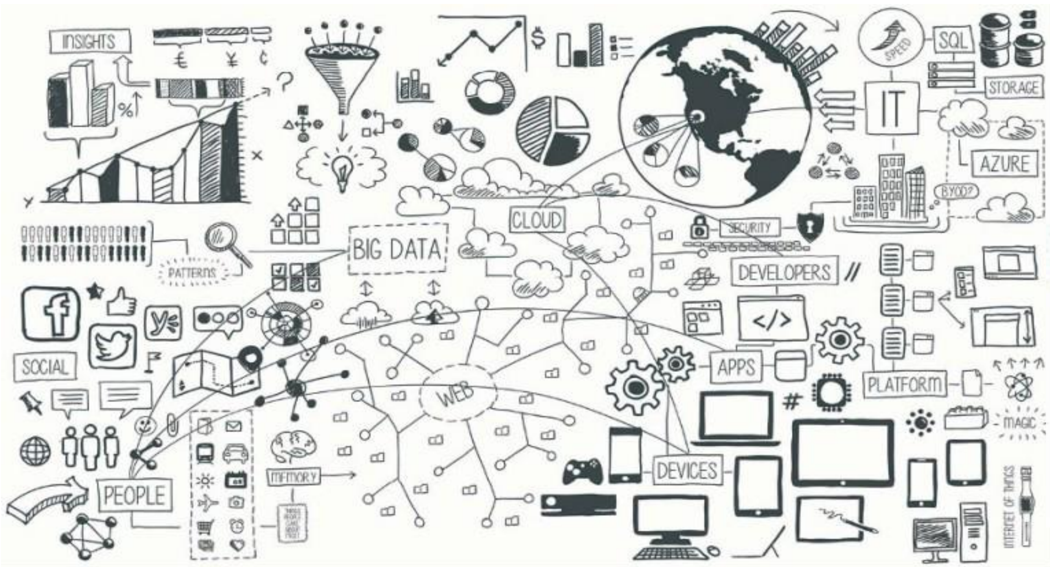
# Data Mining (Minería de Datos)

# The k-NN technique






Rodrigo Manzanas

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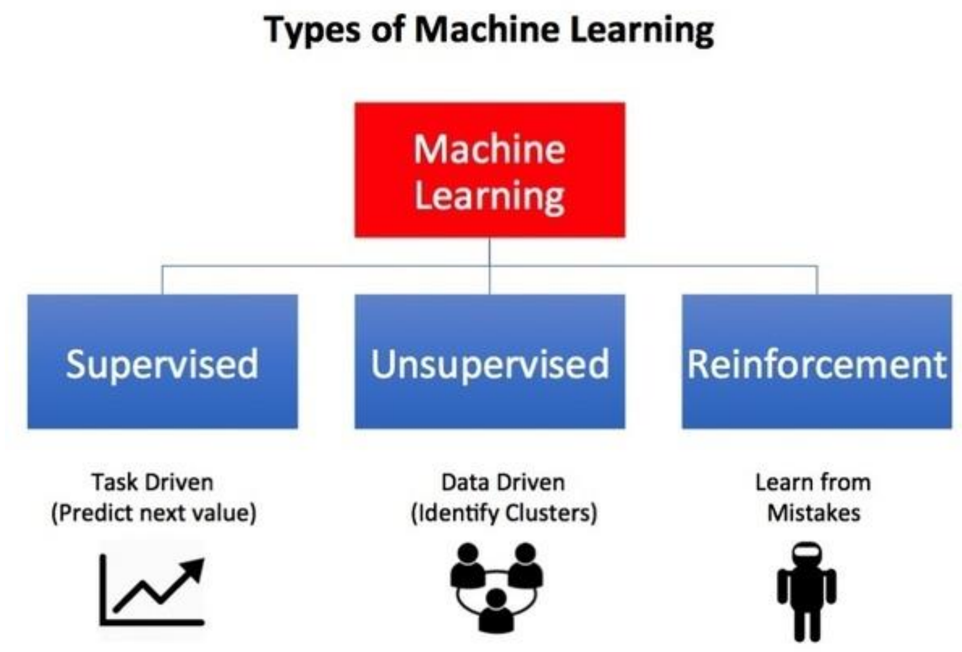
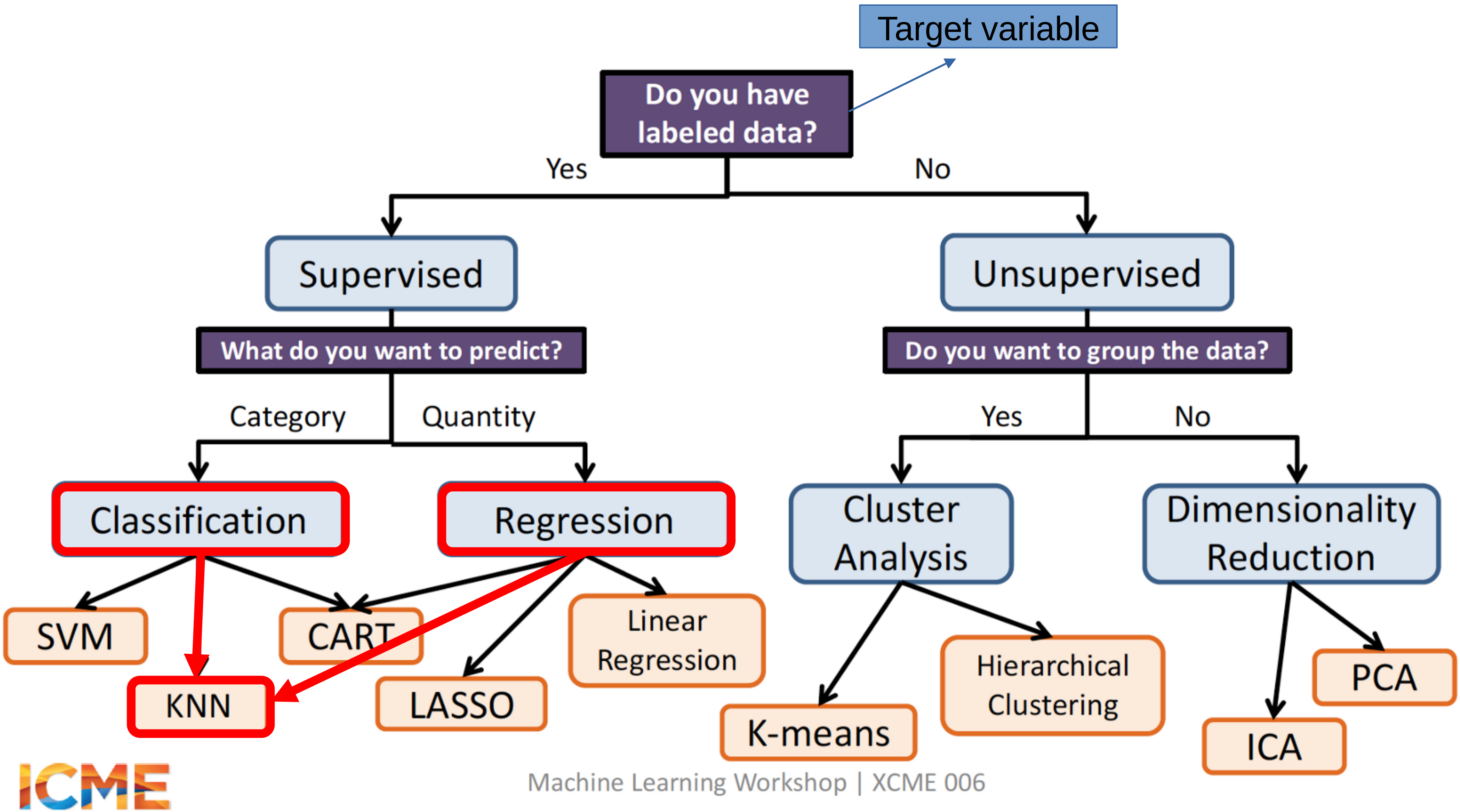


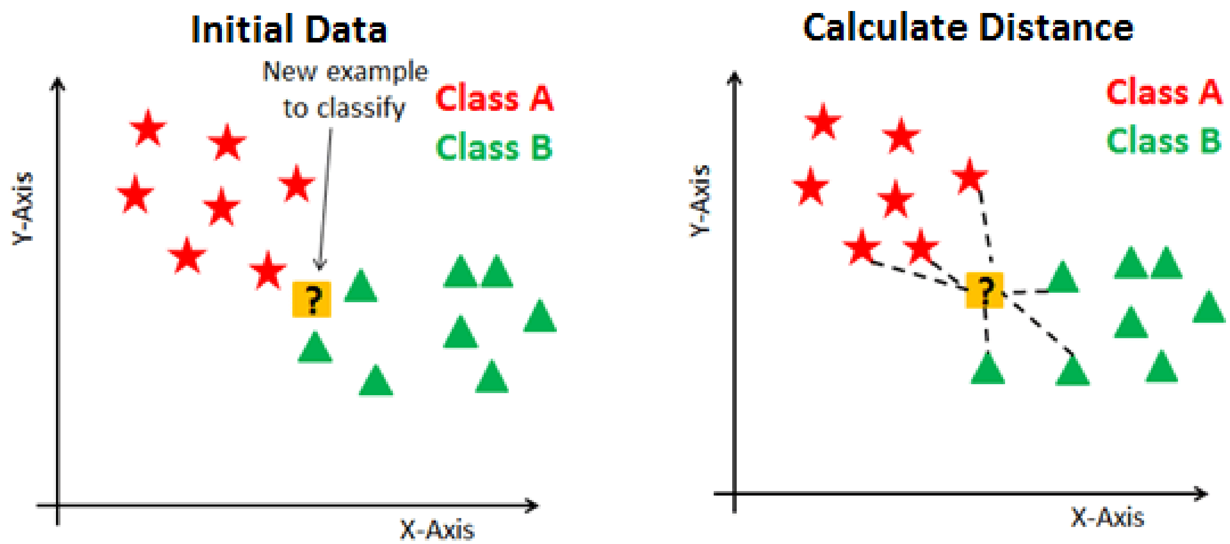

NOTA: Las líneas de código de R en esta presentación se muestran sobre un fondo gris

| | | |
|---|---|---|
| Oct | 30 | Aplazada (sesión de refuezo) |
| Nov | 6 | Presentación, introducción y perspectiva histórica |
| | 8 | Paradigmas, problemas canónicos y data challenges |
| | 13 | Reglas de asociación |
| | 15 | Práctica: Reglas de asociación |
| | 20 | Evaluación, sobreajuste y cross-validación |
| | 22 | Práctica: Cross-validación |
| | 27 | Árboles de clasificación |
| | 29 | Práctica: Árboles de clasificación |
| | | T01. Datos discretos |
| Dic | 4 | Técnicas de vecinos cercano (k-NN) |
| | 11 | Práctica: Vecinos cercanos |
| | 13 | Reducción de dimensión lineal |
| | 18 | Práctica: LDA y PCA |
| | 20 | Reducción no lineal |
| | | T02. Clasificación |
| Ene | 8 | Árboles de clasificación y regresión (CART) |
| | 10 | Práctica: CART |
| | 15 | Ensembles: Bagging and Boosting |
| | 17 | Práctica: Random forests |
| | | T03. Predicción |
| | 22 | Práctica: Gradient boosting |
| | 24a | Técnicas de agrupamiento |
| | 24b | Práctica: Técnicas de agrupamiento |
| | 29a | Práctica: El paquete CARET |
| | 29b | Examen |


Target variable
Do you have labeled data?
Yes
No
Supervised
Unsupervised
What do you want to predict?
Do you want to group the data?
Category
Quantity
Yes
No
Classification
Regression
Cluster Analysis
Dimensionality Reduction
SVM
CART
KNN
LASSO
Linear Regression
K-means
Hierarchical Clustering
PCA
ICA
Machine Learning Workshop | XCME 006

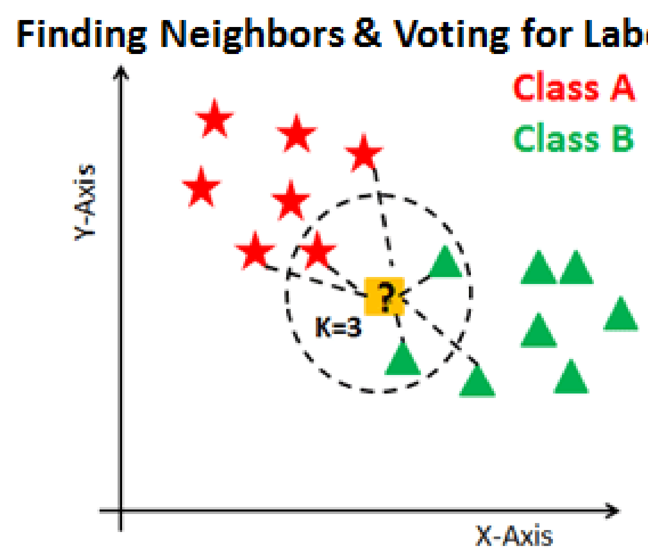
## How does it work?

*"… dime con quién vas y te diré quién eres …"*




**Non-parametric:**
No assumption is made on the underlying data distribution

**Lazy (or instance-based) learning:**
There is no explicit training phase. All the training data is needed during the testing phase



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| … | | | | | |
| 148 | 6.5 | 3.0 | 5.2 | 2.0 | virginica |
| 149 | 6.2 | 3.4 | 5.4 | 2.3 | virginica |
| 150 | 5.9 | 3.0 | 5.1 | 1.8 | virginica |

| 151 | 5.4 | 2.7 | 4.6 | 1.4 | ? |
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*1) Computing distances*

$$d_{151,1} = \sqrt{(5.4-5.1)^2+(2.7-3.5)^2+(4.6-1.4)^2+(1.4-0.2)^2} = 3.52$$

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*3) Classification based on NN*

$\xrightarrow{k = 1}$ *151 = Versicolor*

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*k = 3* → *151 = Versicolor*

**Pros:**

- Easy to understand
- Versatile: Classification and regression problems
- High accuracy (benchmark method)

**Cons**:

- High memory requirements, computationally expensive
- Sensitive to scale of the data
- Can suffer from biases towards skewed distributions
- Performance can be severely degraded in high-dimensional problems

**Applications:**

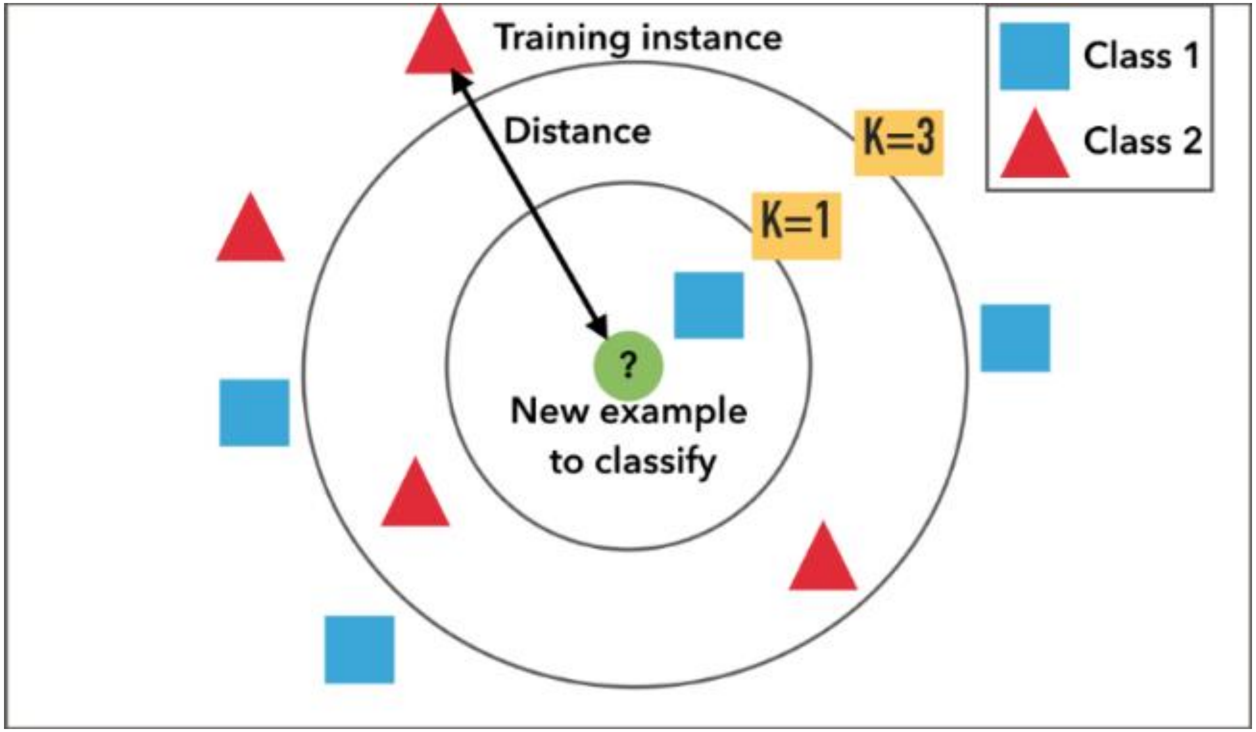
- Economic sciences: concession of loans
- Political sciences: classifying potential voters
- Handwriting detection (e.g. OCR)
- Image/video recognition
- Genetics

# Fitting the method

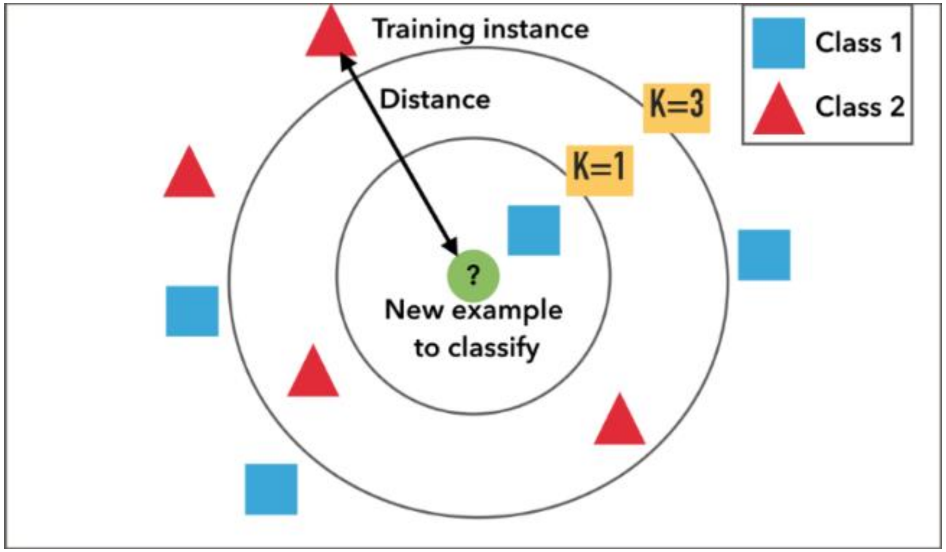
**Distance metric**
Different distances are used, depending on the application. *Euclidean* is the most common

**Number of neighbors (*k*)**
This is the unique model parameter. Must be properly chosen

**Classifying criterion**
- Majority vote
- Weighted vote
- Random
- etc.



# Distance metric




**Minkowsky:**

$$D(\boldsymbol{x},\boldsymbol{y}) = \left( \sum_{i=1}^{m} |x_i - y_i|^r \right)^{1/r}$$

**Euclidean:**

$$D(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

**Manhattan / city-block:**

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} |x_i - y_i|$$

**Camberra:**

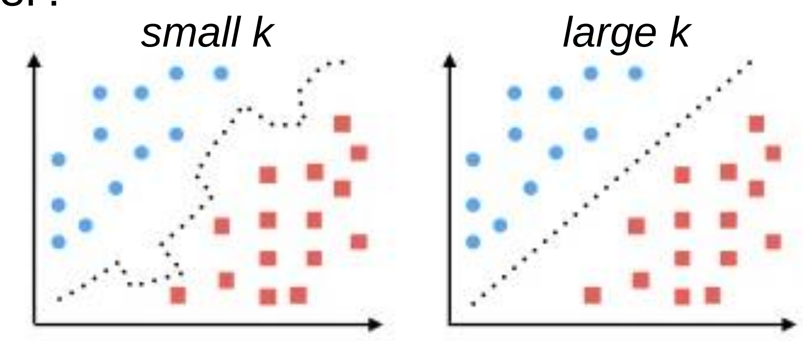
$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{|x_i - y_i|}{|x_i + y_i|}$$

**Chebychev:**

$$D(\boldsymbol{x},\boldsymbol{y}) = \max_{i=1}^{m} |x_i - y_i|$$

# Number of neighbors (*k*)

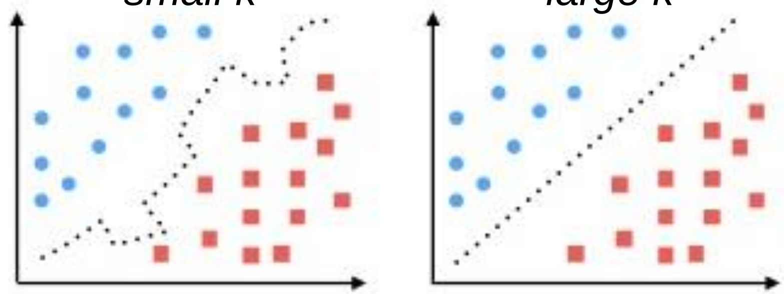
Which one classifies better?



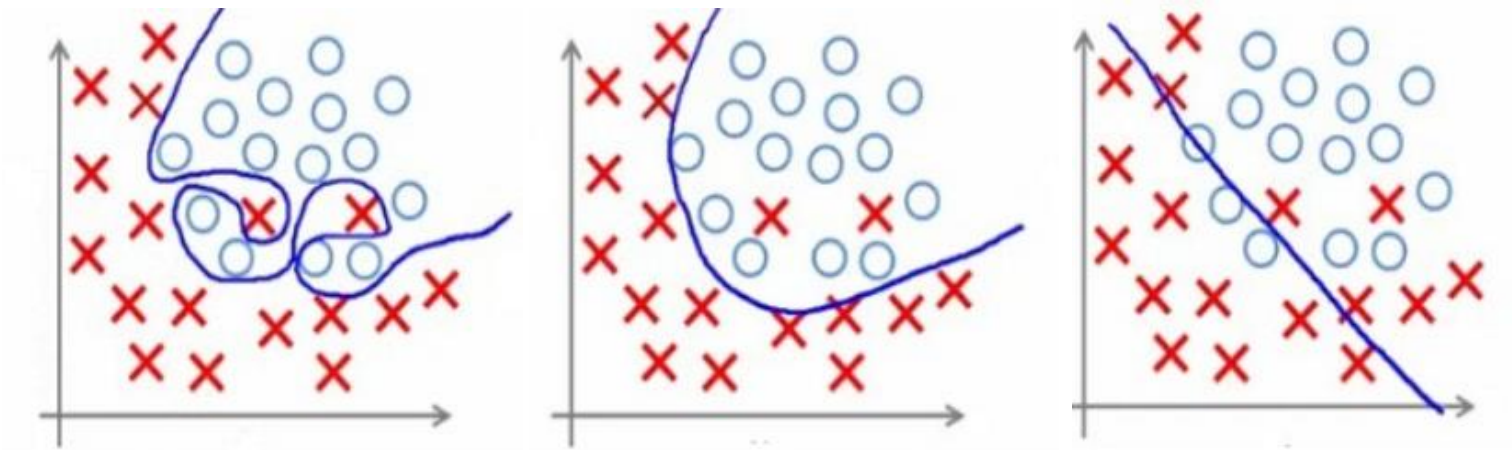
# Number of neighbors (*k*)

Which one classifies better?

*small k* *large k*



*too small k* *optimum k* *too large k*



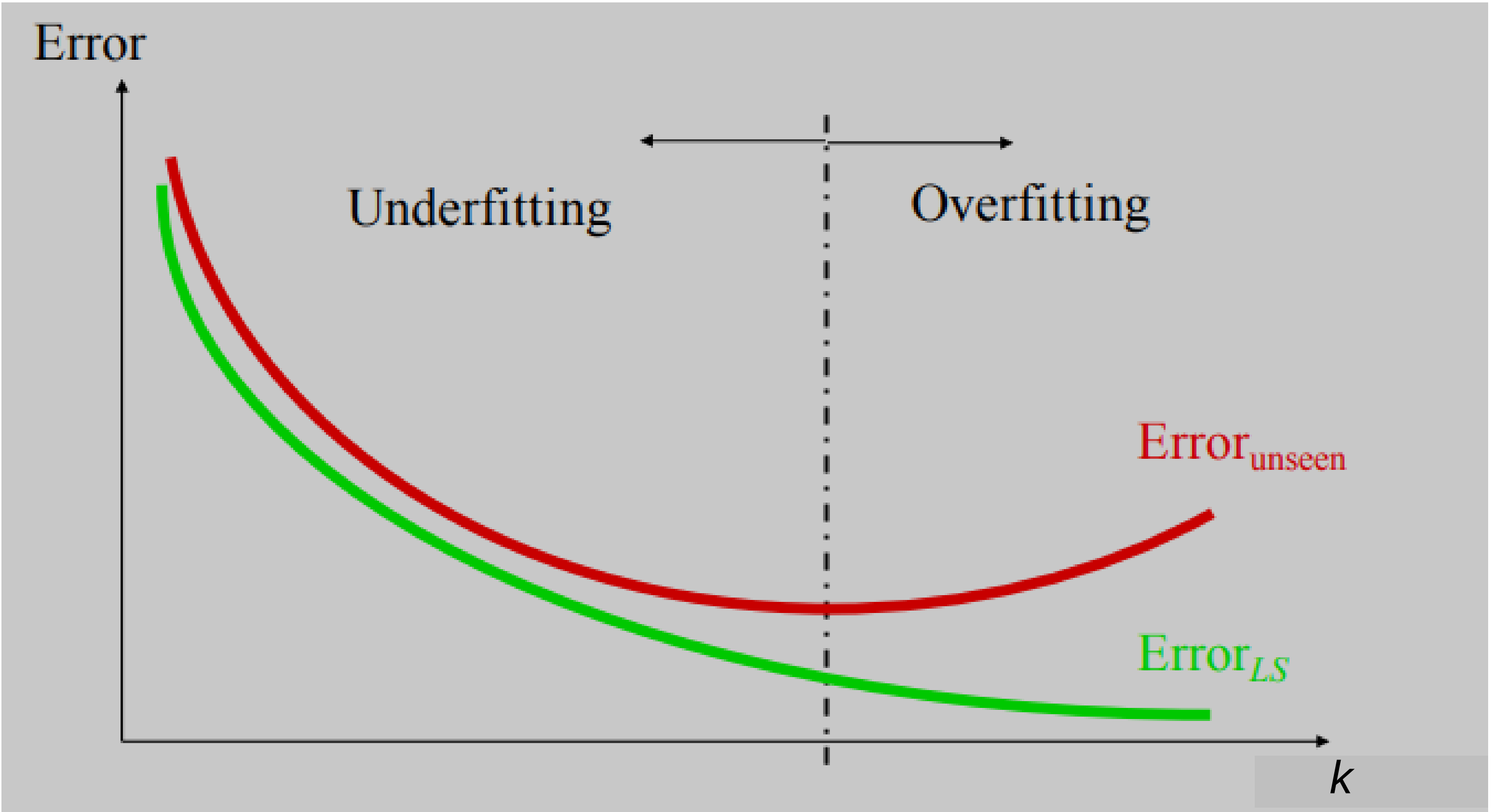
**Over-fitting** **Appropriate-fitting** **Under-fitting**

(forcefitting -- too good to be true)

(too simple to explain the variance)

# Number of neighbors (*k*)

Cross-validation is needed to find the optimal *k*



# Examples in R

*<u>Based on the iris dataset, classify the following new instance:</u>*
*(sepal l., sepal w., petal l., petal w.) = (5.4, 2.7, 4.6, 1.4)*

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# new instance
d.new = c(5.4, 2.7, 4.6, 1.4)
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eucli = c()
for (i in 1:nrow(iris)) {
  eucli[i] = sqrt(sum((d.new - iris[i,-5])^2))
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```

```
# classifying based on the 10 nearest neighbors
pred.k10 = iris$Species[ind.sort$ix[1:10]]
summary(pred.k10)
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## Examples in R

*Divide iris into train y test (75% and 25% of the total dataset, respectively) and find the test error for the nearest neighbor method. Use the function "knn" from package "class"*

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```
# train/test division
n = nrow(iris)
indtrain = sample(1:n, round(0.75*n))
indtest = setdiff(1:n, indtrain)
iris.train = iris[indtrain,]
iris.test = iris[indtest,]
```

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indtrain = sample(1:n, round(0.75*n))
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iris.train = iris[indtrain,]
iris.test = iris[indtest,]
```

```
# classifying using the nearest neighbor method
library(class)
pred = knn(train = iris.train[,-5], test = iris.test[,-5], cl = iris.train$Species, k = 1)
```

# Examples in R

*Divide iris into train y test (75% and 25% of the total dataset, respectively) and find the test error for the nearest neighbor method. Use the function “knn” from package “class”*

```
# train/test division
n = nrow(iris)
indtrain = sample(1:n, round(0.75*n))
indtest = setdiff(1:n, indtrain)
iris.train = iris[indtrain,]
iris.test = iris[indtest,]
```

```
# classifying using the nearest neighbor method
library(class)
pred = knn(train = iris.train[,-5], test = iris.test[,-5], cl = iris.train$Species, k = 1)
```

```
# validating method
table(pred, iris.test$Species)
pred         setosa versicolor virginica
  setosa         11          0         0
  versicolor      0         14         1
  virginica       0          1        11
acc.class(pred, iris.test$Species)
```

```
# evaluation function
acc.class = function(x, y) {
  stopifnot(length(x) == length(y))
  return(sum(diag(table(x, y))) / length(x))
}
```

## Examples in R

*Use the package "caret" (method "knn") to find the optimal k. To do so, check how the test error varies with increasing k (for values from 1 to 50) under a hold-out cross-validation scheme.*

```
library(caret)
# defining hold-out cross-validation
trctrl = trainControl(method = "cv", number = 2)
# searching the optimal k
knn.fit = train(Species ~ ., iris.train,
                method = "knn",
                trControl = trctrl,
                tuneGrid = expand.grid(k = 1:50))
plot(knn.fit)
```

)

# Examples in R

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```

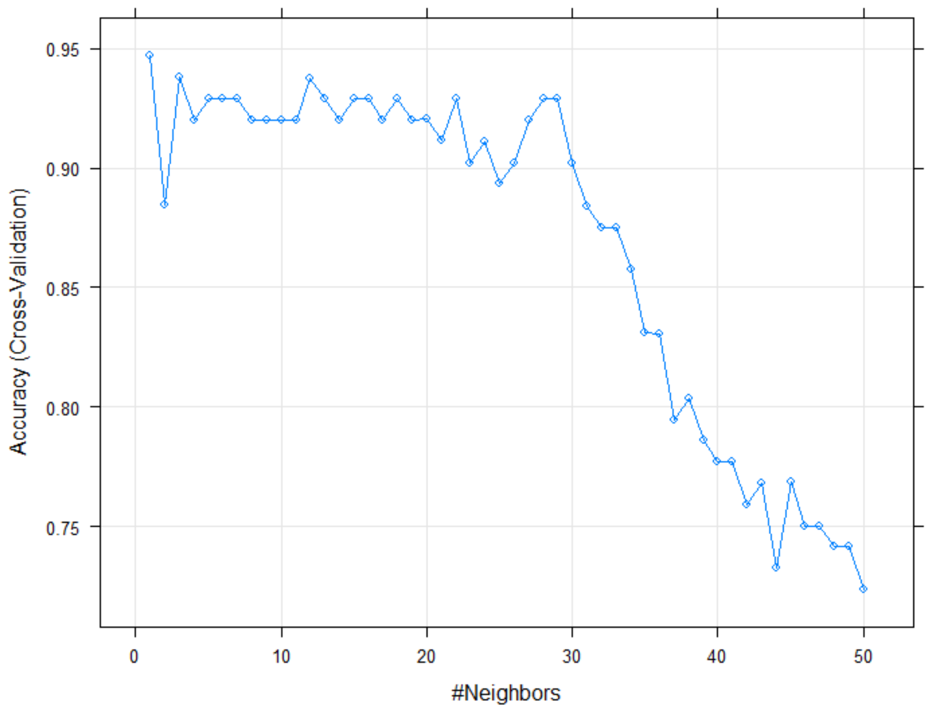

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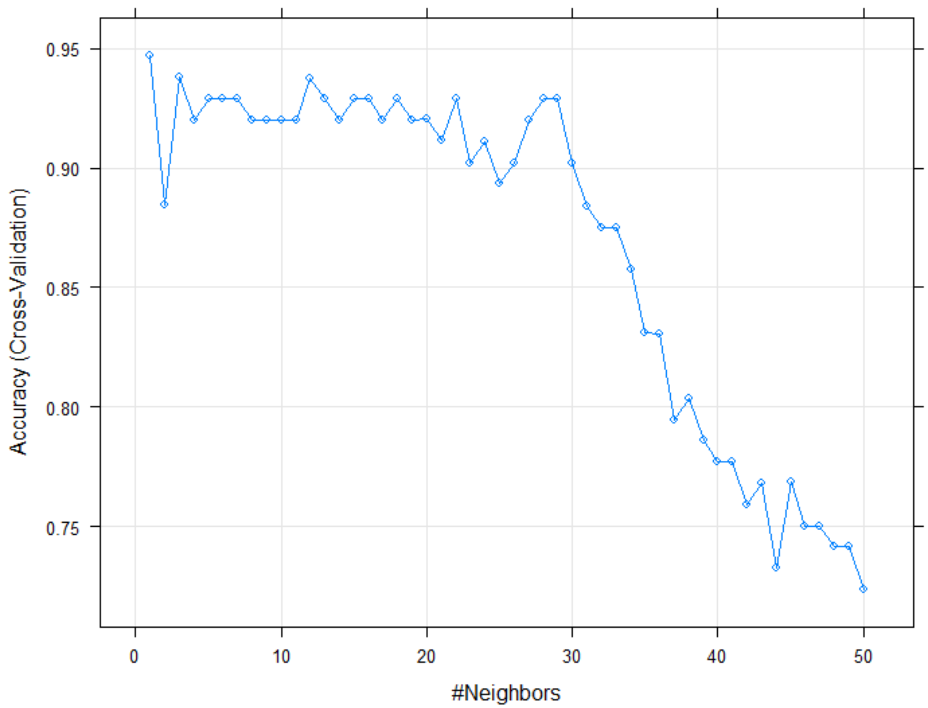



```
# predicting in test with the optimal k
pred = predict(knn.fit, iris.test)
acc = acc.class(pred, iris.test$Species)
```

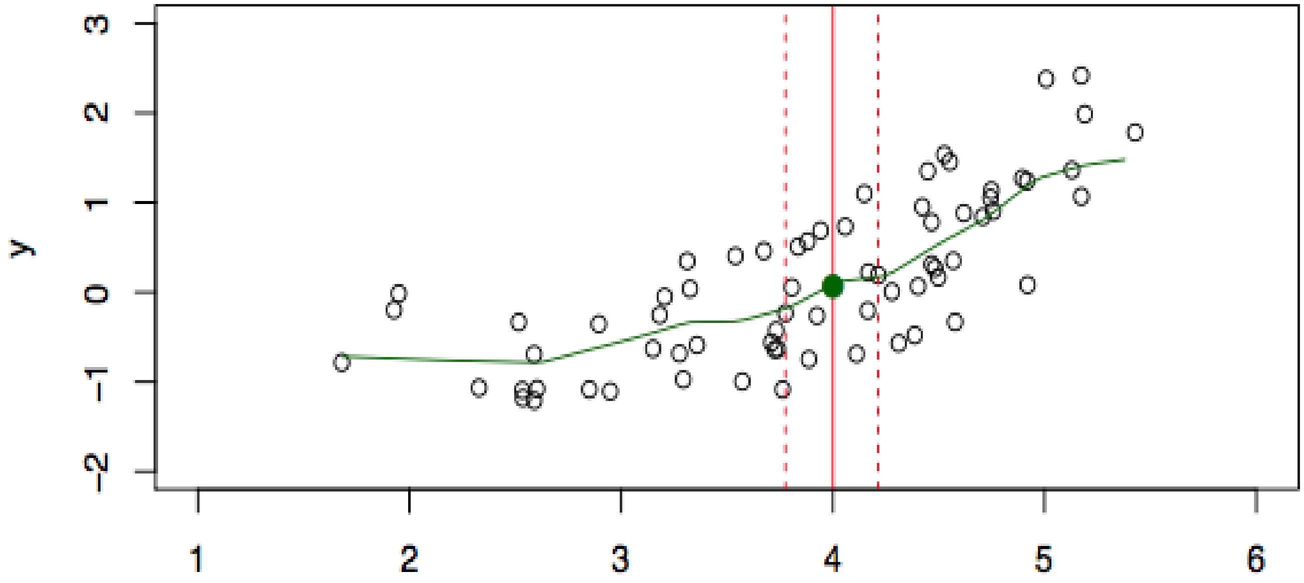
## k-NN for regression

***Aim:***
Predicting a continuous target variable

***What do we need?***
An inference criterion: It can be a simple mean, a particular percentile, etc.

***To take into account:***
Predictor variables covering larger ranges may have more weight in the search of neighbours. Rescaling the predictor data is recommended to make the distance metric more meaningful

$$Z = \frac{X - \mu}{\sigma}$$




| | Ozone | Solar.R | Wind | Temp |
|---|---|---|---|---|
| 1 | 41 | 190 | 7.4 | 67 |
| 2 | 36 | 118 | 8.0 | 72 |
| 3 | 12 | 149 | 12.6 | 74 |
| 4 | 18 | 313 | 11.5 | 62 |
| 5 | 25 | 297 | 14.3 | 56 |
| … | | | | |
| 500 | 23 | 234 | 9.3 | 65 |
| 501 | 45 | 321 | 16.7 | ? |

# Examples in R

*For regression, we will work with the dataset “carseats” (included in the package “ISLR”). Our target variable will be “Sales”. First, we will remove the all the categorical variables from the dataset, retaining only the continuous ones. We will use the function “knn.reg” from the package “FNN”. As you did for the case of classification, divide the total dataset in 75% for train and 25% for test and see how the test error varies with k*

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```
library(ISLR)
attach(Carseats)
dataset = Carseats[, -c(7,10,11)]

# evaluation function
rmse <- function(x, y) {
  sqrt(mean((x - y)^2))
}

# train/test division
n = nrow(dataset)
indtrain = sample(1:n, round(0.75*n));
dataset.train = dataset[indtrain, ]
indtest = setdiff(1:n, indtrain);
dataset.test = dataset[indtest, ]
```

# Examples in R

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# train/test division
n = nrow(dataset)
indtrain = sample(1:n, round(0.75*n));
dataset.train = dataset[indtrain, ]
indtest = setdiff(1:n, indtrain);
dataset.test = dataset[indtest, ]
```

```
# test error as a function of k
library(FNN)
kmax = 50
test.err = c()
for (k in 1:kmax) {
  pred = knn.reg(dataset.train[,-1], dataset.test[,-1],
dataset.train$Sales, k = k)
  test.err[k] = rmse(pred$pred, as.numeric(dataset.test$Sales))
}
plot(1:kmax, test.err, type = "o", pch = 19,
xlab = "k", ylab = "RMSE"); grid()
```

## Examples in R

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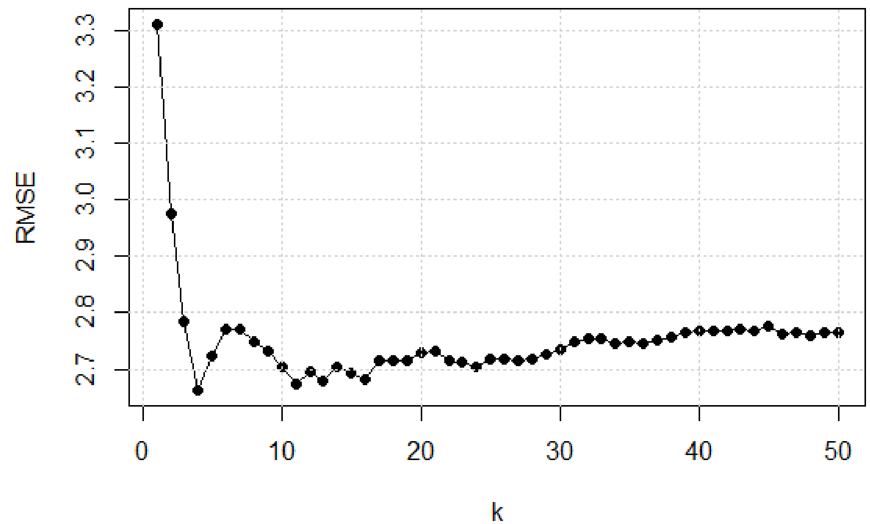
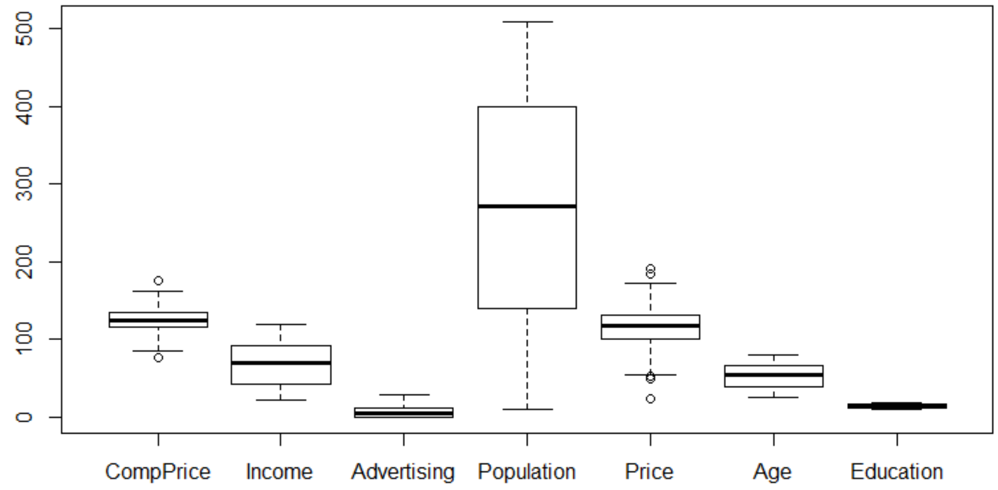


# Examples in R

*Let's continue by seeing the effect of properly rescaling the predictor data. Use the function "scale"*

```
# predictor ranges
boxplot(dataset[,-1])
```

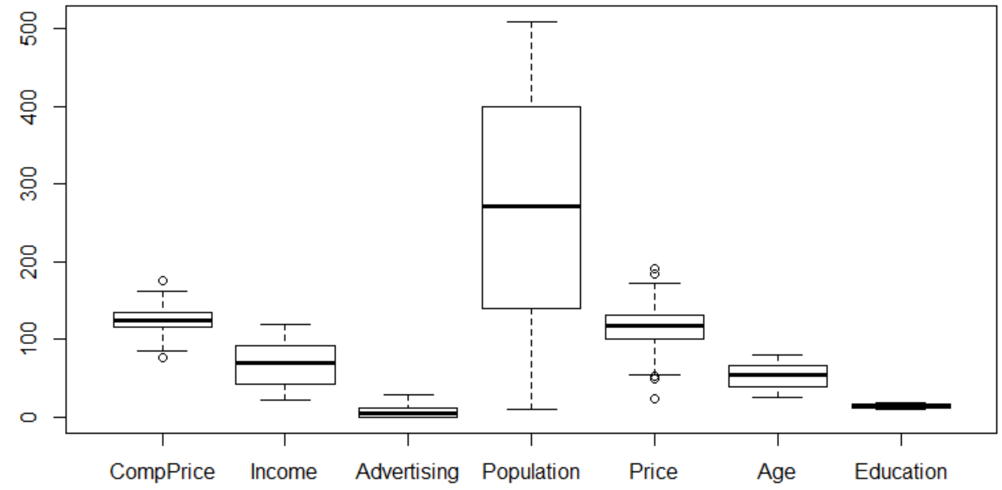


# Examples in R

*Let's continue by seeing the effect of properly rescaling the predictor data. Use the function "scale"*

```
# predictor ranges
boxplot(dataset[,-1])
```

```
# test error as a function of k (for standardized data)
test.err2 = c()
for (k in 1:kmax) {
  pred = knn.reg(scale(dataset.train[,-1]),
scale(dataset.test[,-1]), dataset.train$Sales, k = k)
  test.err2[k] = rmse(pred$pred,
as.numeric(dataset.test$Sales))
}
```



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*Let's continue by seeing the effect of properly rescaling the predictor data. Use the function "scale"*

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boxplot(dataset[,-1])
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# test error as a function of k (for standardized data)
test.err2 = c()
for (k in 1:kmax) {
  pred = knn.reg(scale(dataset.train[,-1]),
scale(dataset.test[,-1]), dataset.train$Sales, k = k)
  test.err2[k] = rmse(pred$pred,
as.numeric(dataset.test$Sales))
}
```
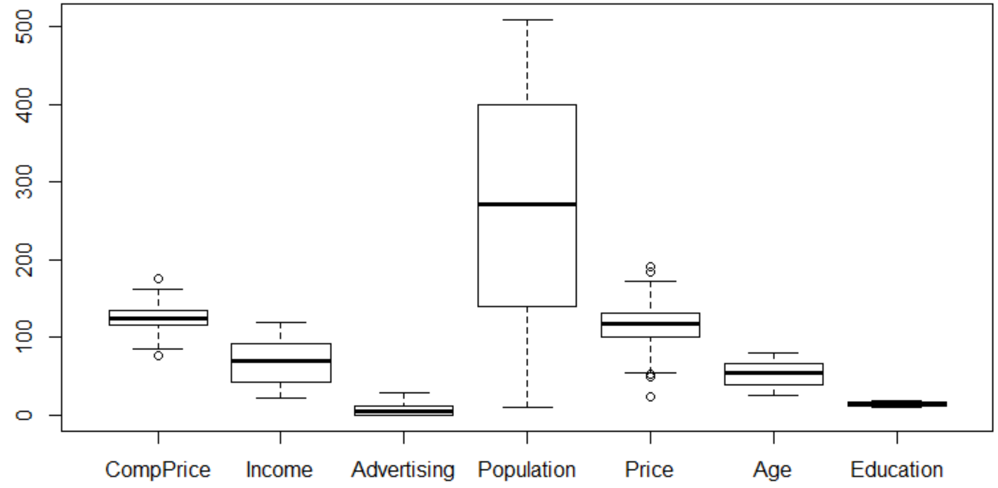
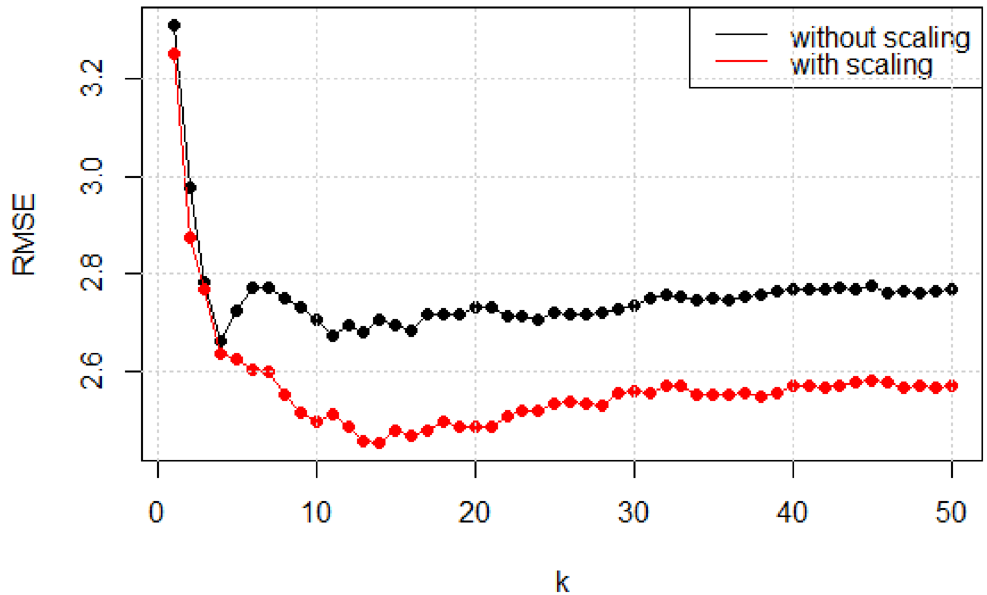

```
# plotting results
matplot(1:kmax, cbind(test.err, test.err2),
        type = "o", pch = 19, lty = 1,
        col = c("black", "red"), xlab = "k", ylab = "RMSE")
legend("topright", c("without scaling", "with scaling"),
       lty = 1, col = c("black", "red"))
grid()
```



# Examples in R

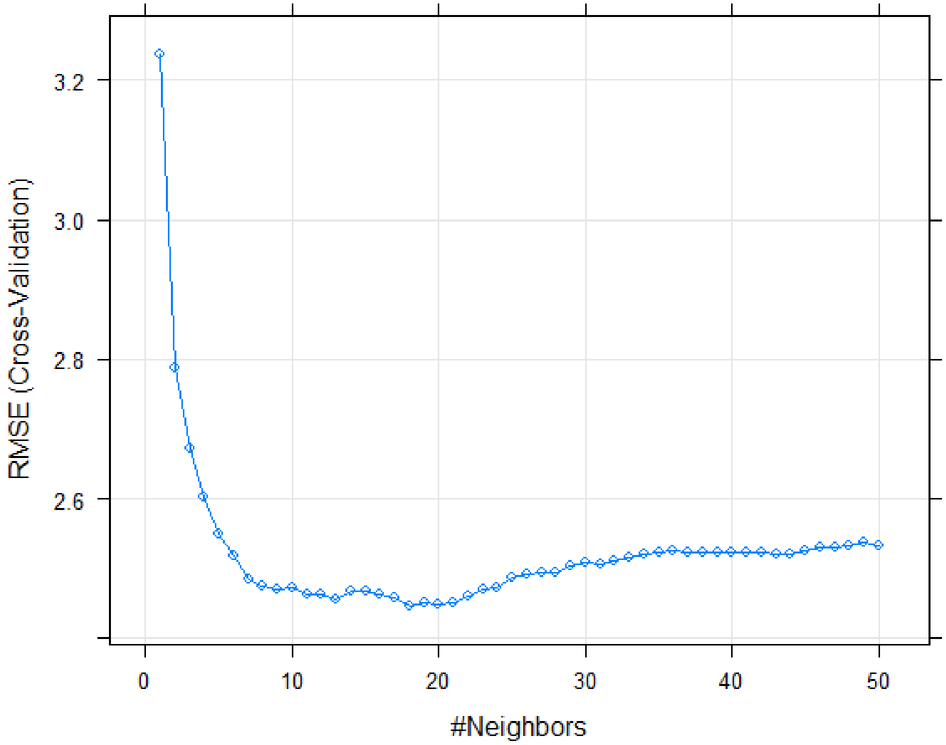
*<u>Do the same exercise, but this time using “caret”. Recall to standardize your predictor data to obtain meaningful results.</u>*

# Examples in R

*Do the same exercise, but this time using “caret”. Recall to standardize your predictor data to obtain meaningful results*

```
# defininig hold-out cross-validation
trctrl <- trainControl(method = "cv", number = 2)
# searching the optimal k (with standardized data)
knn.fit <- train(Sales ~ ., data = dataset.train,
                 method = "knn",
                 trControl = trctrl,
                 preProcess = c("center","scale"),
                 tuneGrid = expand.grid(k = 1:50))
plot(knn.fit)
```

```
# predicting in test with the optimal k
pred = predict(knn.fit, dataset.test)
rmse(pred, dataset.test$Sales)
```

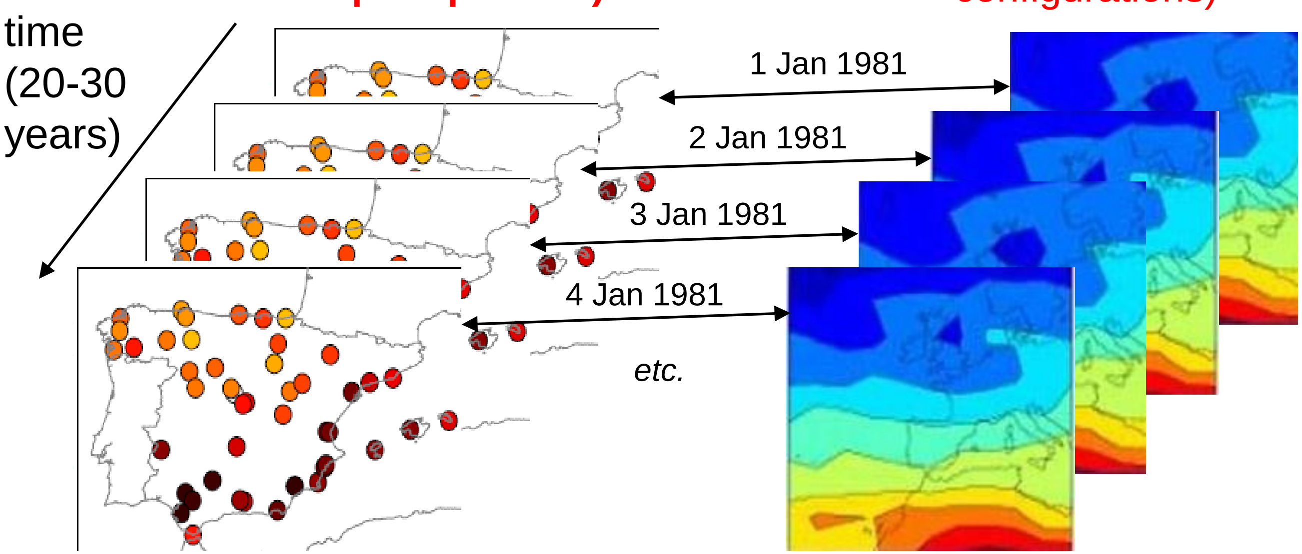


# k-NN in meteorology

The analog technique (Lorenz, 1969): Similar atmospheric patterns lead to similar meteorological conditions

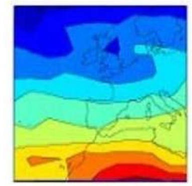
**Y**: historical observations of the **target variable (e.g. precipitation)**

**X**: historical model simulations (large-scale atmospheric configurations)

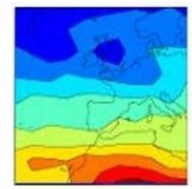



**Problem: Y' (**prediction) for 26 Mar 2046?

*1) Take X' for 26 Mar 2046: $X_{2046}$*

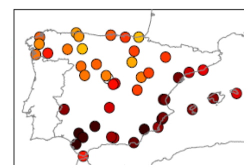


*2) Search the nearest neighbor/s to $X_{2046}$ within X*



*X (3-Jan-1981)*

*3) Infer a prediction based on the observed values in the days selected in 2)*

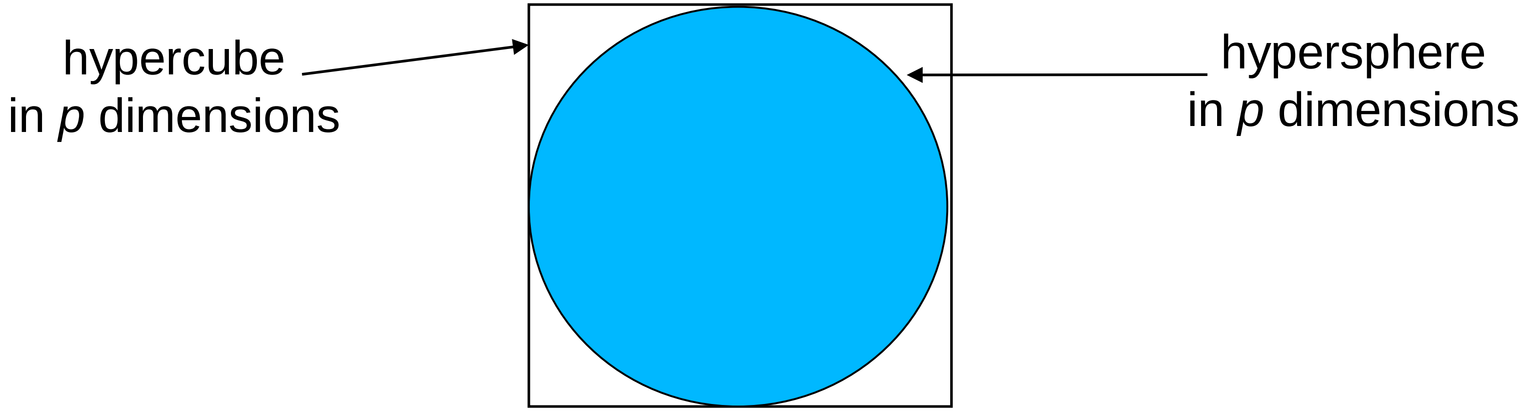


In meteorology, two important factors must be taken into account for the application of k-NN technique:

1) Predictor scaling
2) High dimensionality (the curse of dimensionality)

# The curse of dimensionality

(David Scott, *Multivariate Density Estimation,* Wiley, 1992)

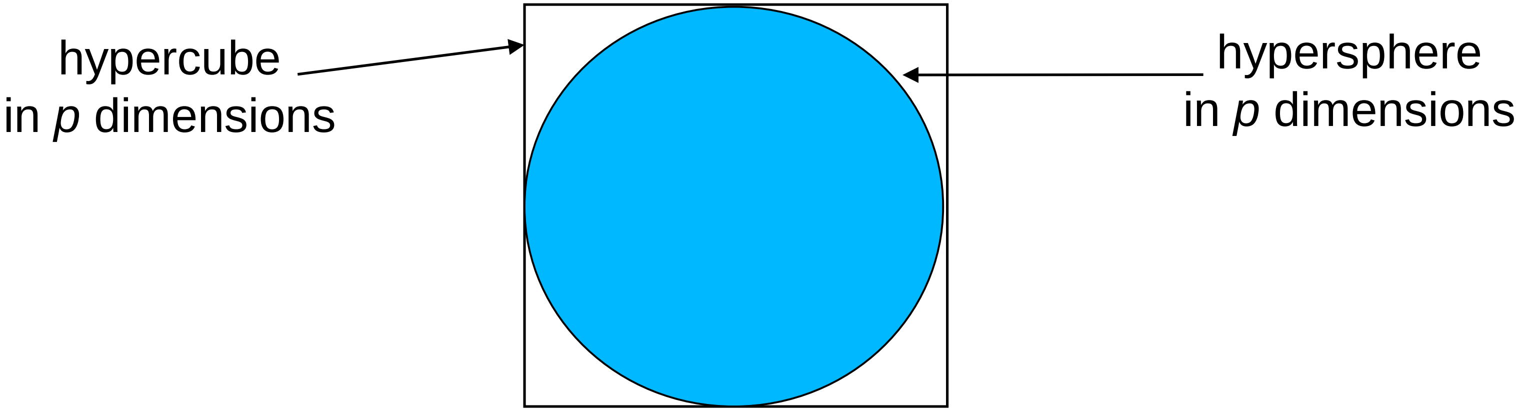



Volume of sphere relative to cube in *d* dimensions?

| | |
|---|---|
| **Dimension** | **2** |
| **Rel. vol.** | **0.79** |

# The curse of dimensionality

(David Scott, *Multivariate Density Estimation,* Wiley, 1992)

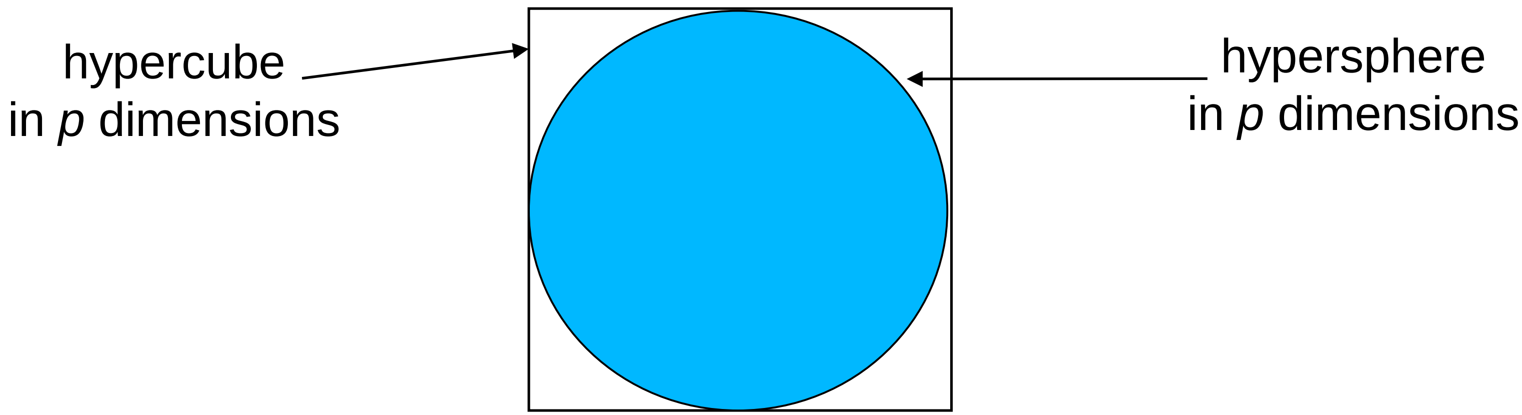



Volume of sphere relative to cube in *d* dimensions?

| **Dimension** | **2** | **3** |
|---|---|---|
| **Rel. vol.** | **0.79** | **0.53** |

# The curse of dimensionality

(David Scott, *Multivariate Density Estimation,* Wiley, 1992)

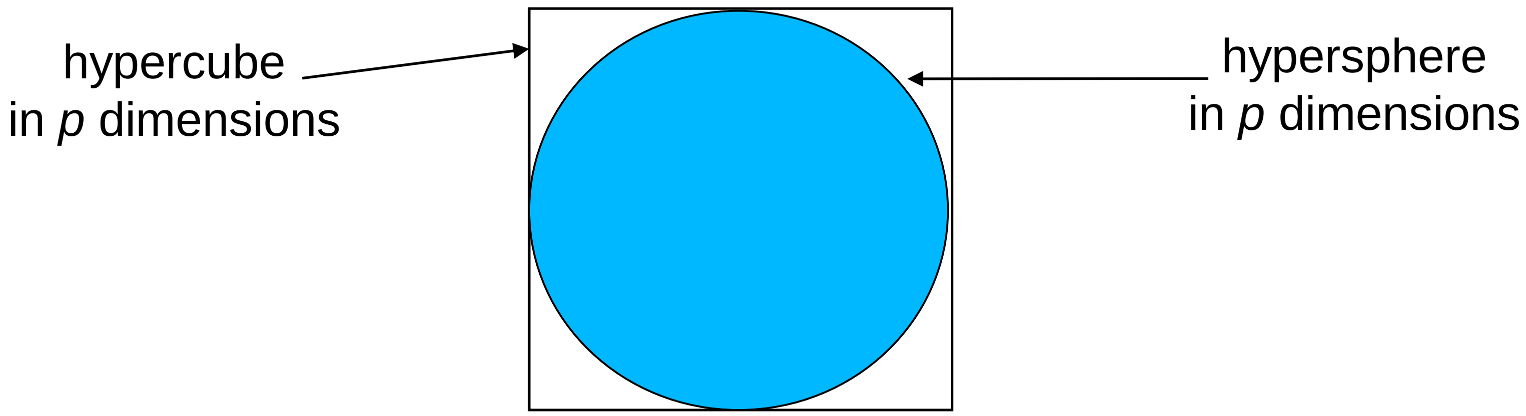



Volume of sphere relative to cube in *d* dimensions?

| **Dimension** | **2** | **3** | **4** |
|---|---|---|---|
| **Rel. vol.** | **0.79** | **0.53** | **0.31** |

# The curse of dimensionality

(David Scott, *Multivariate Density Estimation,* Wiley, 1992)

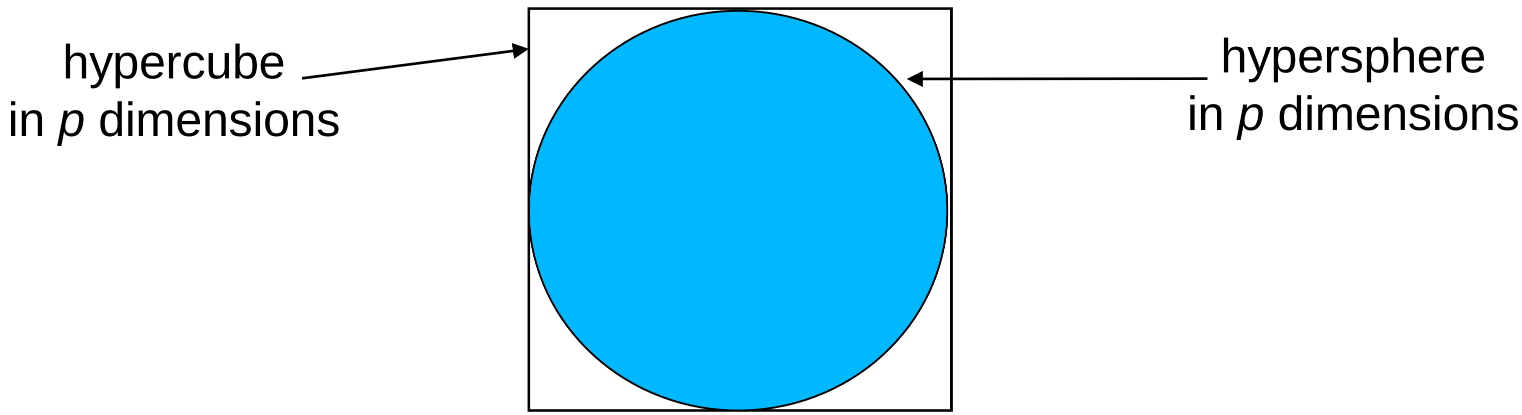



Volume of sphere relative to cube in *d* dimensions?

| **Dimension** | **2** | **3** | **4** | **5** |
|---|---|---|---|---|
| **Rel. vol.** | **0.79** | **0.53** | **0.31** | **0.16** |

# The curse of dimensionality

(David Scott, *Multivariate Density Estimation,* Wiley, 1992)




Volume of sphere relative to cube in *d* dimensions?

| **Dimension** | **2** | **3** | **4** | **5** | **6** |
|---|---|---|---|---|---|
| **Rel. vol.** | **0.79** | **0.53** | **0.31** | **0.16** | **0.08** |

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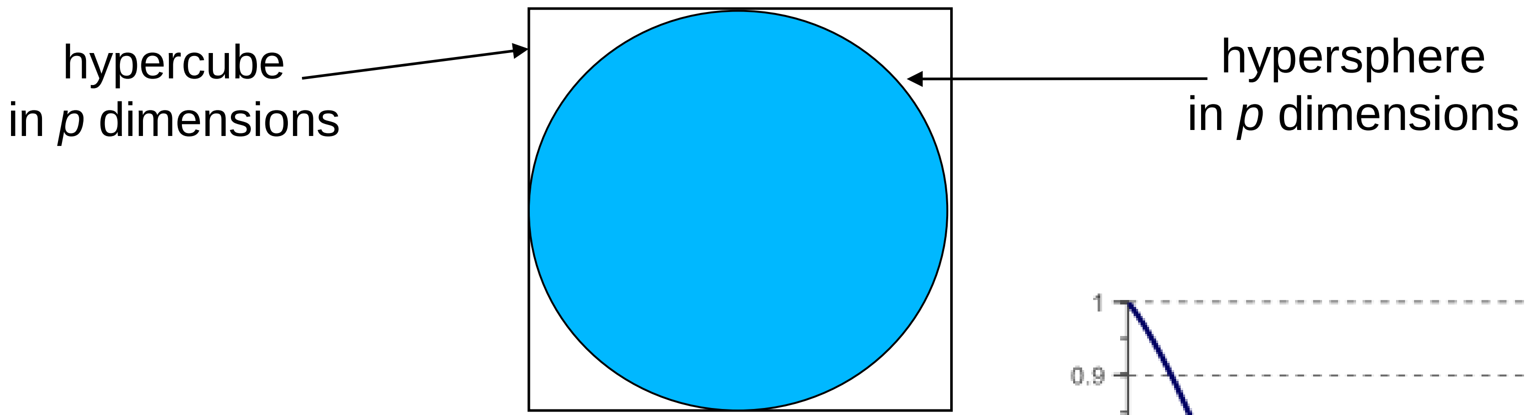
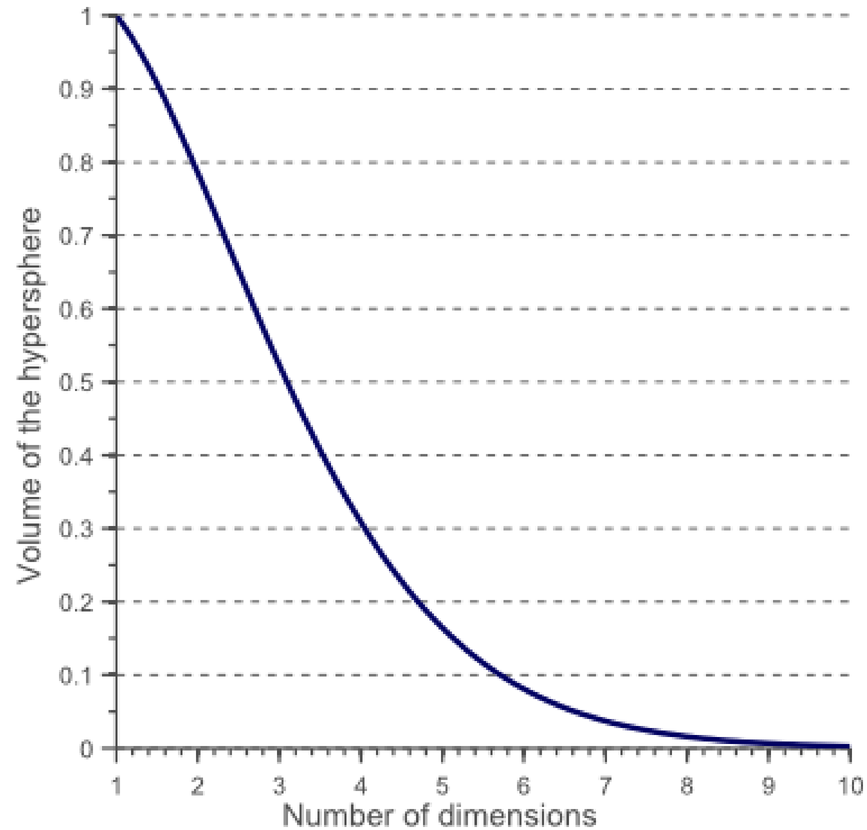
(David Scott, *Multivariate Density Estimation,* Wiley, 1992)



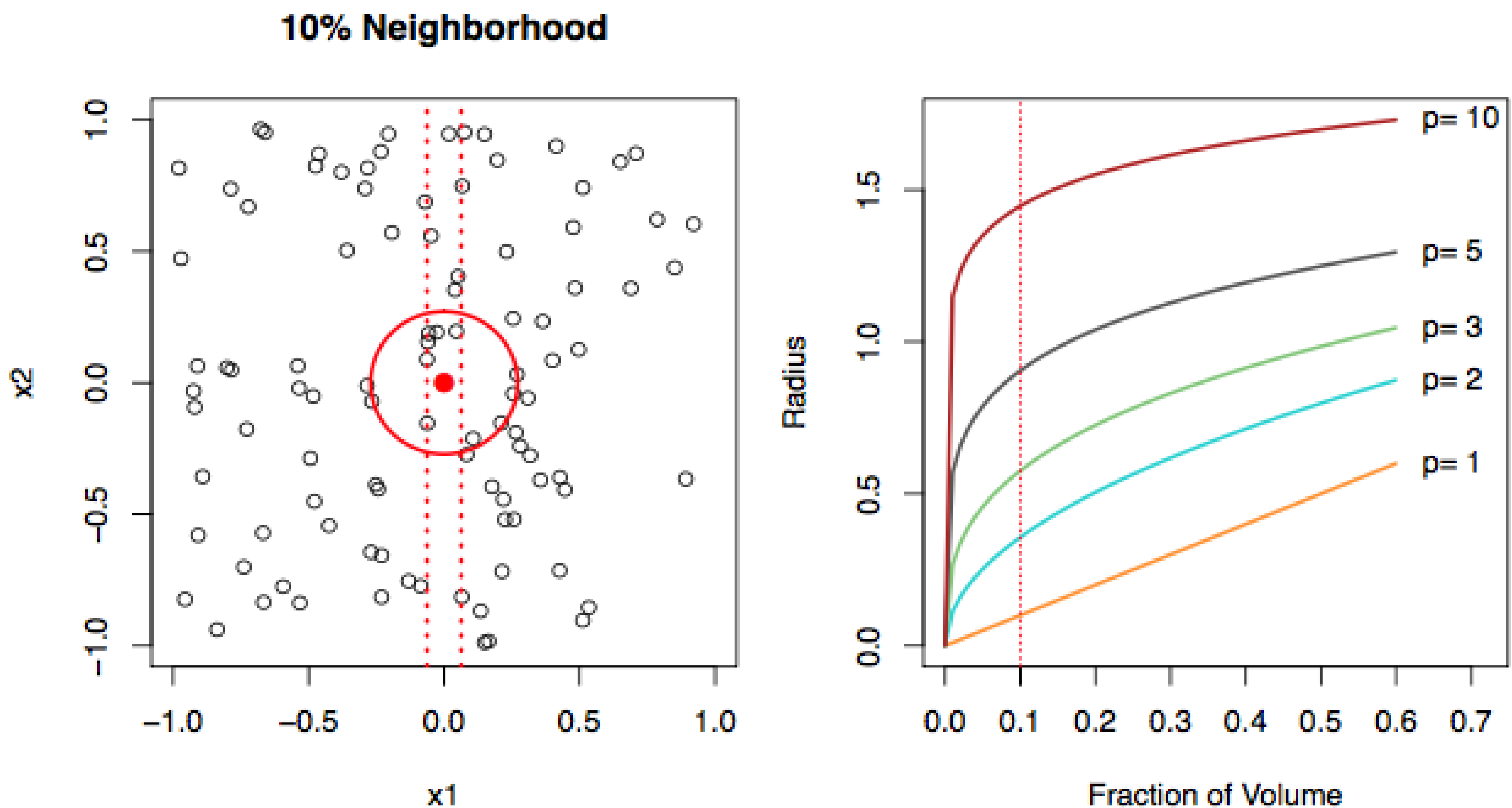

Volume of sphere relative to cube in *d* dimensions?

| **Dimension** | **2** | **3** | **4** | **5** | **6** | **7** |
|---|---|---|---|---|---|---|
| **Rel. vol.** | **0.79** | **0.53** | **0.31** | **0.16** | **0.08** | **0.04** |

As the dimensionality increases, a larger percentage of the training data resides in the corners of the feature space. Therefore, k-NN is unhelpful in high dimensional problems because there is little difference between the nearest and the farthest neighbor



# The curse of dimensionality




The amount of training data needed to cover 10% of the feature range grows exponentially with the number of dimensions

Dimensionality reduction techniques (e.g. PCA ~ effective degrees of freedom) should be applied prior to using k-NN in order to help make the distance metric more meaningful