Minería de Datos

La Técnica k-NN

Máster en Ciencia de Datos

Con la colaboración de:

Rodrigo García Manzanas (rodrigo.manzanas@unican.es)
Departamento de Matemática Aplicada y Ciencias de la Computación
Universidad de Cantabria

Contents

- k-NN for classification
- k-NN for regression
- The curse of dimensionality
- k-NN in the climate science

Aprendizaje supervisado

- Clasificación (Cla)
- Regresión/predicción (Reg)

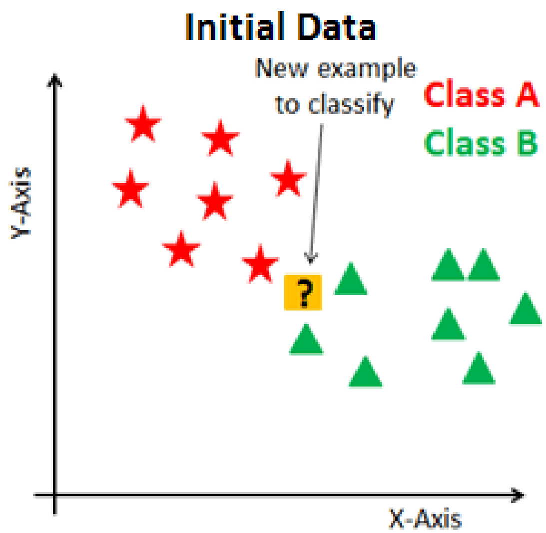
- Regresión logística (Cla)
- Regresión lineal (Reg)
- **k-NN (Cla, Reg)**
- Árboles de decisión (Cla, Reg)
- Métodos de ensembles: Random forests (Cla,Reg); AdaBoost (Cla); GBoost (Cla, Reg)
- Métodos de kernels (Cla, Reg)
- Máquinas de vector soporte (Cla, Reg)
- Redes neuronales (Cla, Reg)
- Redes probabilísticas (Cla, Reg)
- etc.

Aprendizaje no supervisado

- Asociación (Aso)
- Clustering (Clu)
- Reducción de la dimensionalidad (RDim)

- Reglas de asociación (Aso): Algoritmo Apriori, Algoritmo Eclat
- Clustering jerárquico (Clu): Dendograma
- Clustering no jerárquico (Clu): k-means
- Reducción de la dimensionalidad lineal (RDim): PCA, LDA
- Reducción de la dimensionalidad no lineal (RDim): MDS, MMF, Isomap, LLE, SNE
- Redes probabilísticas (Rdim)
- etc.

Minería de Datos Estadística Aprendizaje Automático Aprendizaje Automático II



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Aim:
To **classify** a **discrete** target variable, based on some similarity measure in the predictors' space.

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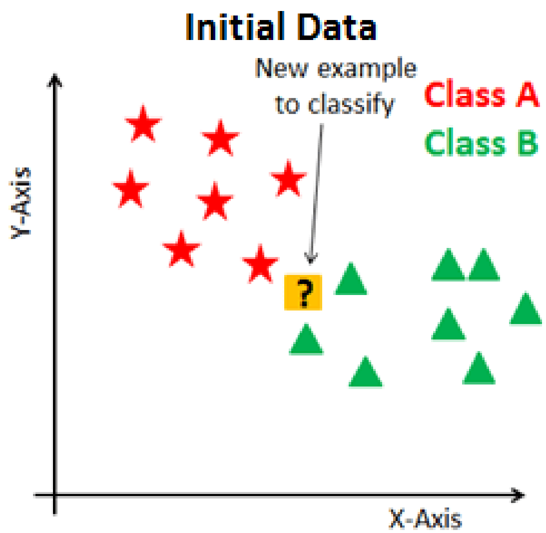

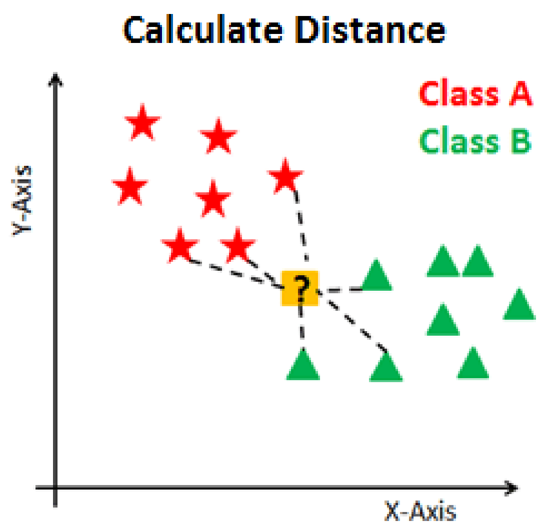

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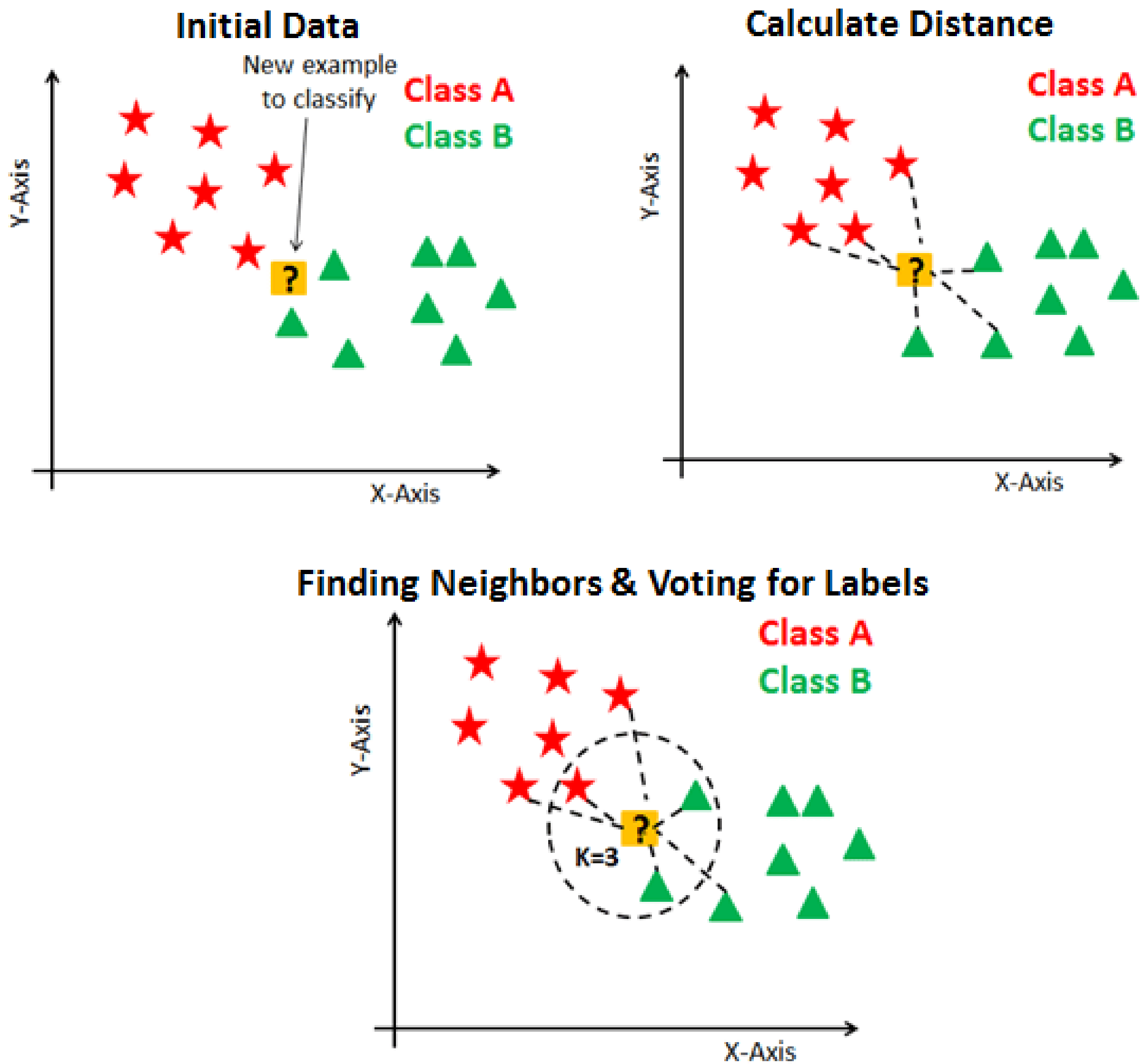
To classify a discrete target variable, based on some similarity measure in the predictors' space.



The Core Idea

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width		Species
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New instance to be classified

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New instance to be classified

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STEP 3: NN-based classification

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Applications:
- Economic sciences
- Political sciences
- Genetics
- Image recognition
- Climate

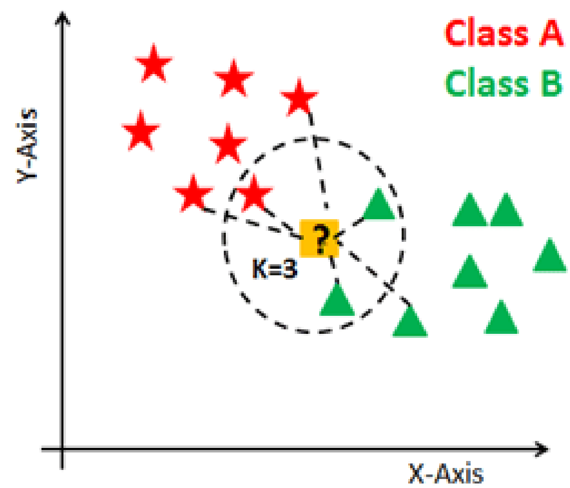
- **Distance metric**
  Different distance metrics can be used, depending on the application.

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

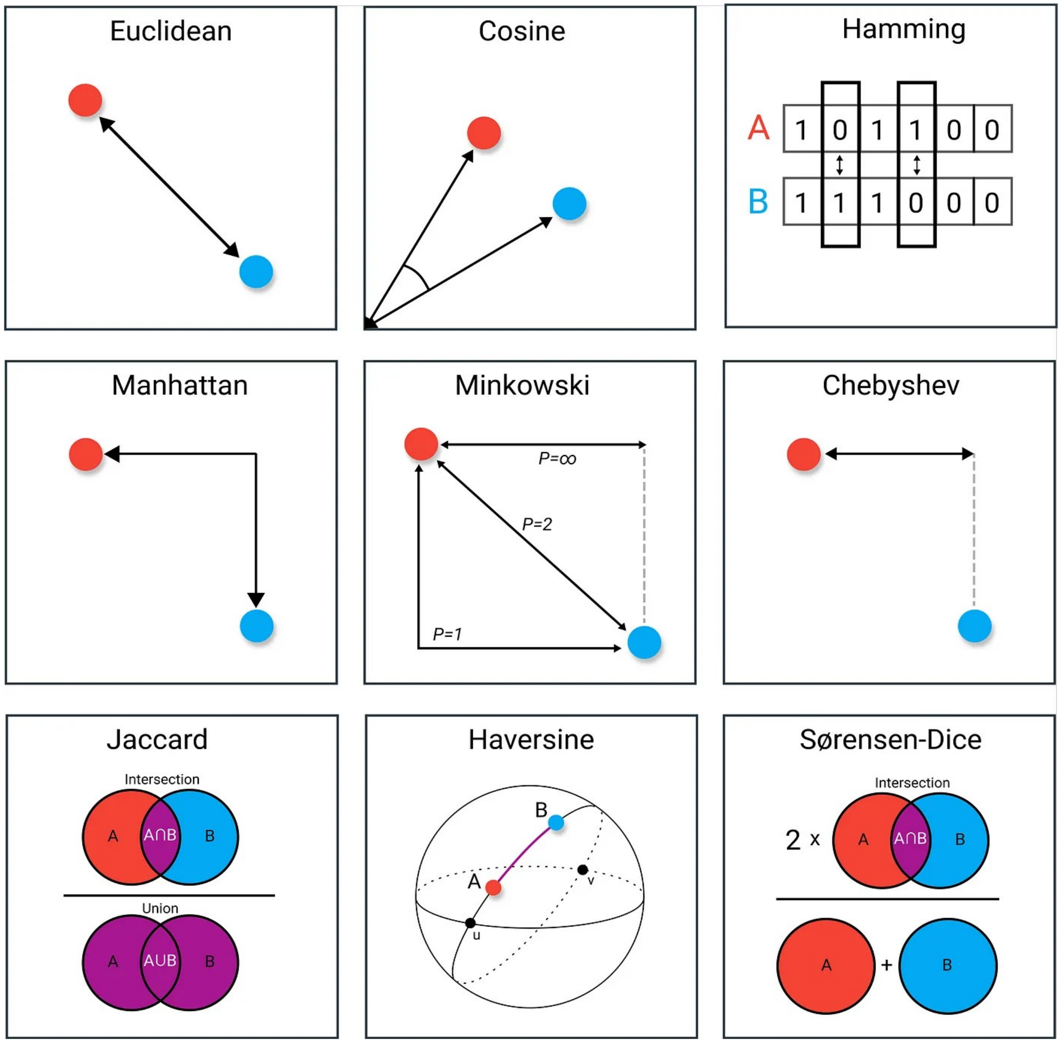
- **Inference criterion**
  - Majority vote
  - Random
  - etc.

Deterministic result

Stochastic result



There is a large number of available distance metrics: see Prasath et al. 2019 and this interesting post for details



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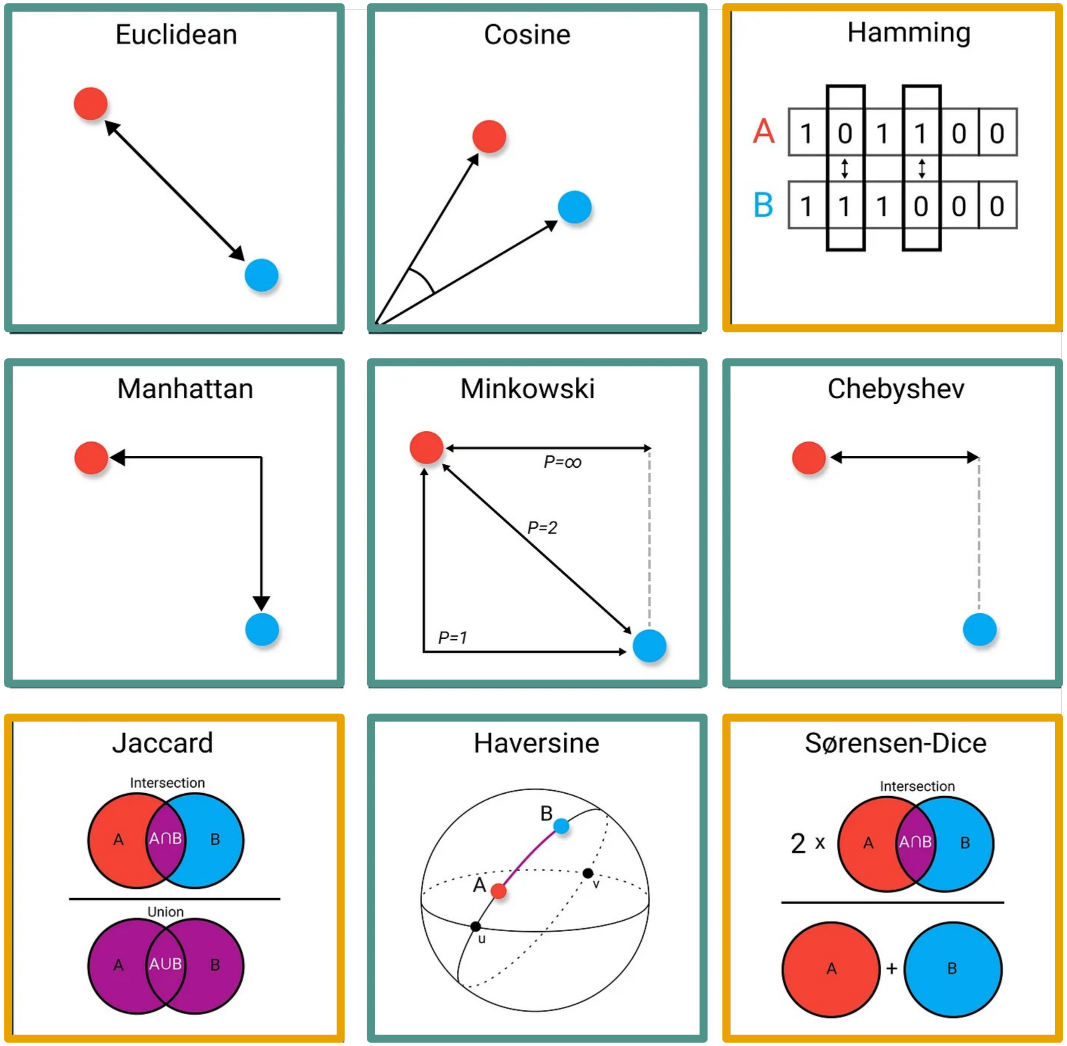

Geometric nature

Topological nature

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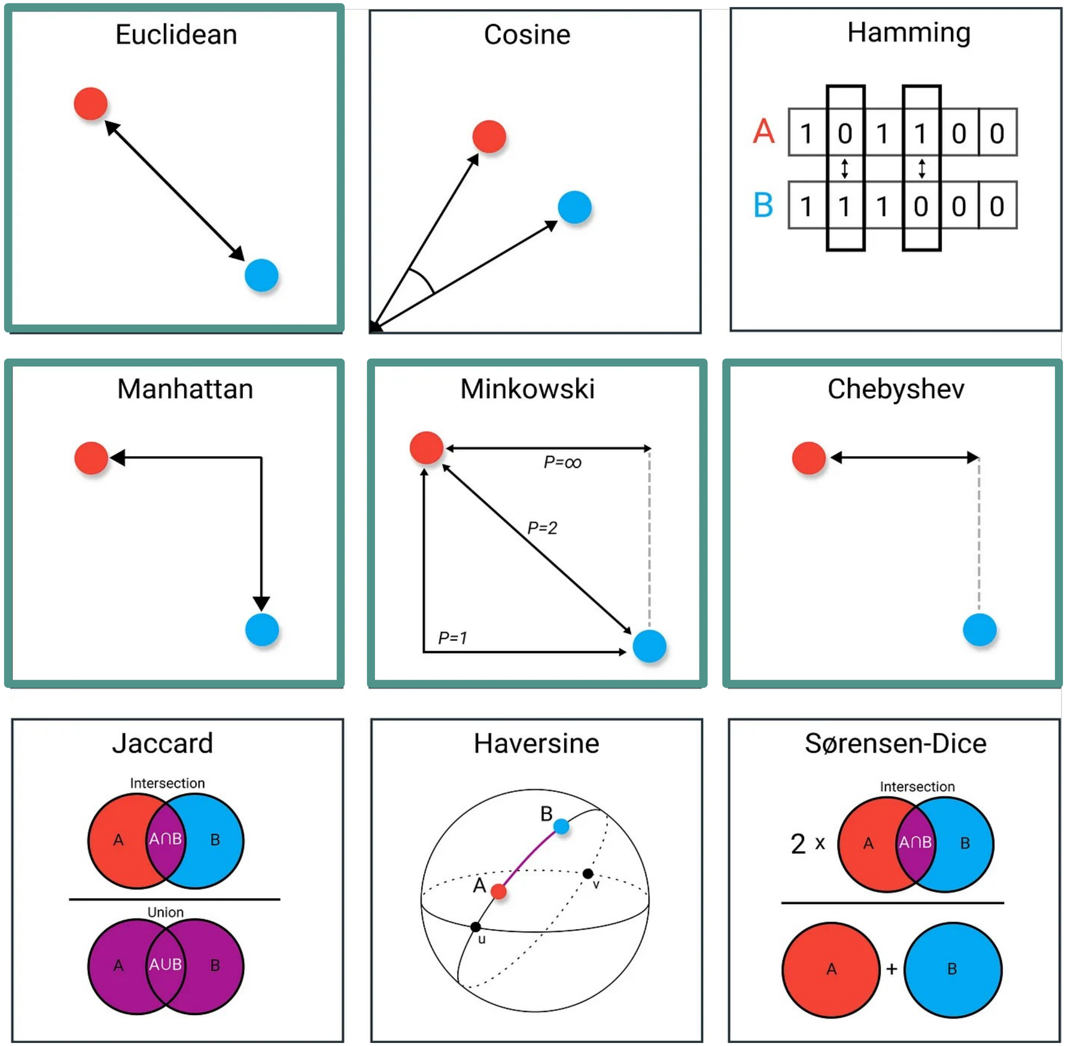

Minkowsky-based geometric distances

$$D_{Minkowsky}(x,y) = \left(\sum_{i=1}^{n}(x_i - y_i)^p\right)^{1/p}$$

$$D_{Manhattan}(x,y) = \sum_{i=1}^{n}|x_i - y_i|$$

$$D_{Euclidean}(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

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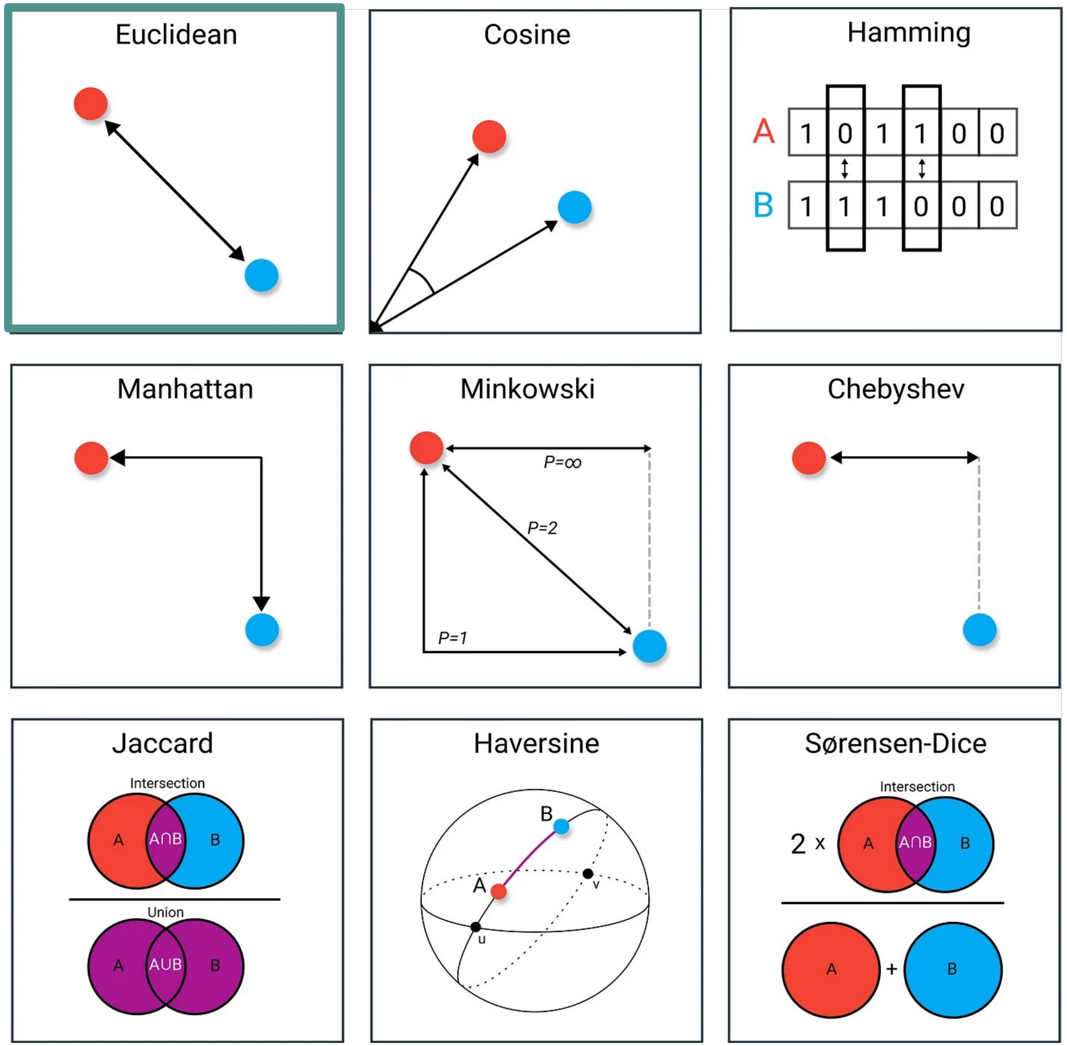

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Most commonly used

$$\boxed{D_{Euclidean}(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}}$$

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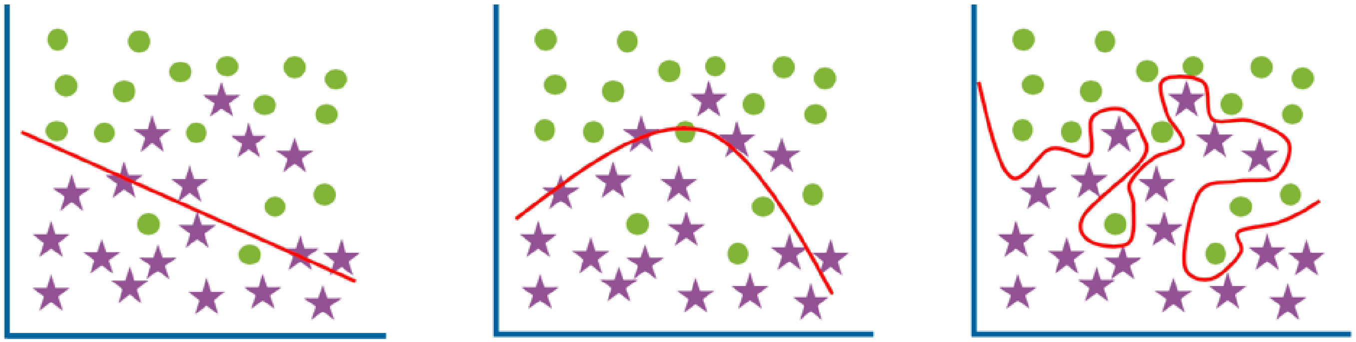
Which model would you prefer?



Classification borders obtained for different values of *k*

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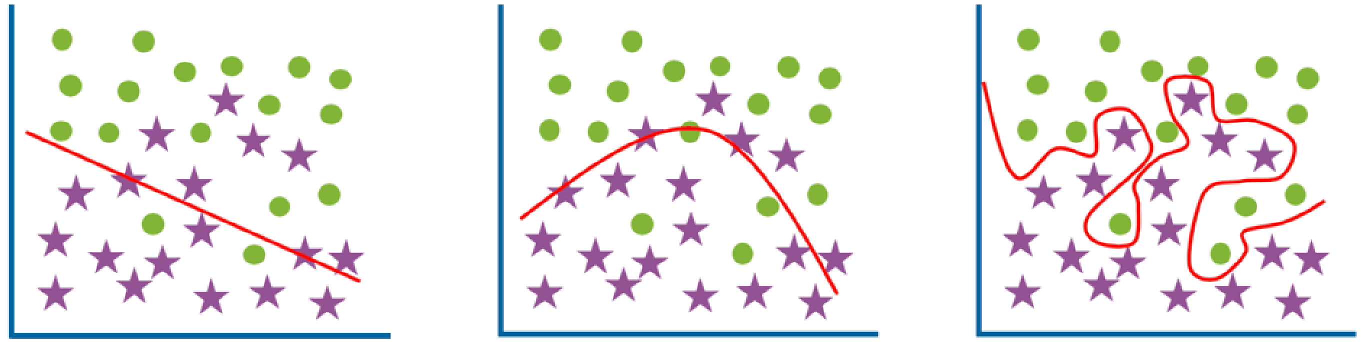

Resulting model	Value of *k*
Overfitted	*Too large k*
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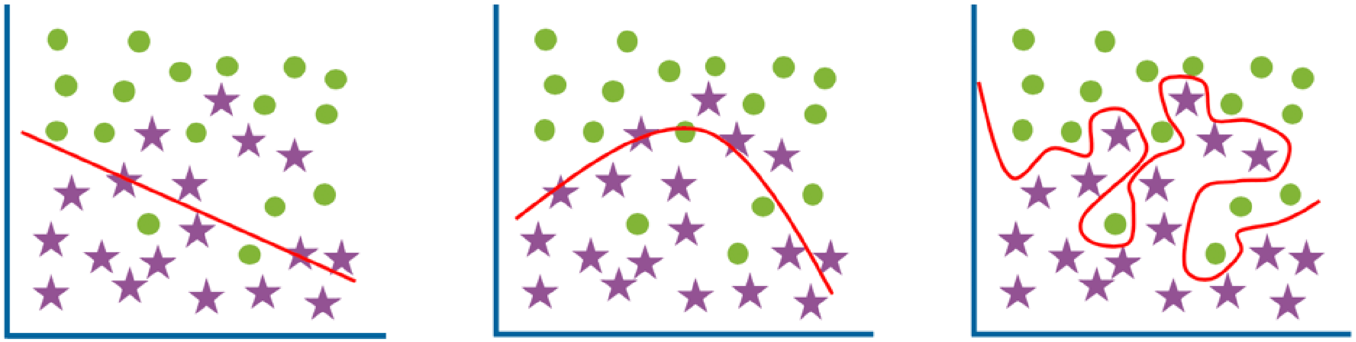

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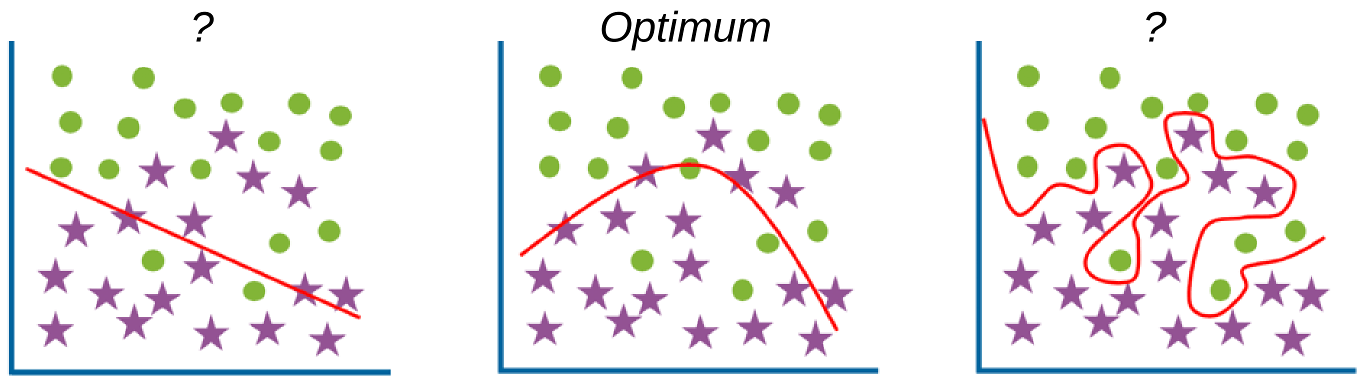

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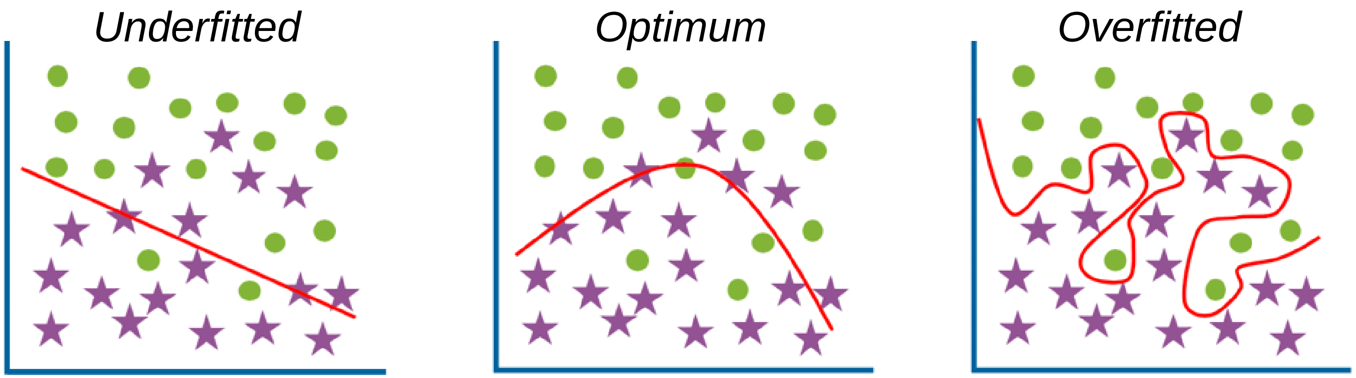

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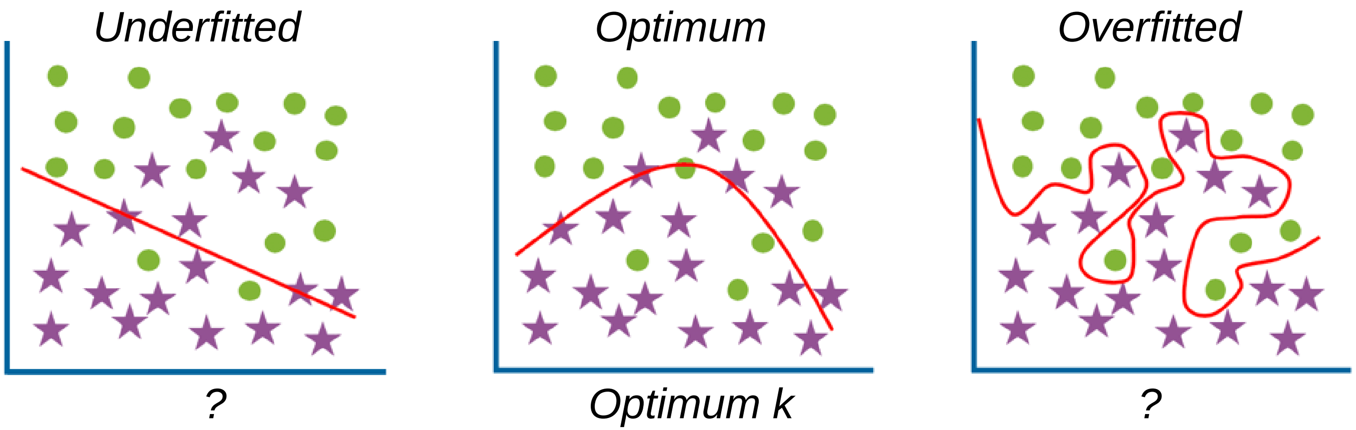

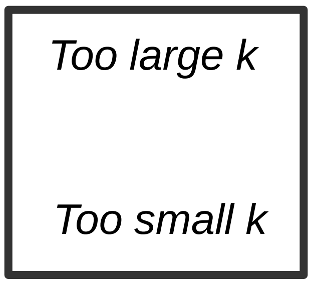

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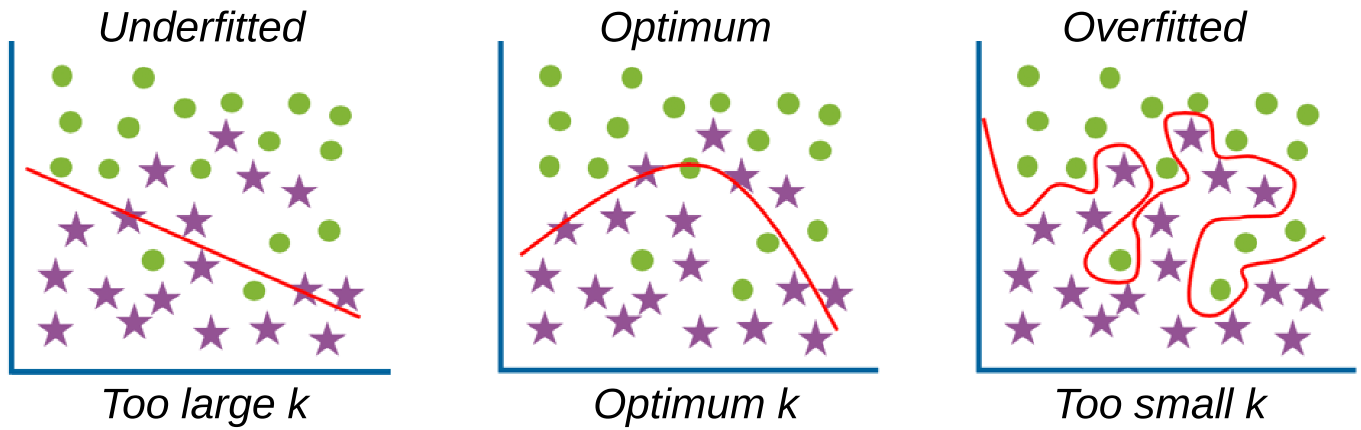

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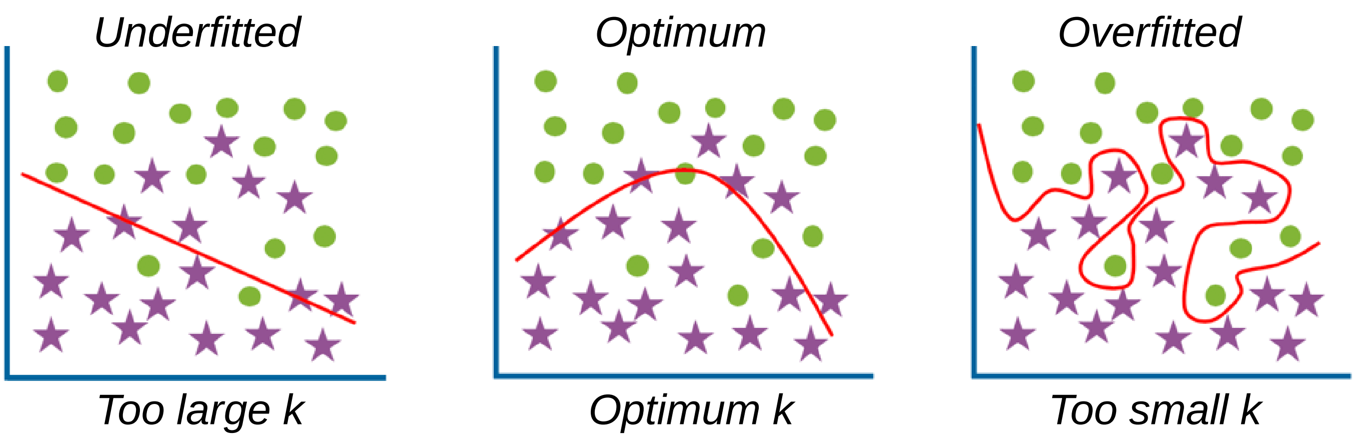
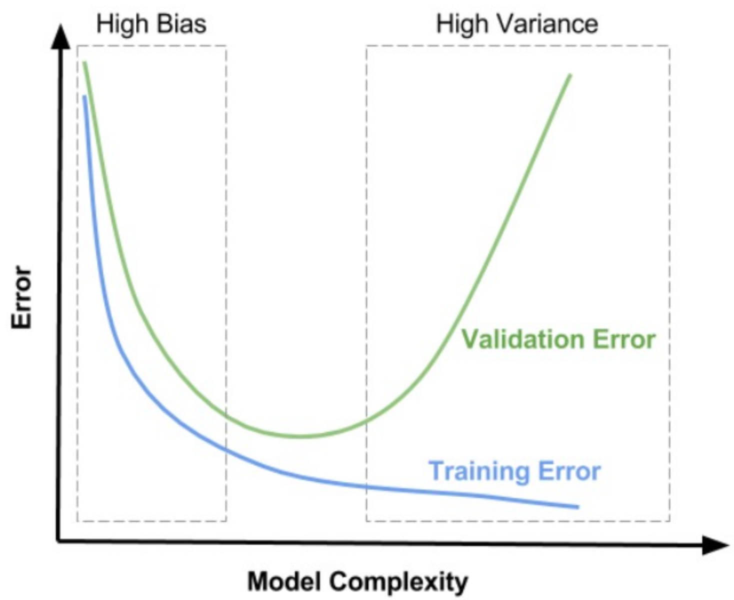


Cross-validation is needed to find the optimal *k*!

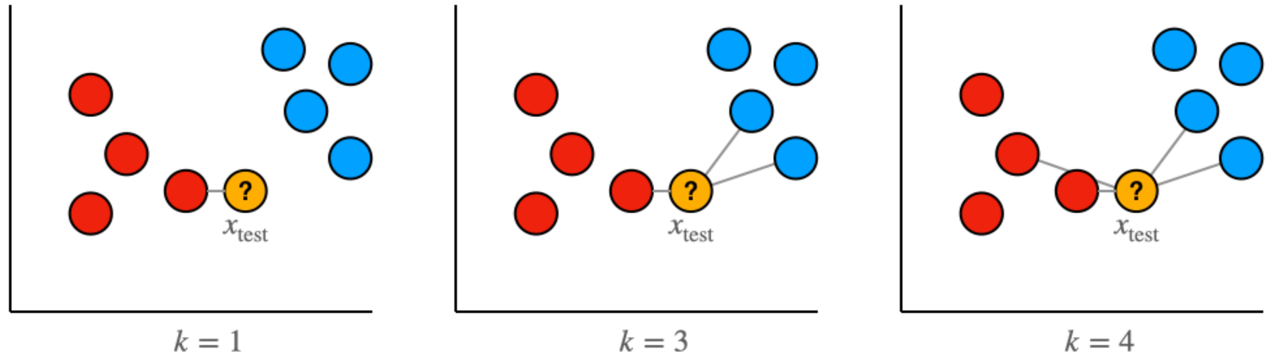
come si stabilisce la larghezza di high bias?



complexity ~ k

In classification problems, the choice of k can lead to **ties**

Binary classification



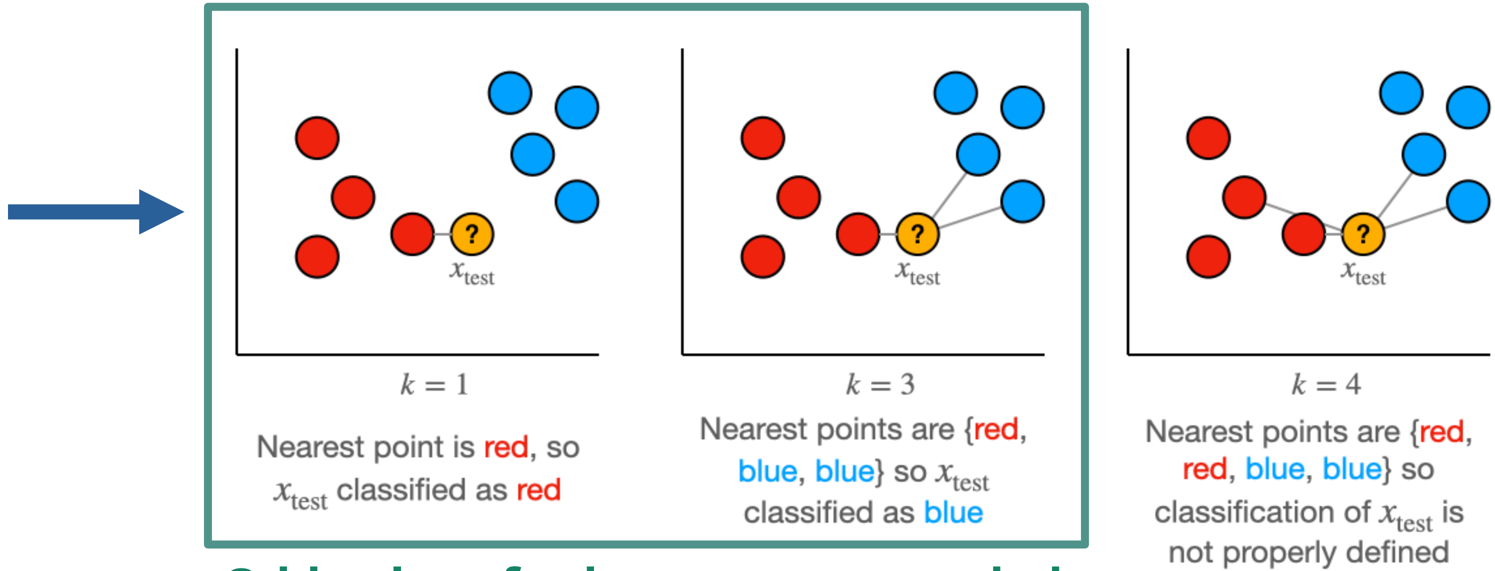
Nearest point is red, so x_{test} classified as red

Nearest points are {red, blue, blue} so x_{test} classified as blue

Nearest points are {red, red, blue, blue} so classification of x_{test} is not properly defined

In classification problems, the choice of k can lead to **ties**

Binary classification



Odd values for k are recommended

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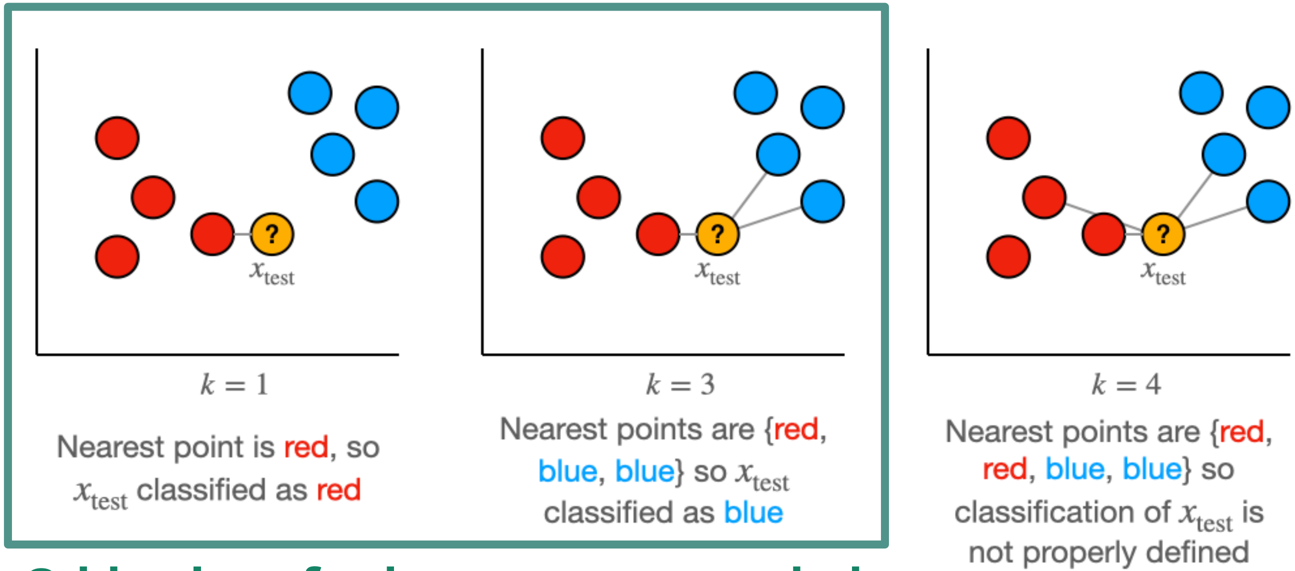
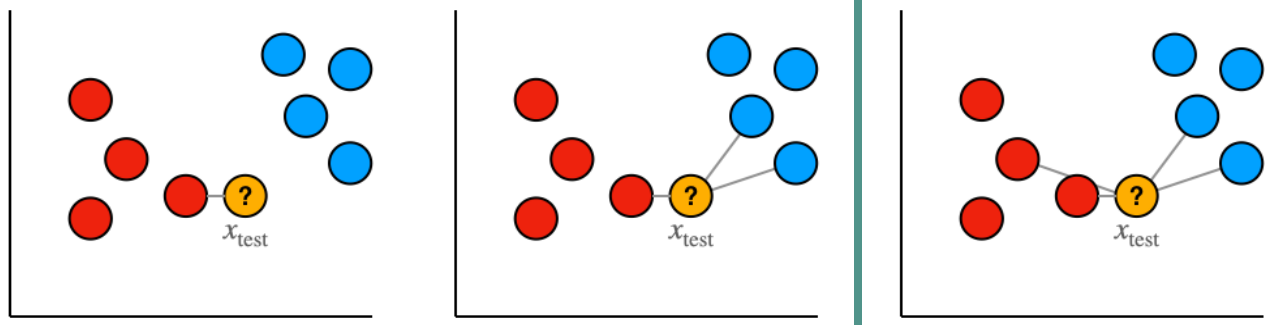


Odd values for k are recommended

Multinomial classification?

In classification problems, the choice of k can lead to **ties**

Binary classification



$k = 1$

Nearest point is red, so x_{test} classified as red

$k = 3$

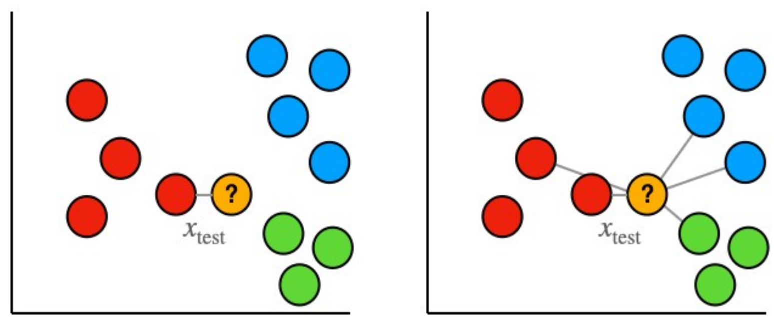
Nearest points are {red, blue, blue} so x_{test} classified as blue

$k = 4$

Nearest points are {red, red, blue, blue} so classification of x_{test} is not properly defined

Odd values for k are recommended

Multinomial classification



$k = 1$

Nearest point is red, so x_{test} classified as red

$k = 5$

Nearest points are {red, red, blue, blue, green}. The model cannot choose between blue and red because both appear twice

*Based on the **iris** dataset, **classify** the following **new instance**:*

(sepal l., sepal w., petal l., petal w.) = (5.4, 2.7, 4.6, 1.4)

```
## new instance
d.new = c(5.4, 2.7, 4.6, 1.4)
```

```
## euclidean distance between the new instance and all the
others
eucli = rep(***)
for (i in 1:nrow(iris)) {
  eucli[i] = ***
}
```

```
## ordering distances
ind.sort = sort(***)
```

```
## classifying based on the nearest
neighbor
pred.k1 = ***
```

```
## classifying based on the 20 nearest
neighbors
pred.k20 = ***
summary(pred.k20)
```

*Divide **iris** into train and test (75% and 25% of the total dataset, respectively) and find the **test error** for the nearest neighbor method (**k=1**). Use the function **knn** from package **class***

```
## train/test partition
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(***)
```

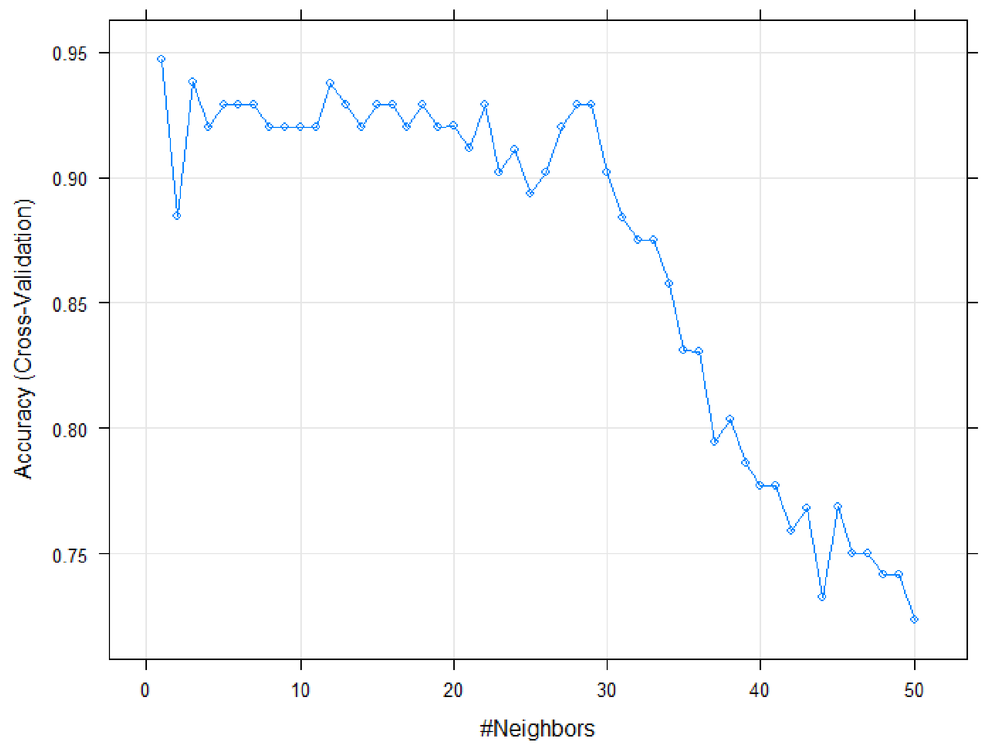
```
## validation (accuracy)
table(***)


acc.class()
```

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

*For the **iris** dataset, use the package **caret** (method knn) to **find the optimal k**. To do so, check **how the validation error varies with increasing k** (for values from **1 to 50**) under a **2-fold cross-validation** scheme. Then, check whether or not the optimal model is overfitted.*

```
library(caret)
## defining 2-fold cross-validation
trctrl = trainControl(method = "***", number =
***)
## searching the optimal k
knn.fit = train(Species ~ ., ***,
              method = "**",
              trControl = ***,
              tuneGrid = )
plot(knn.fit)
```




```
## predicting in test with the optimal k
pred = predict(knn.fit, iris.test)
acc = acc.class(pred, iris.test$Species)
0.9392613
```

Would you say your model is overfitted/underfitted?

In **regression** problems…

Aim:
To **predict** a **continuous** target variable, based on some **similarity measure in the predictors' space**.

	Wind (m/s)	Pressure (hPa)	Humidity (%)	Temperature (ºC)
1	4.1	1018	68	21
2	7.9	1020	64	23
3	1.6	1015	72	18
…				
498	12.3	1008	83	14
499	15.1	1010	80	16
500	4.3	1014	71	17
501	7.8	1013	74	?

New instance
to be predicted

In **regression** problems…

Aim:
To **predict** a **continuous** target variable, based on some **similarity measure in the predictors' space**.

What do we need?
As for classification:
- A distance metric (e.g. Euclidean)
- A value for *k*
- An inference criterion (e.g. the mean, a particular percentile, a random value, etc.)

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New instance to be predicted

To take into account:
- Predictor variables which are larger in magnitude and/or variability may have more weight in the search of neighbors. Thus, **standardizing the predictor data is highly recommended** to make the distance metric more meaningful $$Z = \frac{X - \mu}{\sigma}$$

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<u>*Note*</u>: In the preceding examples this was not important because all predictor variables in the iris dataset are similar in terms of magnitude and variability

In **regression** problems…

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To **predict** a **continuous** target variable, based on some **similarity measure in the predictors' space.**

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New instance to be predicted

To take into account:
- Predictor variables which are larger in magnitude and/or variability may have more weight in the search of neighbors. Thus, **standardizing the predictor data is highly recommended** to make the distance metric more meaningful $Z = \frac{X - \mu}{\sigma}$
- Likewise, outlier values in the predictors' space may bias the search for neighbors. Thus, if needed, the **removal of outliers is recommended**

For regression, we will work with the dataset ***carseats*** *(included in the package* ***ISLR****). Our target variable will be* ***Sales****. First, we will remove 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 (in terms of the RMSE) varies with k***

Examples in R

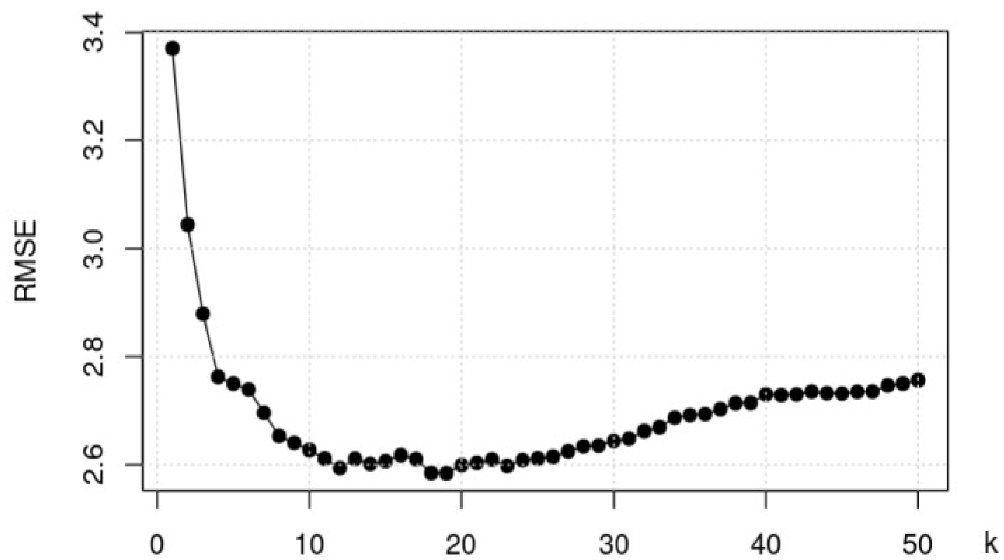
*For regression, we will work with the dataset **carseats** (included in the package **ISLR**). Our target variable will be **Sales**. First, we will remove all the categorical variables from the dataset, retaining only the continuous ones. We will use the function **knn.reg** from the package **FNN**. 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 (in terms of the RMSE) varies with k***

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

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

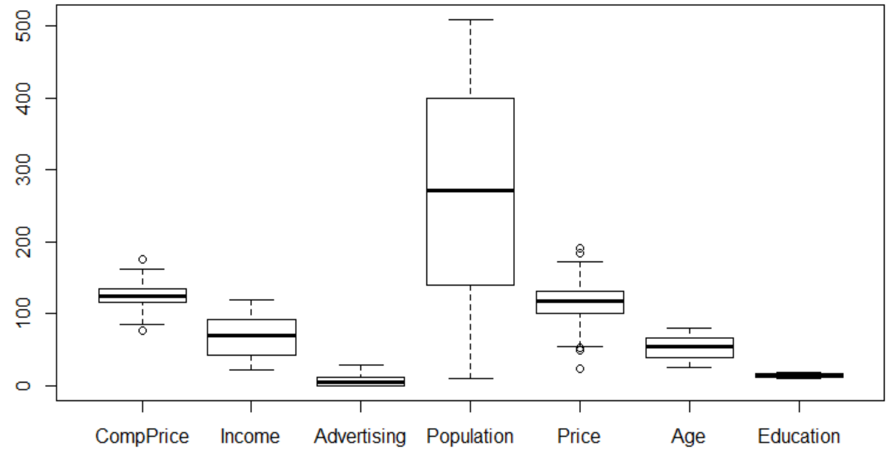
## train/test division
n = nrow(dataset)
indtrain = sample(1:n, round(0.75*n));
dataset.train = dataset[indtrain, ]
indtest = setdiff(1:n, indtrain);
dataset.test = dataset[indtest, ]
```

```
## test error as a function of k, from k=1 to k=50
library(FNN)
kmax = 50
test.err = rep(***)
for (k in 1:kmax) {
  pred = knn.reg(***)
  test.err[k] = rmse(***)
}
plot(1:kmax, test.err, type = "o", pch = 19,
xlab = "k", ylab = "RMSE"); grid()
```



Continue with the same example. Let's now assess the ***effect of standardizing the predictor data****. Use the function* ***scale***

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



*Continue with the same example. Let's now assess the **effect of standardizing the predictor data**. Use the function **scale***

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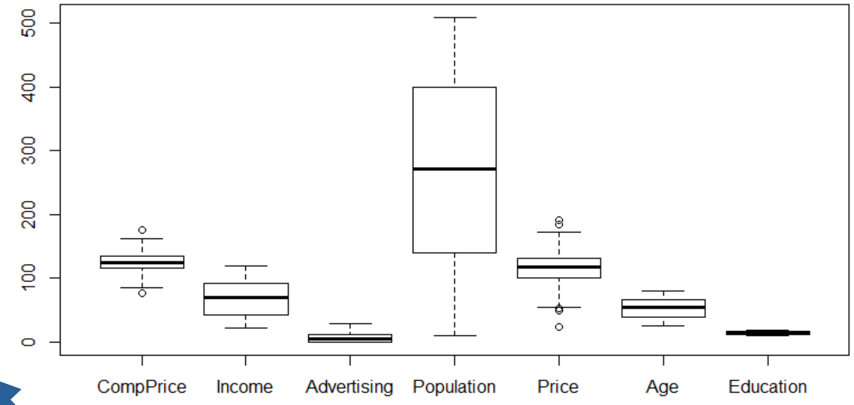
## predictor ranges
boxplot(dataset[,-1])
```




```
## predictor standardization
params.scaling = preProcess(***,
                method = ***)
x.train.scaled = scale(***,
              center = ***, scale = ***)
x.test.scaled = scale(***,
              center = ***, scale = ***)
```

```
## test error as a function of k (for standardized predictors)
test.err2 = rep(***)
for (k in 1:kmax) {
  ## prediction
  pred = knn.reg(***)
  ## validation
  test.err2[k] = rmse(***)
}
```

```
## plotting results
matplot(1:kmax, cbind(***),
        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()
```

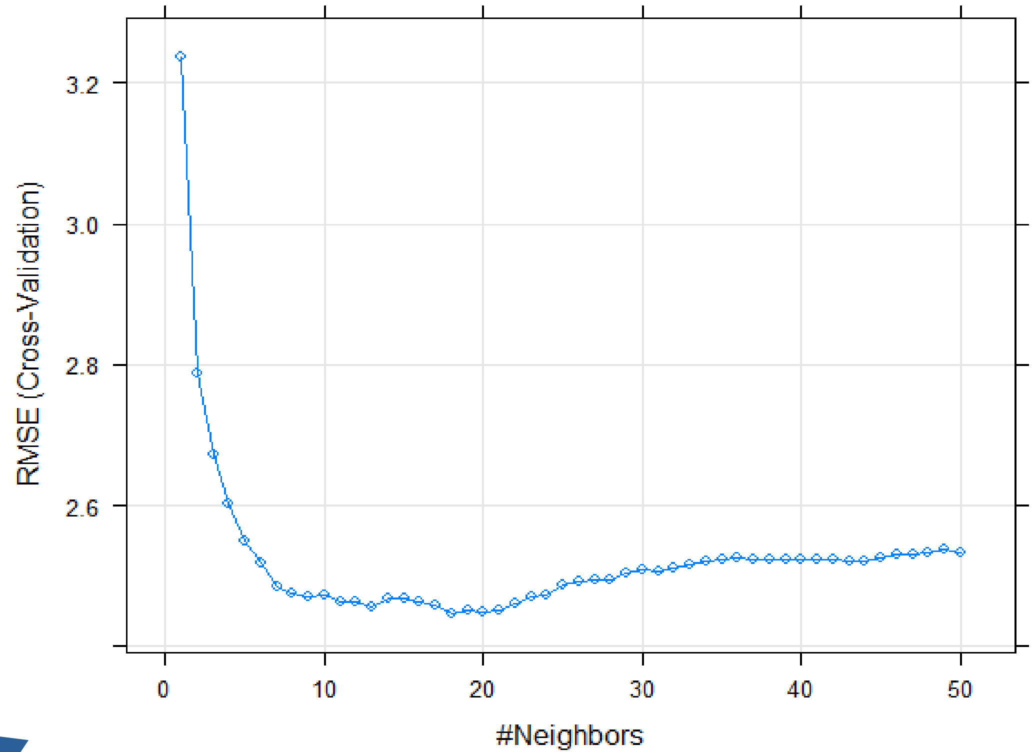
Be careful: Standardization must be properly done!

*Do the **same exercise**, but this time using **caret**, under a **2-fold cross-validation scheme**. Recall to standardize your predictor data to obtain meaningful results*

```
## defininig 2-fold cross-validation
trctrl <- trainControl(***)
```

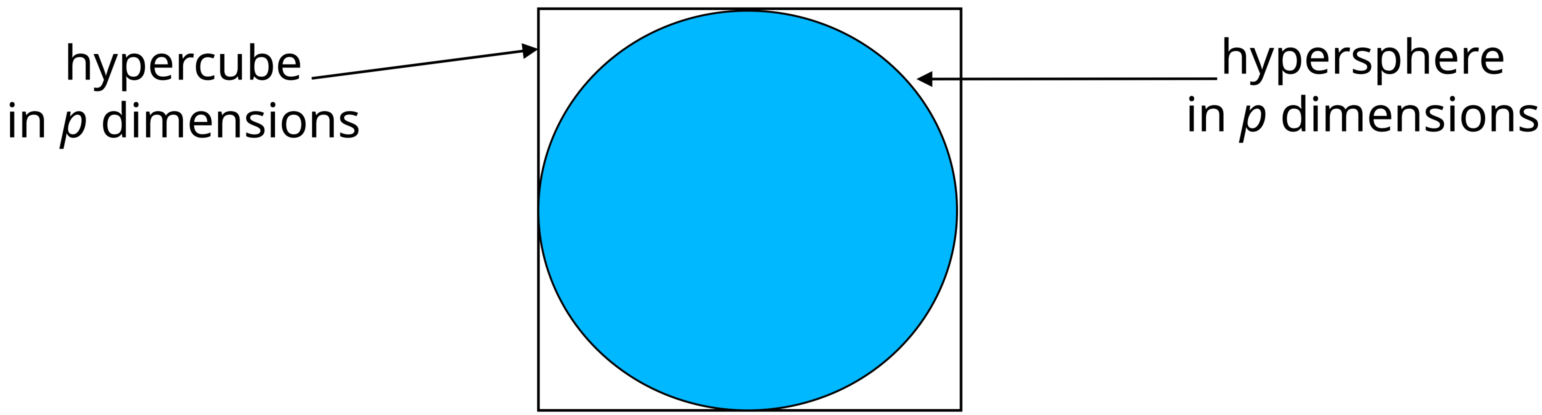
```
## searching the optimal k
(with standardized data)
knn.fit <- train(, data = ***,
              method = "***",
              trControl = ***,
              preProcess = ***,
              tuneGrid = ***)
plot(***)
```

```
## predicting in test with the optimal k
pred = predict(***)
## evaluation of test error
rmse(***)
```



Would you say your model is overfitted/underfitted?

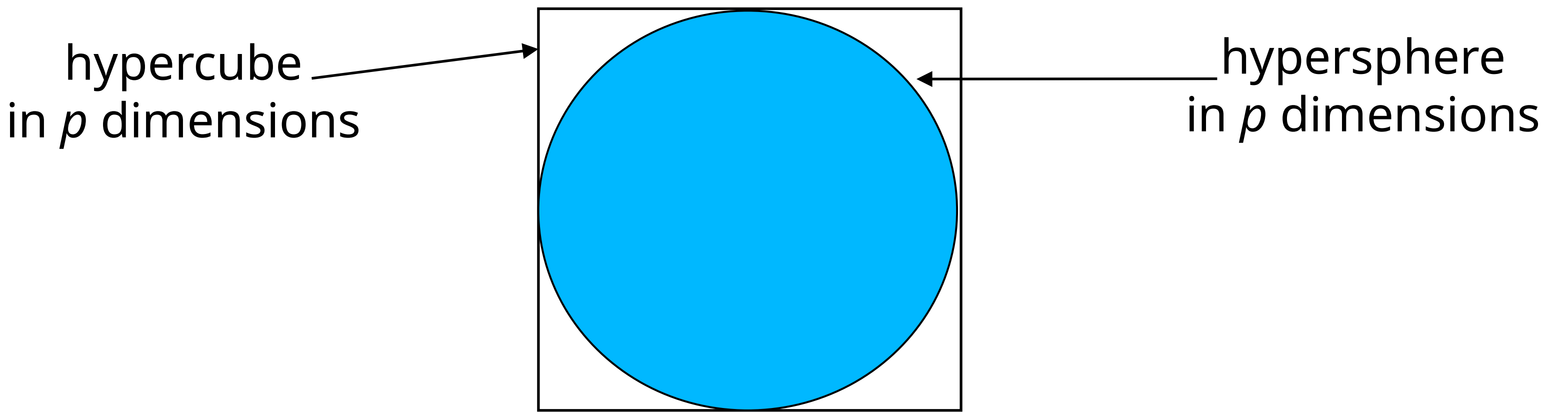
David Scott, Multivariate Density Estimation, Wiley, 1992



Volume of the sphere relative to that of the cube?

Dimension	**2**
Rel. vol.	**0.79**

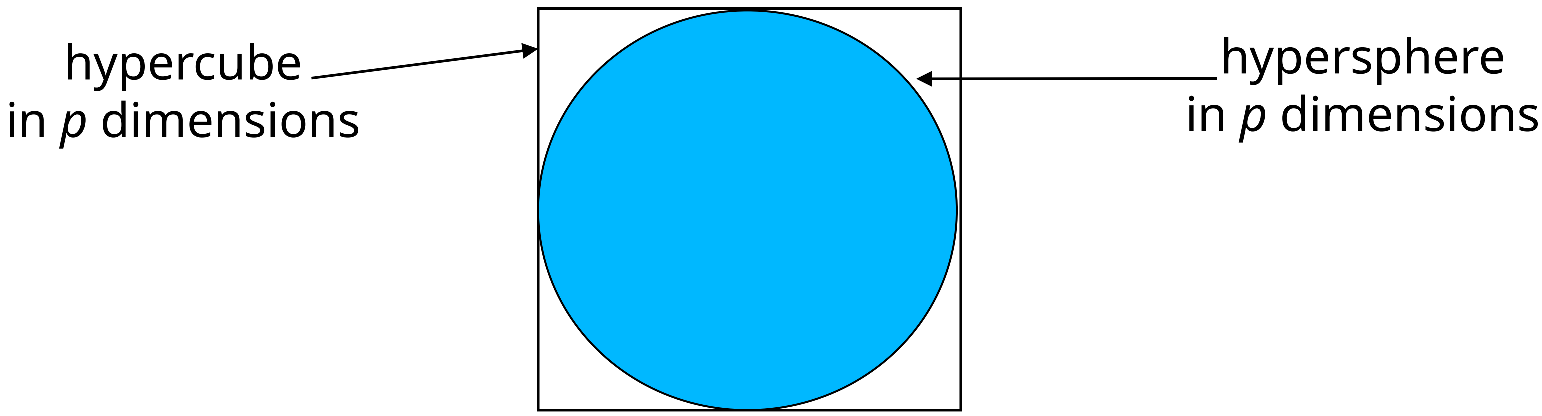
David Scott, Multivariate Density Estimation, Wiley, 1992



Volume of the sphere relative to that of the cube?

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

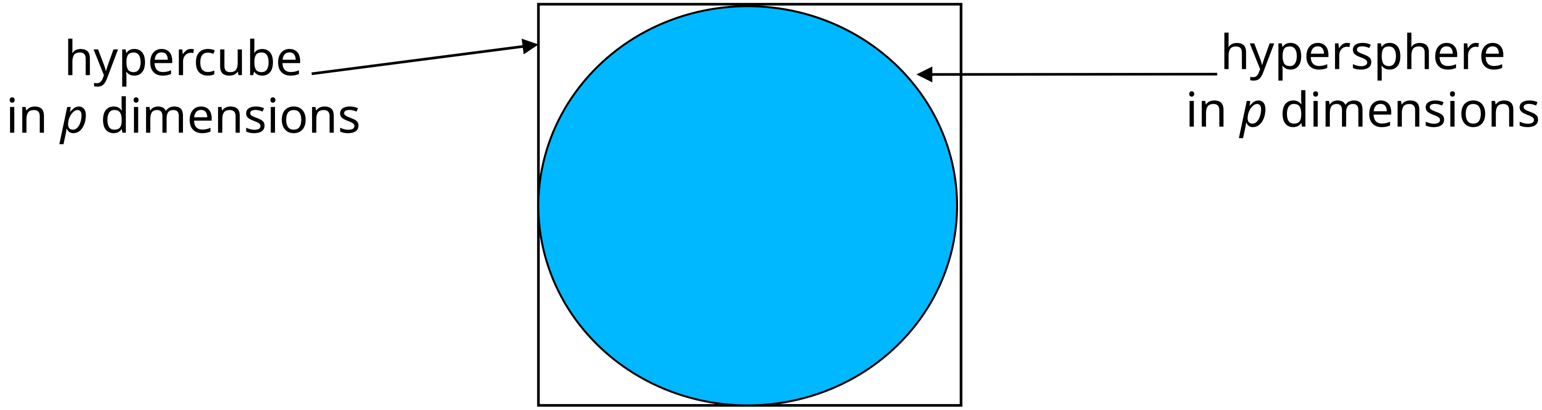
David Scott, Multivariate Density Estimation, Wiley, 1992



Volume of the sphere relative to that of the cube?

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

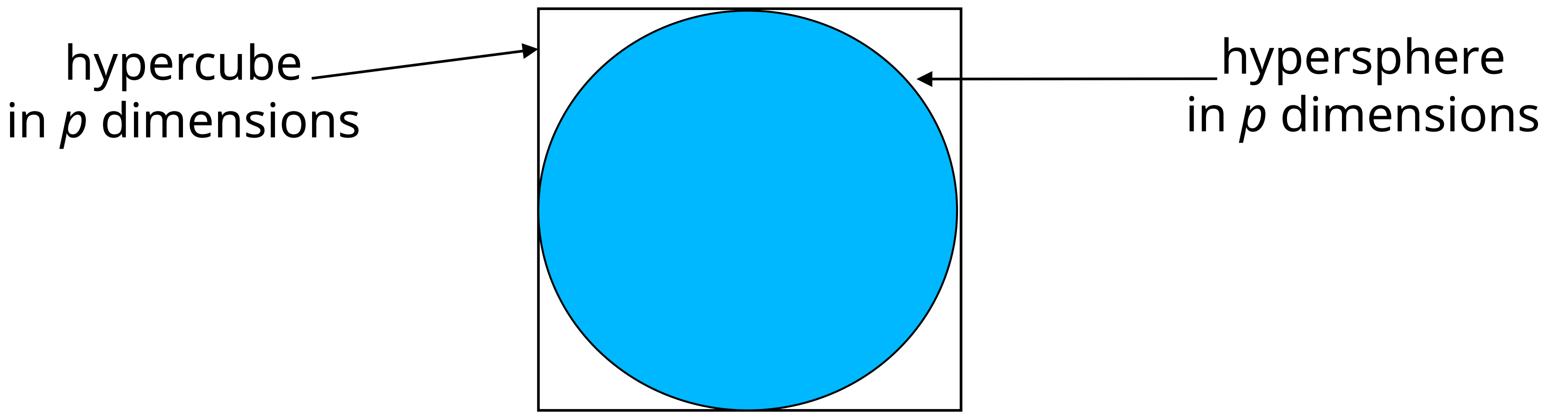
David Scott, Multivariate Density Estimation, Wiley, 1992



Volume of the sphere relative to that of the cube?

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

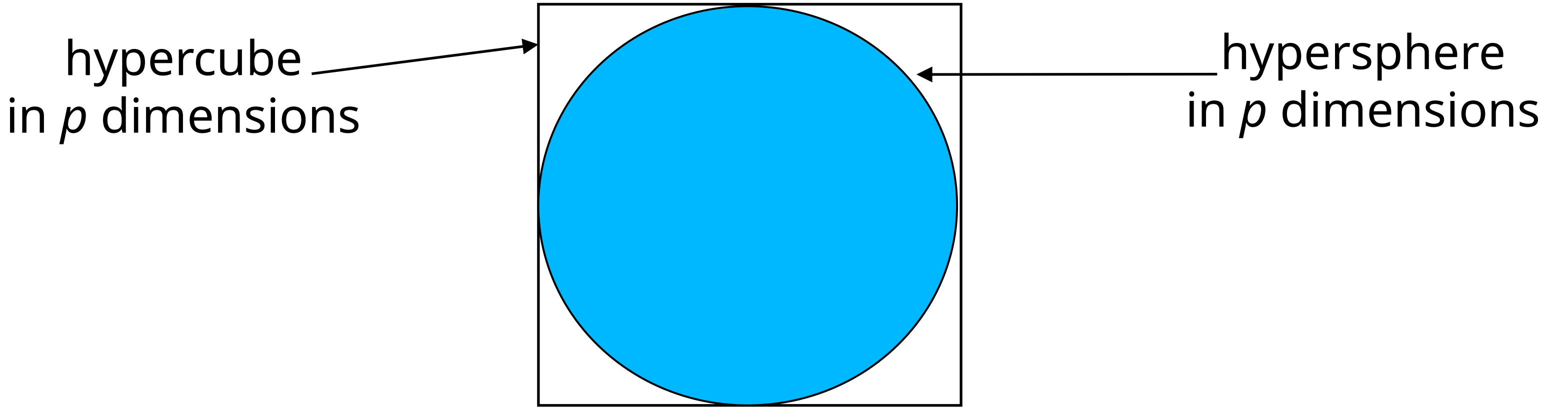
David Scott, Multivariate Density Estimation, Wiley, 1992



Volume of the sphere relative to that of the cube?

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

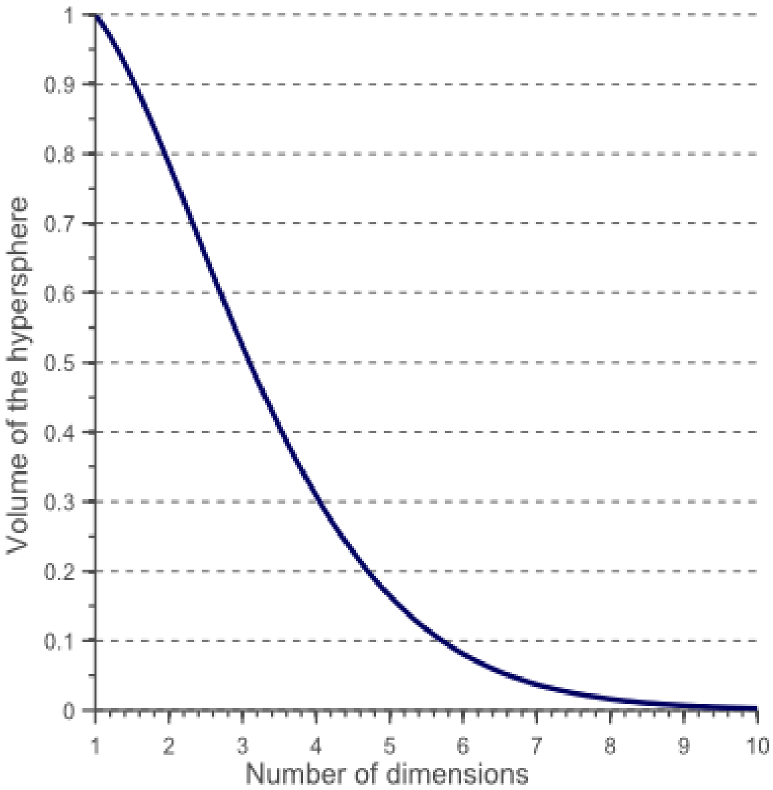
David Scott, Multivariate Density Estimation, Wiley, 1992



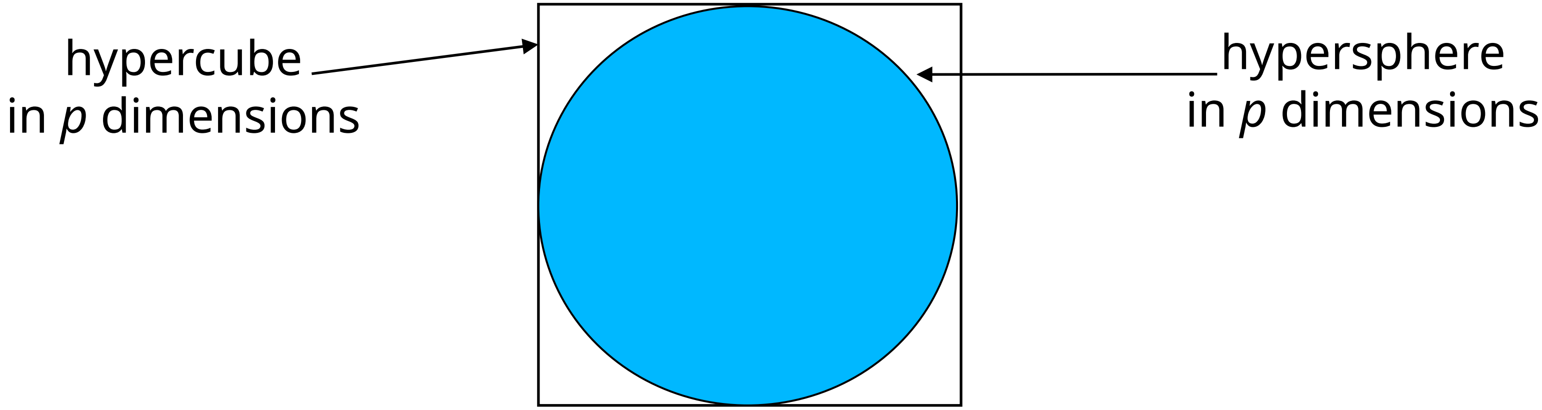
Volume of the sphere relative to that of the cube?

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

Any thought?

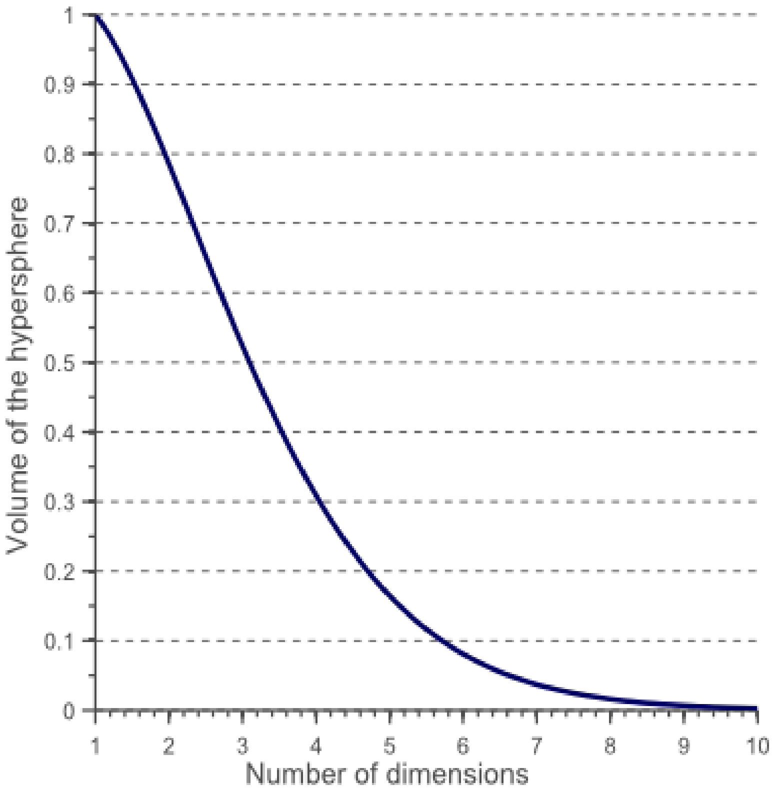


David Scott, Multivariate Density Estimation, Wiley, 1992



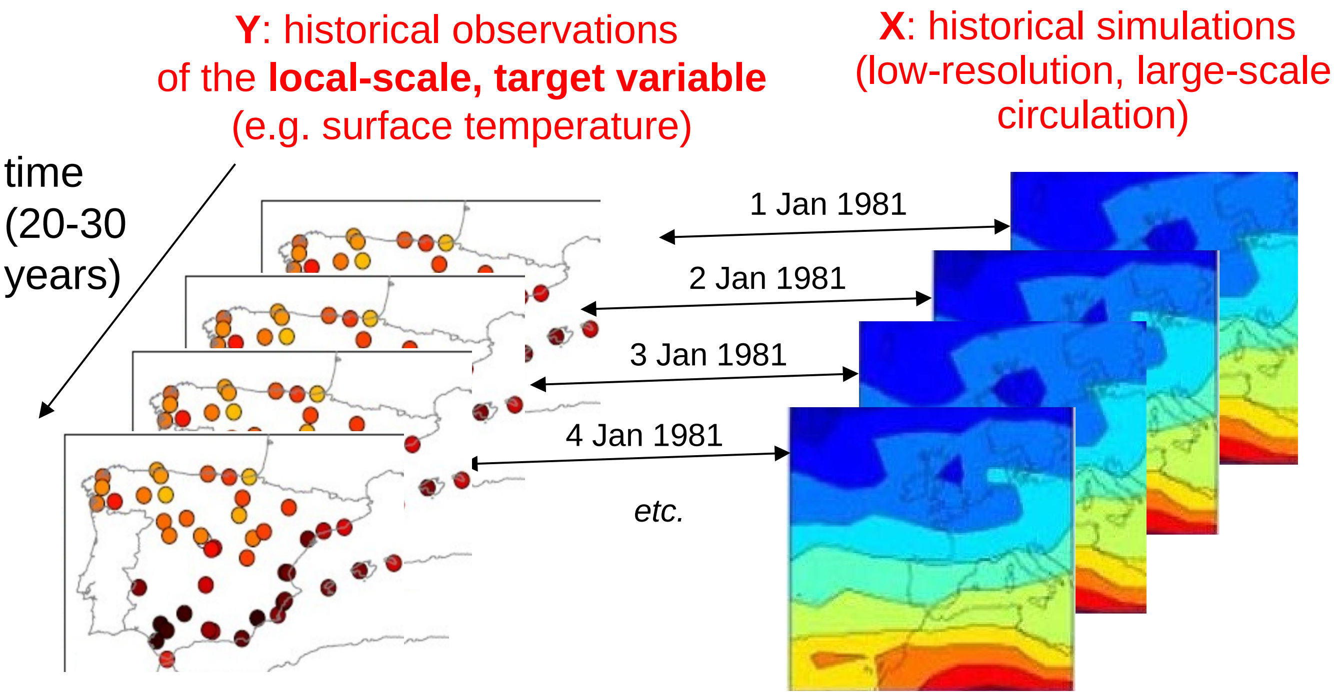
Volume of the sphere relative to that of the cube?

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



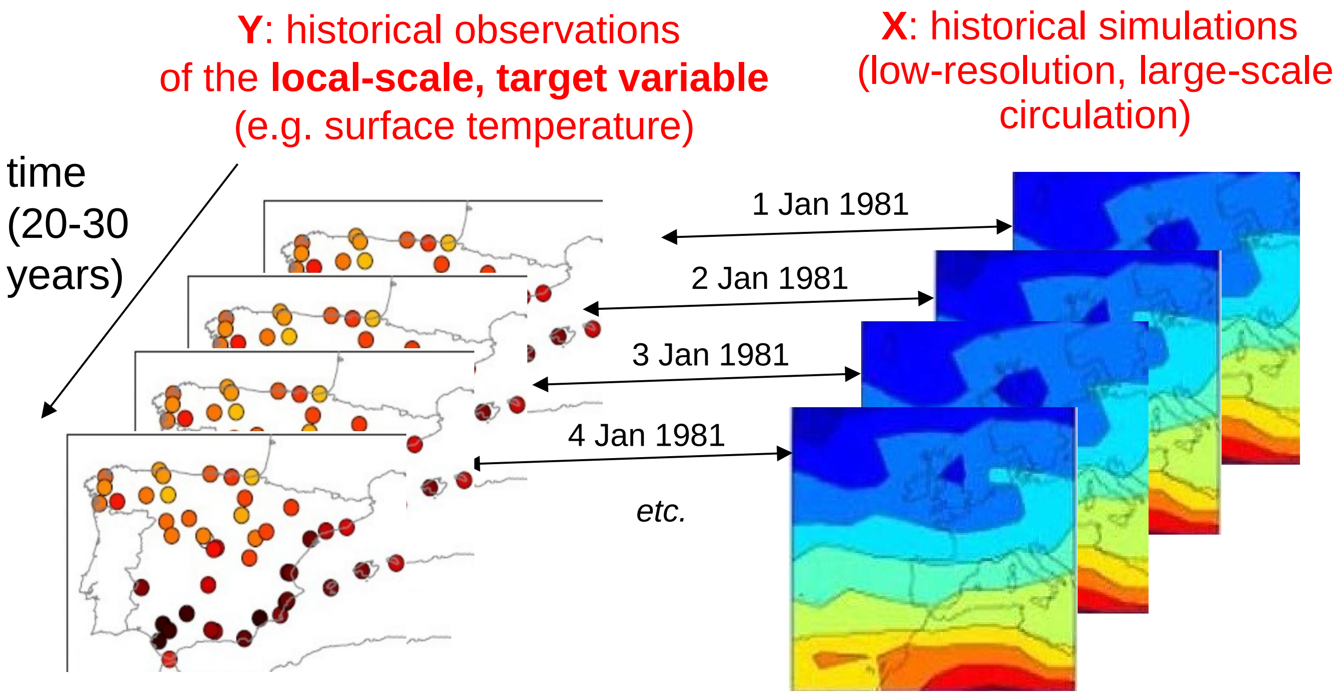
As dimensionality increases, a larger percentage of the training data resides in the corners of the predictors' space. Therefore, ***k*-NN is unhelpful in high dimensional problems** because distances are less meaningful.

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



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

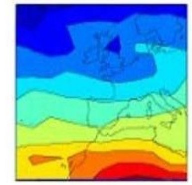
Problem: Y' (projection) for 26 Mar 2046?



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

Problem: Y' (projection) for 26 Mar 2046?

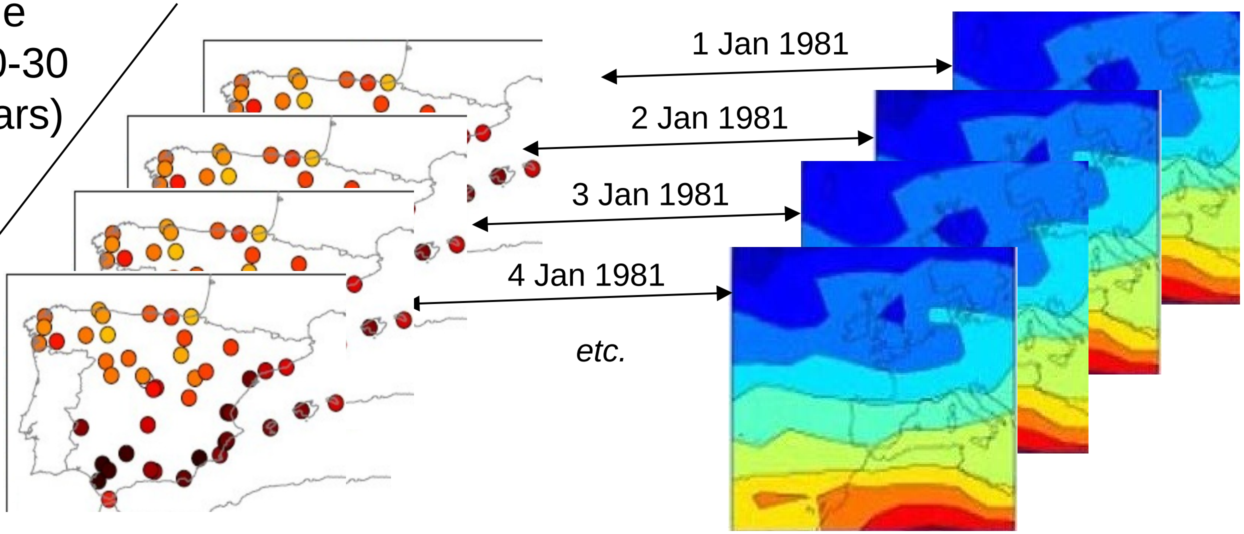
1) Take X' for 26 March 2046: $X'_{26\text{-}03\text{-}2046}$



Y: historical observations of the **local-scale, target variable** (e.g. surface temperature)

X: historical simulations (low-resolution, large-scale circulation)

time (20-30 years)



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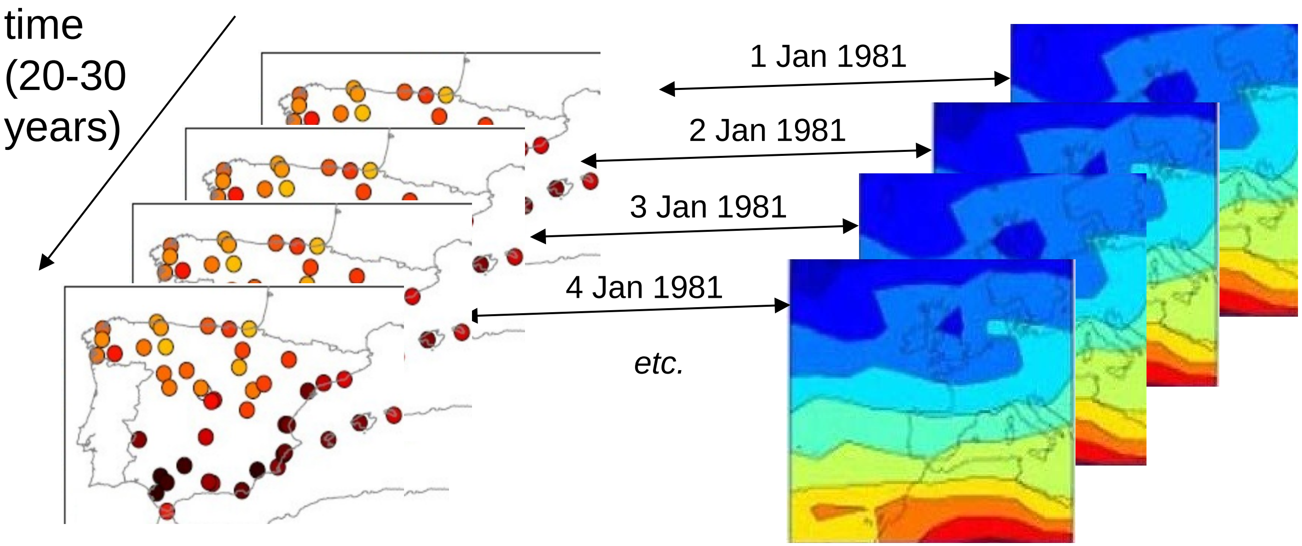
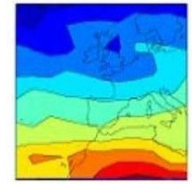
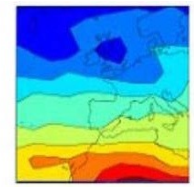


1) Take X’ for 26 March 2046: $X'_{26\text{-}03\text{-}2046}$



2) Search the nearest neighbor/s to $X'_{26\text{-}03\text{-}2046}$ within X. Let’s suppose k=1



$X_{03\text{-}01\text{-}1981}$

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

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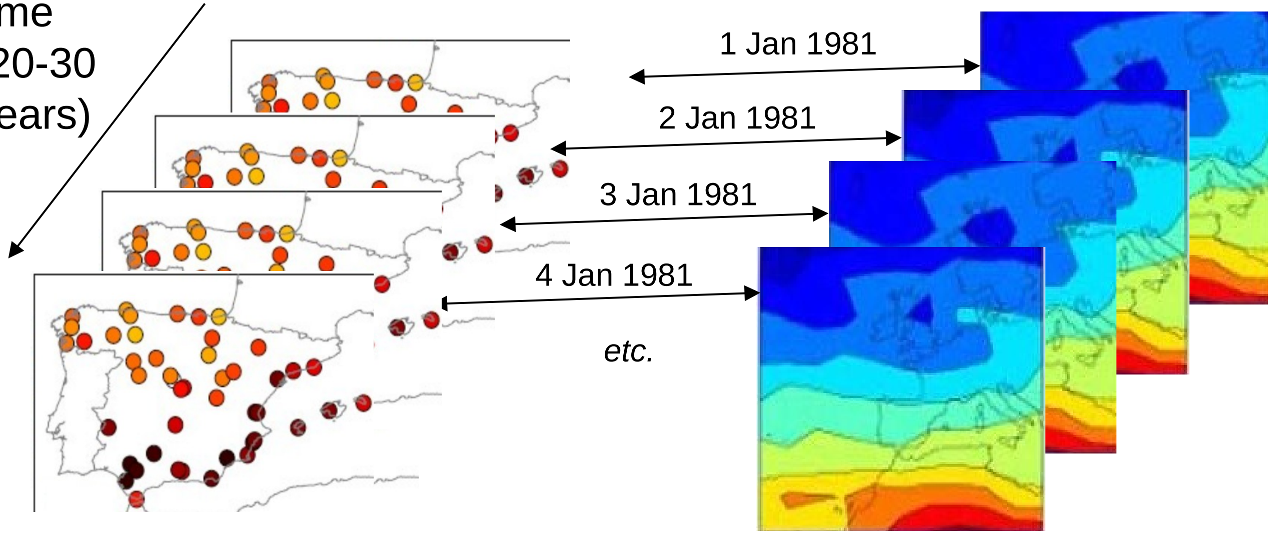

Problem: Y' (projection) for 26 Mar 2046?

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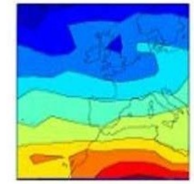

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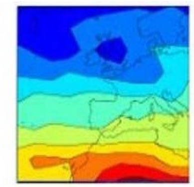

$X_{03\text{-}01\text{-}1981}$

Can you imagine what the projection for 26 Mar 2046 will be?

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

Problem: Y' (projection) for 26 Mar 2046?

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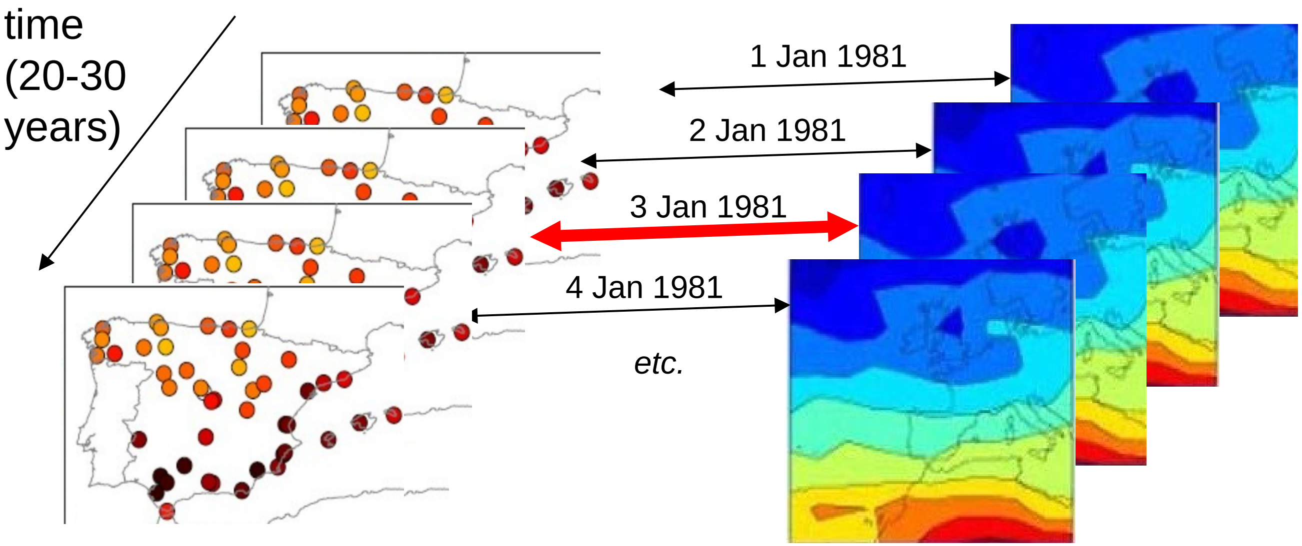
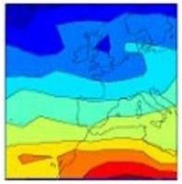
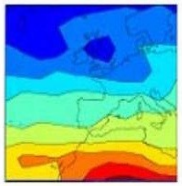


1) Take X' for 26 March 2046: $X'_{26\text{-}03\text{-}2046}$

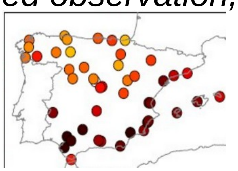


2) Search the nearest neighbor/s to $X'_{26\text{-}03\text{-}2046}$ within X. Let's suppose k=1



$X_{03\text{-}01\text{-}1981}$

3) The projection made, $Y'_{26\text{-}03\text{-}2046}$, is the recorded observation, $Y_{03\text{-}01\text{-}1981}$

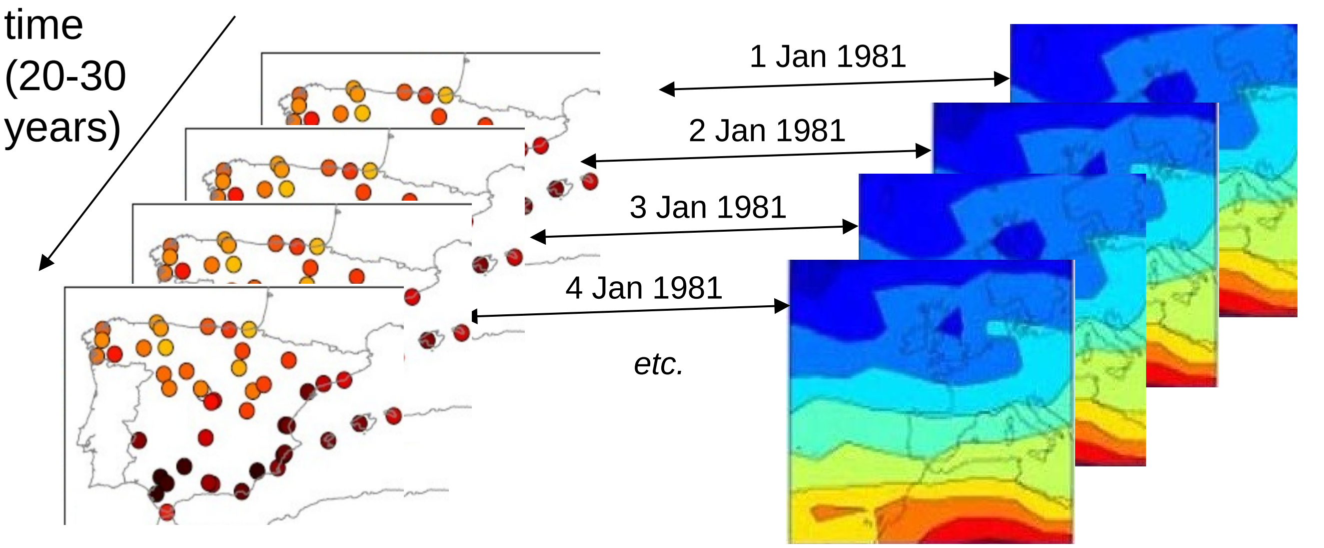


The analog technique (Lorenz, 1969): Similar atmospheric patterns lead to similar meteorological conditions

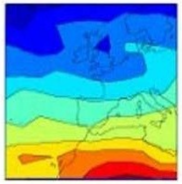
Problem: Y' (projection) for 26 Mar 2046?

Y: historical observations of the **local-scale, target variable** (e.g. surface temperature)

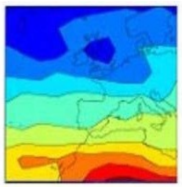
X: historical simulations (low-resolution, large-scale circulation)



1) Take X' for 26 March 2046: $X'_{26\text{-}03\text{-}2046}$

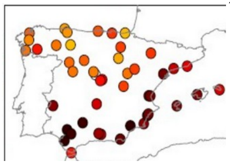


2) Search the nearest neighbor/s to $X'_{26\text{-}03\text{-}2046}$ within X. Let's suppose k=1



$X_{03\text{-}01\text{-}1981}$

3) The projection made, $Y'_{26\text{-}03\text{-}2046}$, is the recorded observation, $Y_{03\text{-}01\text{-}1981}$



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

- Large differences exist, in magnitude and variability, across predictors: **Scaling** must be applied
- The dimensionality of the predictors' space can be very large: **Dimensionality reduction** techniques (e.g. PCA) are commonly used

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

Y: historical observations of the **local-scale, target variable** (e.g. surface temperature)

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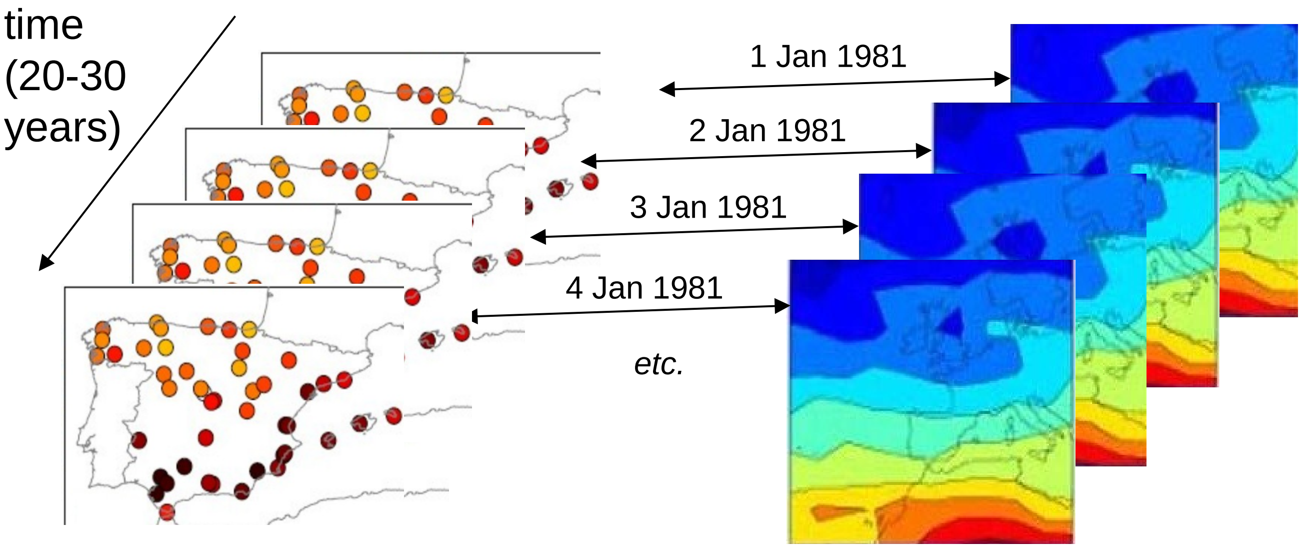
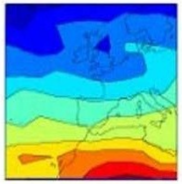
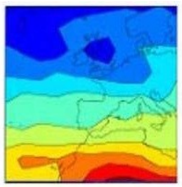


Problem: Y' (projection) for 26 Mar 2046?

1) Take X' for 26 March 2046: $X'_{26\text{-}03\text{-}2046}$

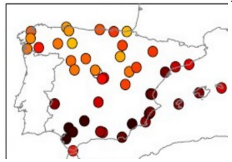


2) Search the nearest neighbor/s to $X'_{26\text{-}03\text{-}2046}$ within X. Let's suppose k=1



$X_{03\text{-}01\text{-}1981}$

3) The projection made, $Y'_{26\text{-}03\text{-}2046}$, is the recorded observation, $Y_{03\text{-}01\text{-}1981}$



Is there any **limitation** you may think of in a **climate change** context?

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

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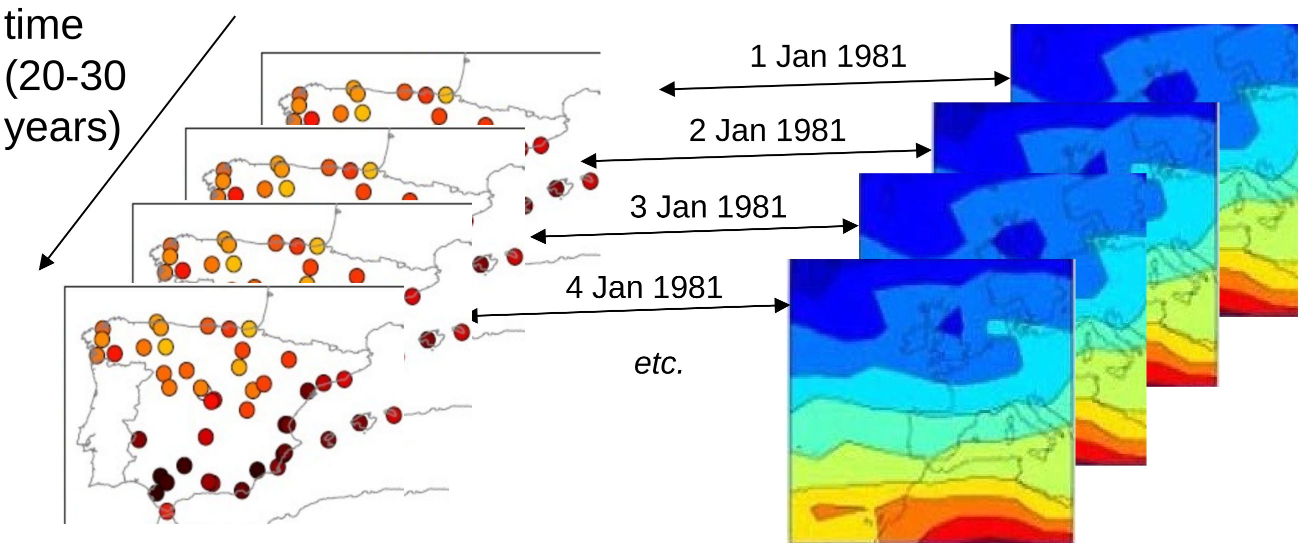
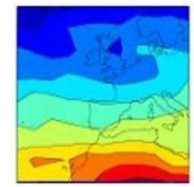


Problem: Y' (projection) for 26 Mar 2046?

1) Take X' for 26 March 2046: $X'_{26\text{-}03\text{-}2046}$



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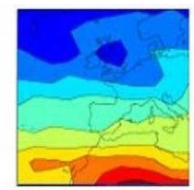

$X_{03\text{-}01\text{-}1981}$

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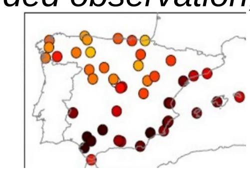

k-NN has **no ability for extrapolation** beyond the learning space!