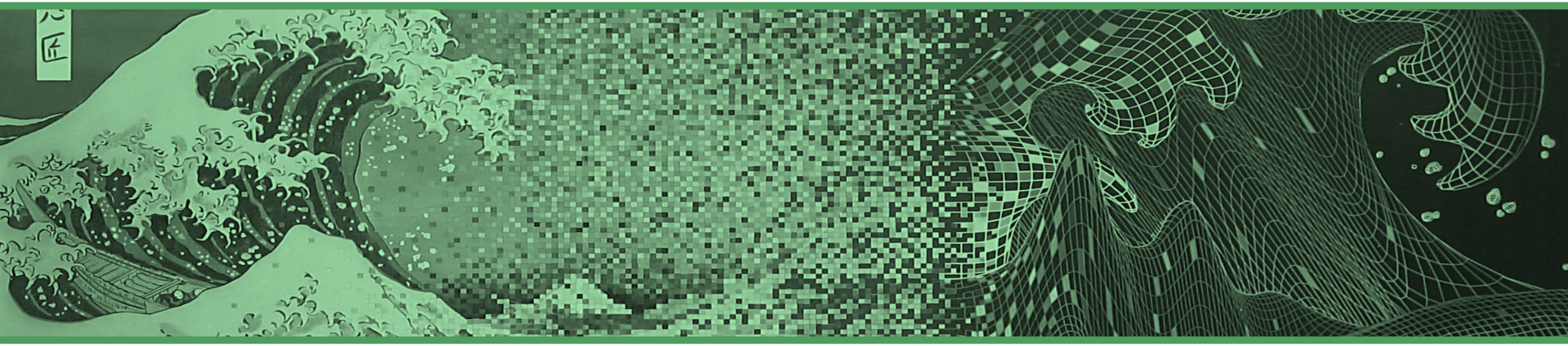
TÉCNICO LISBOA

Lazy learning

Local learning in the vector space



Aprendizagem 2024

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Outline

- **Learning in the vector space**
  - from univariate to multivariate data spaces
  - Minkowski distances
  - norm and cosine similarity
  - encodings for categoric variables and mixed data
- **Instance-based learning**
  - parametric vs non-parametric models
  - k-nearest neighbor classifier
  - k-nearest neighbor regressor
  - distance-based kNN
  - challenges: non-iid variables and dimensionality

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  - **Minkowski distances**
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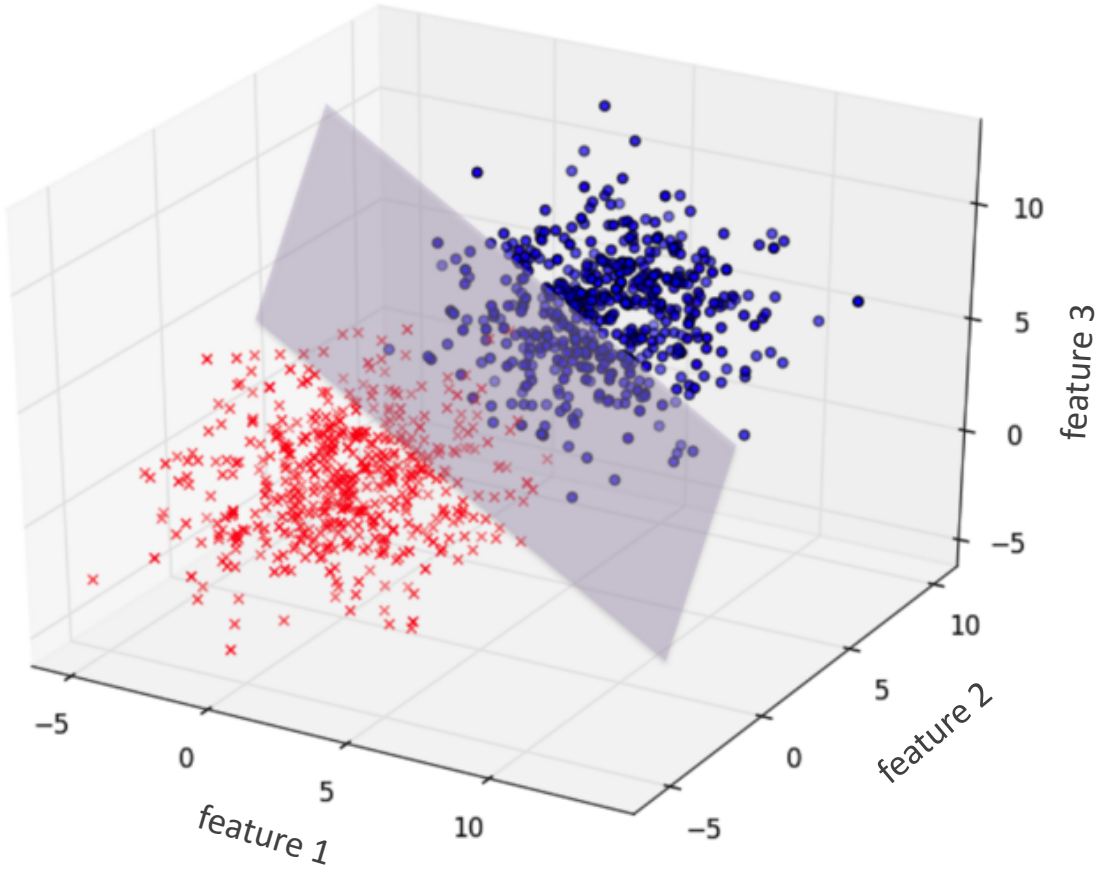
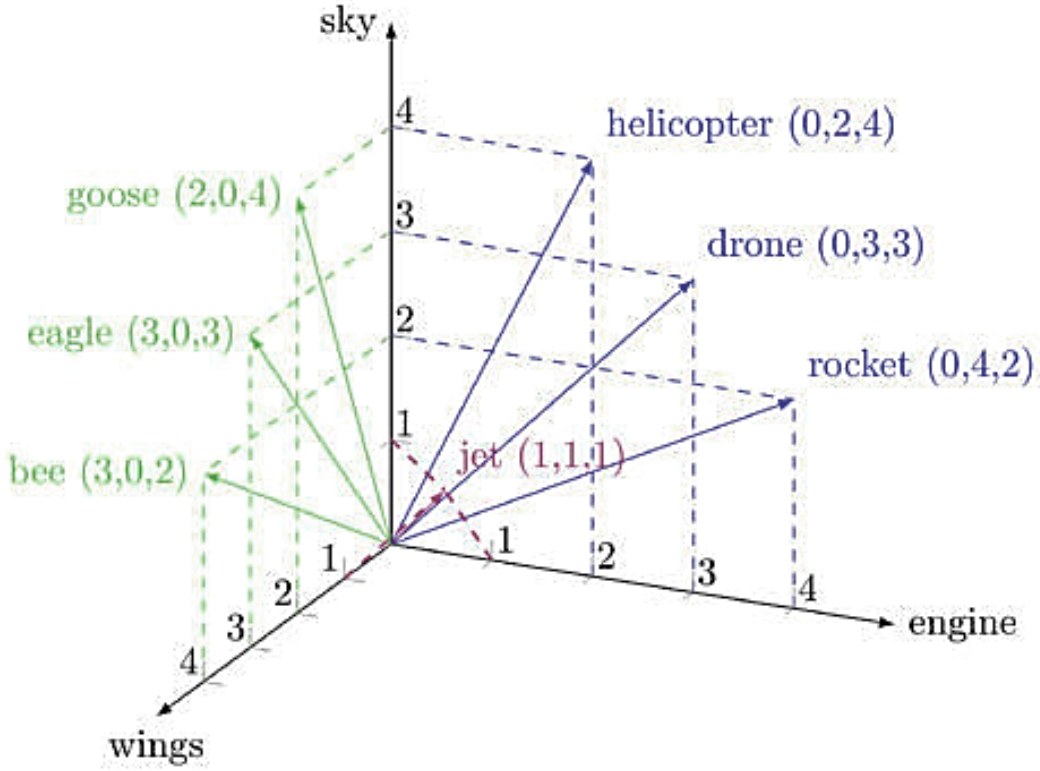
Multivariate feature space



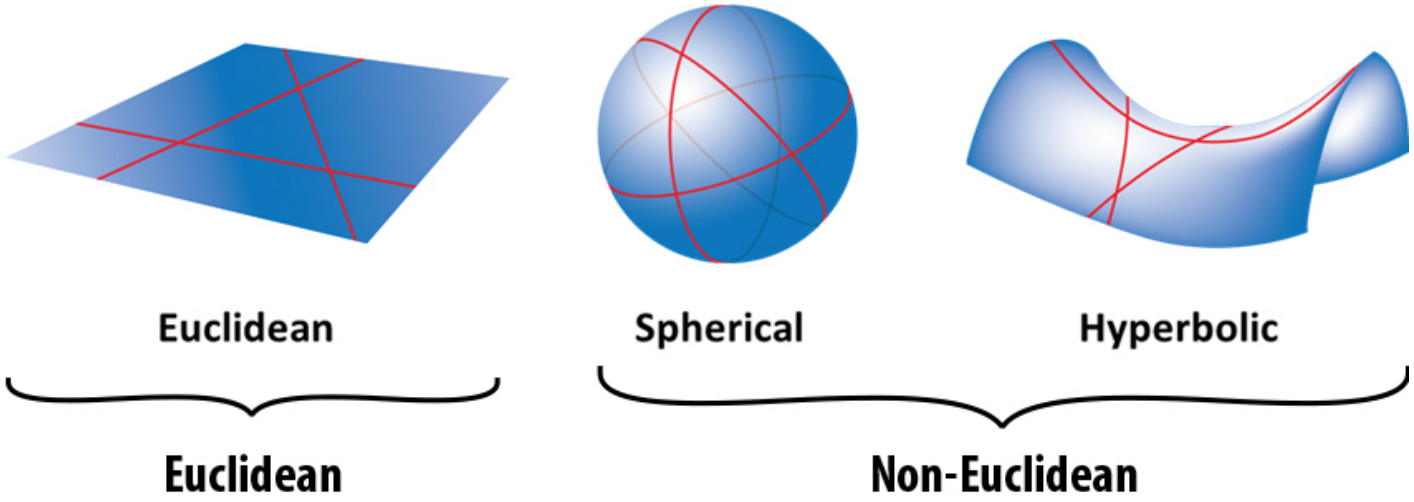


Feature space

- Recall the principles behind the feature space
  - a **feature** is an individual measurable property or characteristic of a phenomenon
    - phenomena is described by a random variable
  - features are usually **numeric** or **categorical**
    - yet **structural features** such as images, videos, strings, time series or graphs can be as well observed
  - recall that a **multivariate observation** of order m is a data instance with m features
  - the set of possible features forms a m-**dimensional feature space** (or m-order multivariate space)
  - when features are numeric:
    - the m-dimensional feature space is a $\mathbb{R}^m$ Euclidean space
    - each observation can be conveniently described by a **point** or **vector** in this $\mathbb{R}^m$ space
  - we will see how can we bring categorical features later on

Feature space

- Bivariate data spaces
  - vector properties and distances are generally assessed on a Euclidean plane
  - alternative continuous spaces yield properties of interest



- Question: consider a single variable that measures the orientation of the wind from 0º to 360º
  - is the univariate Euclidean space that best option for this univariate data space?

Distances and metrics

- A distance function is a **metric** if the following conditions are met:
  - nonnegative:

    $$d(\mathbf{x},\ \mathbf{y})\ \geq\ 0$$

  - distance of a point to itself is zero:

    $$d(\mathbf{x},\ \mathbf{x})\ =\ 0$$

  - symmetry:

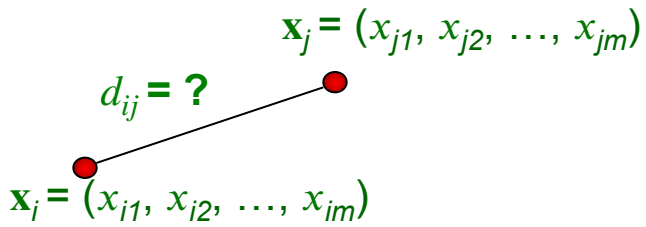
    $$d(\mathbf{x},\ \mathbf{y})\ =\ d(\mathbf{y},\ \mathbf{x})$$

  - triangular inequality:

    $$\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V,\ d(\mathbf{x}, \mathbf{y}) \leq d(\mathbf{x}, \mathbf{z}) + d(\mathbf{z}, \mathbf{y})$$

Common distance metrics

(numeric data)



Minkowski distance

$$d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt[q]{\left|x_{i1} - x_{j1}\right|^q + \left|x_{i2} - x_{j2}\right|^q + \ldots + \left|x_{im} - x_{jm}\right|^q}$$

1st dimension 2nd dimension pth dimension

Euclidean distance

q = 2

$$d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\left|x_{i1} - x_{j1}\right|^2 + \left|x_{i2} - x_{j2}\right|^2 + \ldots + \left|x_{im} - x_{jm}\right|^2}$$

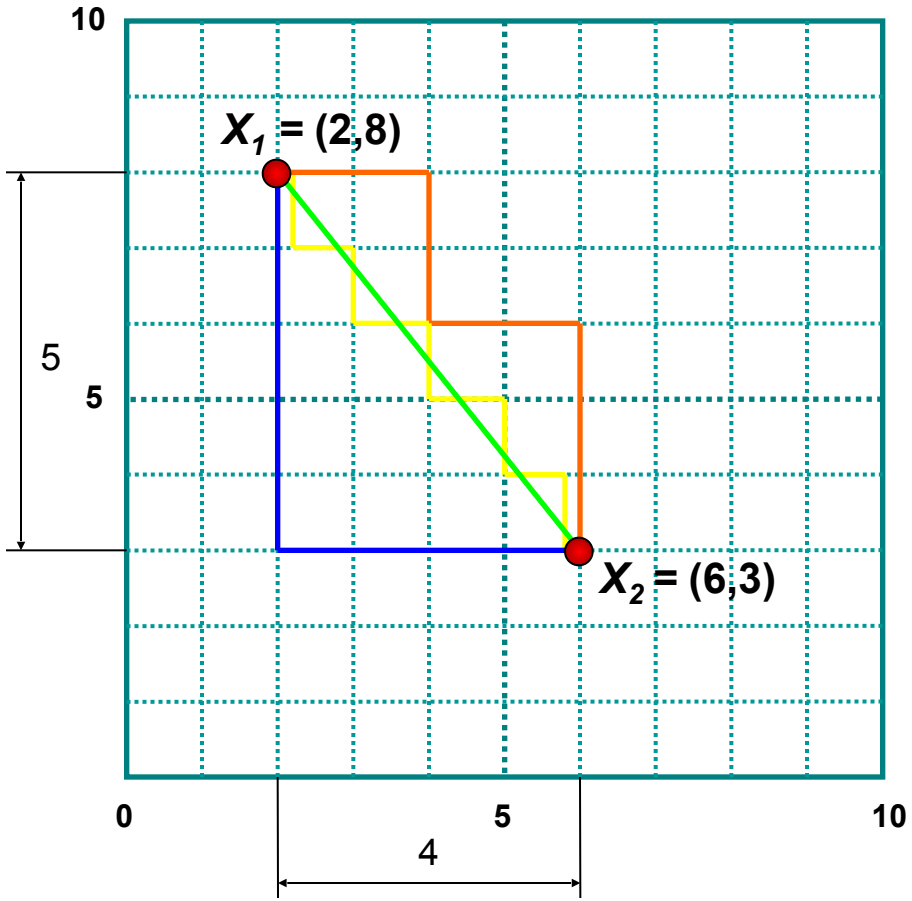
Manhattan distance

q = 1

$$d(\mathbf{x}_i, \mathbf{x}_j) = \left|x_{i1} - x_{j1}\right| + \left|x_{i2} - x_{j2}\right| + \ldots + \left|x_{im} - x_{jm}\right|$$

Common distance metrics

(numeric data)



2D example

$\mathbf{x}1$ = (2,8)

$\mathbf{x}2$ = (6,3)

Euclidean distance

$$d(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{\left|2-6\right|^2 + \left|8-3\right|^2} = \sqrt{41}$$

Manhattan distance

$$d(\mathbf{x}_1, \mathbf{x}_2) = \left|2-6\right| + \left|8-3\right| = 9$$

Chebyshev distance

(numeric data)

- In case of $q \to \infty$, the metric selects the error associated with the highest dissimilar feature
- Useful if the worst case must be avoided:

$$d_{\infty}(\mathbf{x}, \mathbf{y}) = \lim_{q \to \infty} \left(\sum_{i=1}^{n} \left| x_i - y_i \right|^q \right)^{\frac{1}{q}}$$

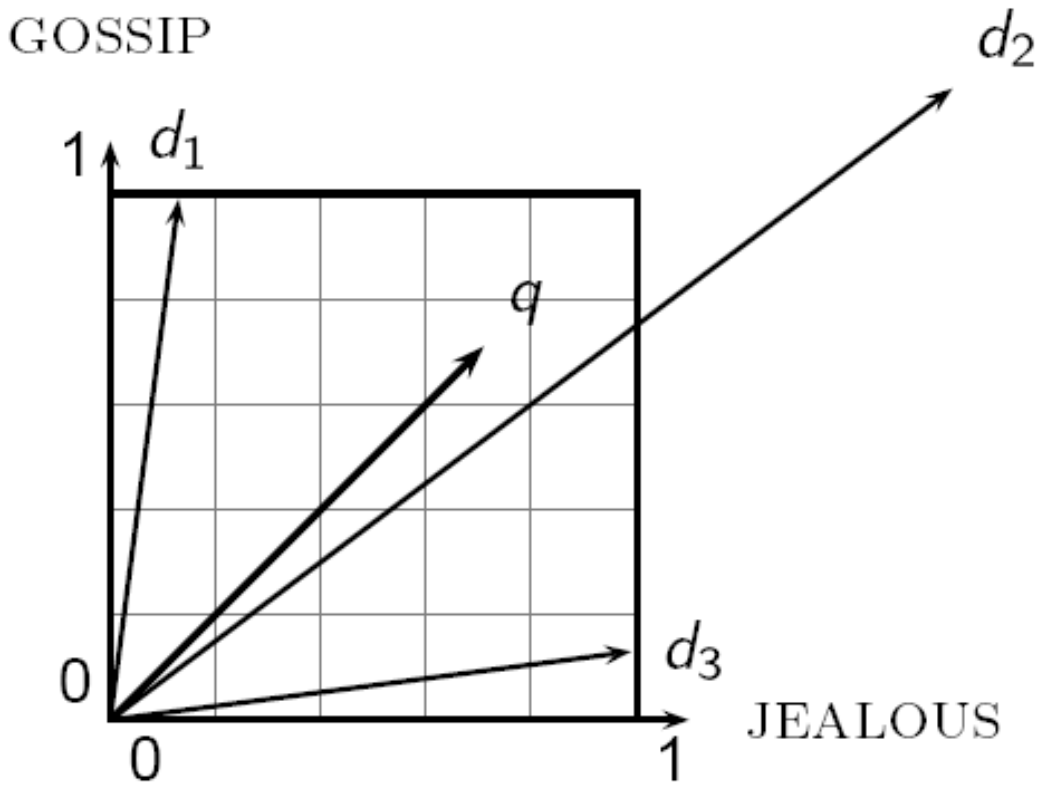
$$= \max\left(\left| x_1 - y_1 \right|, \left| x_2 - y_2 \right|, \ldots, \left| x_n - y_n \right| \right)$$

Example:

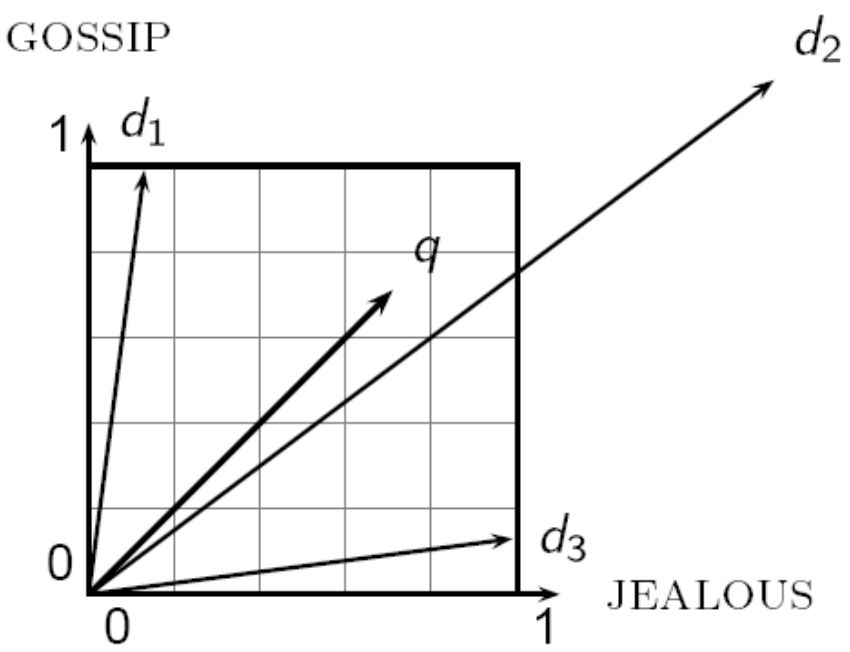
$$d_{\infty}\big((2,8),(6,3)\big) = \max\Big(\big|2-6\big|, \big|8-3\big| \Big) = \max\big(4,5\big) = 5$$

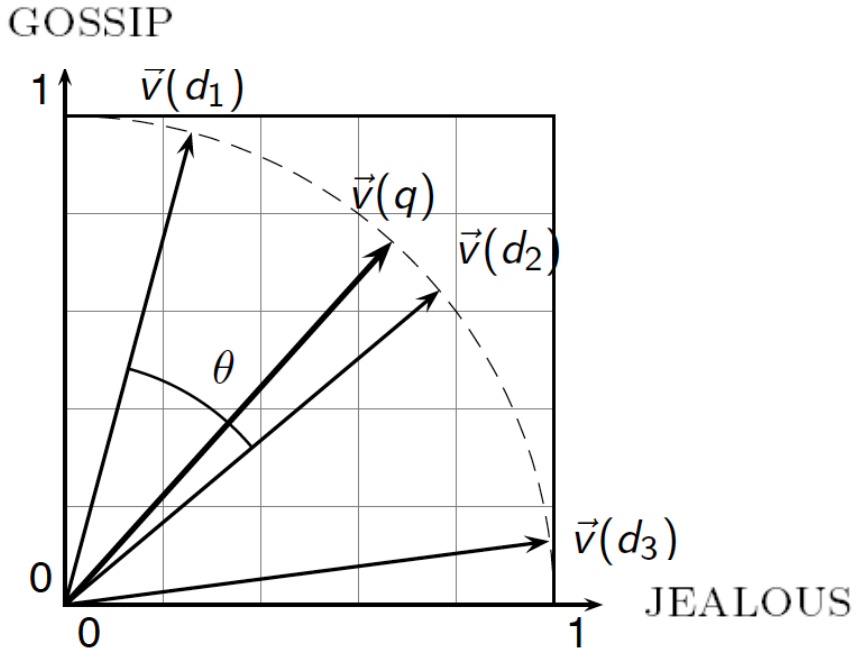
Normalizing vectors?

- Consider the scenario where you have three documents (observations): $\mathbf{d}_1$, $\mathbf{d}_2$ and $\mathbf{d}_3$
  - each document is characterized by the frequency of terms in the text (features)
- Now consider we enter a query $\mathbf{q}$ to retrieve documents similar to $\mathbf{q}$
- Euclidean distance is… a bad idea as it is large for vectors of different lengths
  - the Euclidean distance between $\mathbf{q}$ and $\mathbf{d}2$ is large even though the distribution of terms in the query $\mathbf{q}$ and $\mathbf{d}2$ are very similar



Vector norm





- the normalization of a multivariate observation, should not be misled with *variable normalization*
  - variable normalization guarantees that the measurements of a given variable (e.g. virus concentration) yield statistical properties of interest, e.g. [0,1] or $N(0,1)$

Vector norm

- Given a vector space $\mathbb{R}^m$, the norm is a function that maps a vector $\mathbf{x} \in \mathbb{R}^m$ into a real number, such that:

$$\|\mathbf{x}\| \geq 0$$

$$\|\alpha \cdot \mathbf{x}\| = |\alpha| \times \|\mathbf{x}\| \text{ where } \alpha \text{ is a scalar}$$

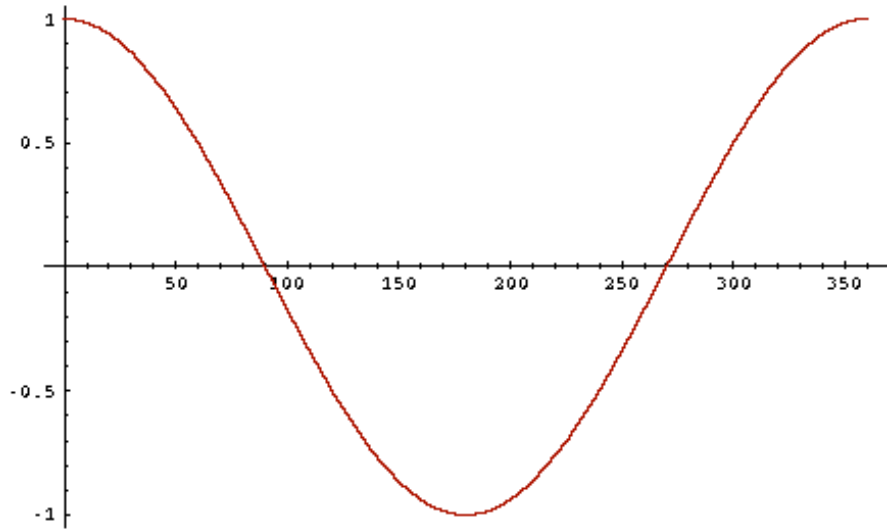
$$\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$$

- The l_p norm (or p-norm), defined by $\|\mathbf{x}\|_p = \left(\sum_{i=1}^{m} x_i^p \right)^{\frac{1}{p}}$
  - $p = 2$ is the Euclidean norm and $\|\mathbf{x}\|_2 = 1$
  - $p = 1$ is the absolute (Manhattan) norm
- To normalize a vector, we divide its values by the vector norm, i.e.:

$$normalize(\mathbf{x}) = \frac{\mathbf{x}}{\|\mathbf{x}\|}$$

From angles to cosines

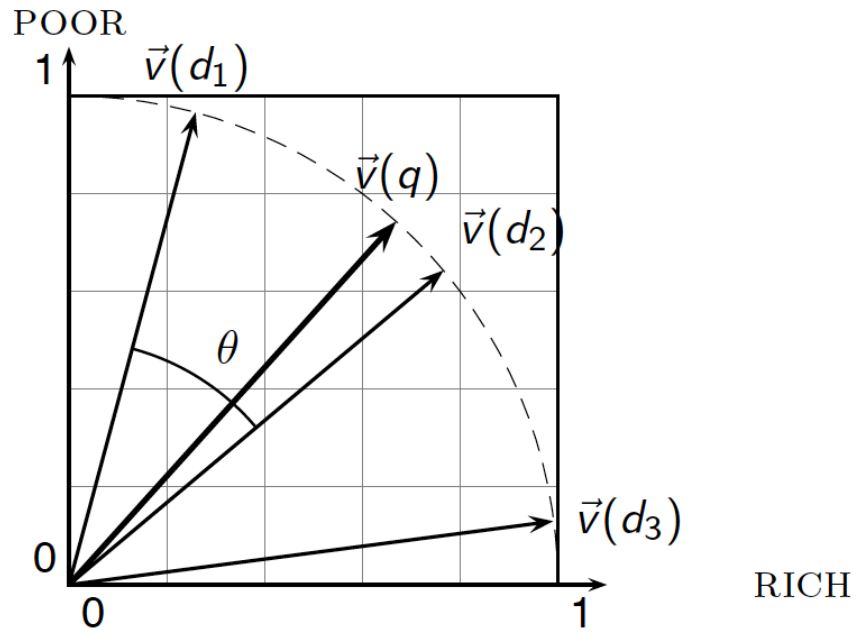
- the following two notions are equivalent:
  - *distance* of the angle between two vectors
  - *similarity* of the cosine between two vectors
- cosine is a monotonically decreasing function on the interval [0°, 180°]



Cosine similarity

$$\cos(\mathbf{x}_1, \mathbf{x}_2) = \frac{\mathbf{x}_1 \bullet \mathbf{x}_2}{\|\mathbf{x}_1\|\|\mathbf{x}_2\|} = \frac{\sum_i x_{1i}\, x_{2i}}{\sqrt{\sum_i x_{1i}^2}\sqrt{\sum_i x_{2i}^2}}$$

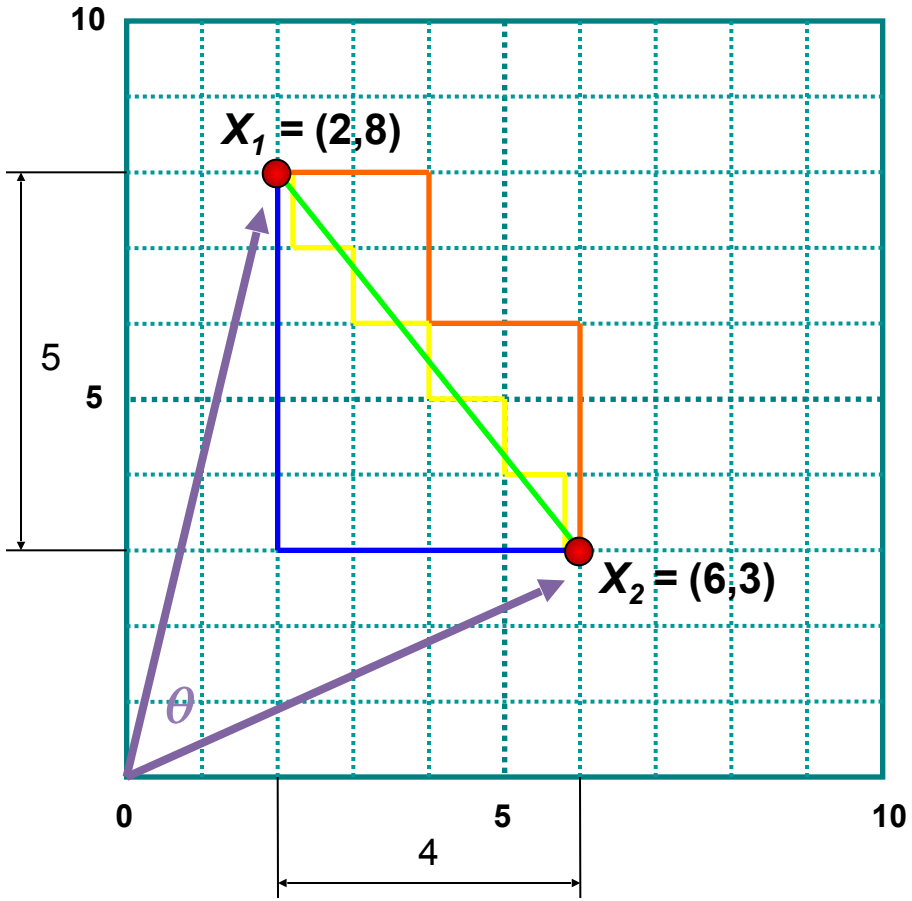
- x_{1i} is the feature from variable y_i in observation $\mathbf{x}_1$
- $\|\mathbf{x}_1\|$ and $\|\mathbf{x}_2\|$ are the (2-norm) lengths of vectors $\mathbf{x}_1$ and $\mathbf{x}_2$
- $\cos(\mathbf{x}_1, \mathbf{x}_2)$ is the (cosine) similarity of $\mathbf{x}_1$ and $\mathbf{x}_2$



For length-normalized vectors, cosine similarity is simply the dot product (or scalar product):

$$\cos(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 \bullet \mathbf{x}_2 = \sum_{i=1}^{m} x_{1i}\, x_{2i}$$

Cosine similarity



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Manhattan distance

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Cosine similarity

$$\cos(\mathbf{x}_1, \mathbf{x}_2) = \frac{\mathbf{x}_1 \bullet \mathbf{x}_2}{\|\mathbf{x}_1\|\|\mathbf{x}_2\|} = \frac{2\times 6 + 8\times 3}{\sqrt{2^2+8^2}\sqrt{6^2+3^2}} = 0.65$$

Correlation

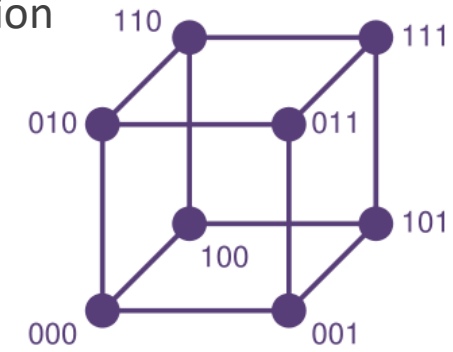
- Assessing similarity between observations can recur to different functions:
  - distance functions
  - cosine angle
  - correlation coefficients
- Recall correlation basics
  - positive (negative): two variables vary in the same (opposite) way
  - maximum (minimum) value of 1 (-1) if $\mathbf{x}_1$ and $\mathbf{x}_2$ are perfectly direct (inverse) correlated
- Example: gene expression arrays

$$\mathbf{x}_1 = (1,2,3,4,5)$$
$$\mathbf{x}_2 = (100,200,300,400,500)$$
$$\mathbf{x}_3 = (5,4,3,2,1)$$

Which genes are similar according to Euclidean and Pearson correlation?

Categorical features

- How do we represent categorical features in a high-dimensional space?
  - Let us start with **binary variables** (e.g. gender)
    - a binary feature can be seen as an axis in a *m*-dimensional where values are constrained to 0 or 1
  - Let us now go to **ordinal variables** (e.g. high-moderate-low)
    - we can find a numeric encoding f for an ordinal variable
      - e.g. $f(high) = 5$, $f(moderate) = 1$, $f(low) = 0$
    - in the absence of an encoding, one can assume equally spaced integers (e.g. 0, 1, 2…)
      - problems?
  - Let us finally consider **nominal variables** with cardinality higher than 2 (e.g. Europe, Africa, America)
    - challenge? As there is no order, we cannot position values along a single axis/dimension
    - solution? Create p axes for a nominal variable with cardinality p
      - only one of the p axes is active (1), while remaining are inactive (0)
      - this operation is called **dummification**
      - some machine learning methods depend on dummification



Hamming distance

(binary and categorical data)

- Simple: number of different features between two feature vectors
  - to compute this distance, we do not need to dummify variables
  - yet if we dummify, the resulting distance is simply $2 \times Hamming$
- Distance of (1011101) and (1001001) is 2
- Distance (2143896) and (2233796) is 3
- Distance between (toned) and (roses) is 3

3-bit binary cube

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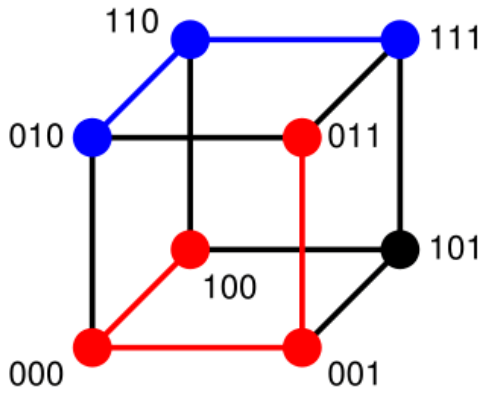
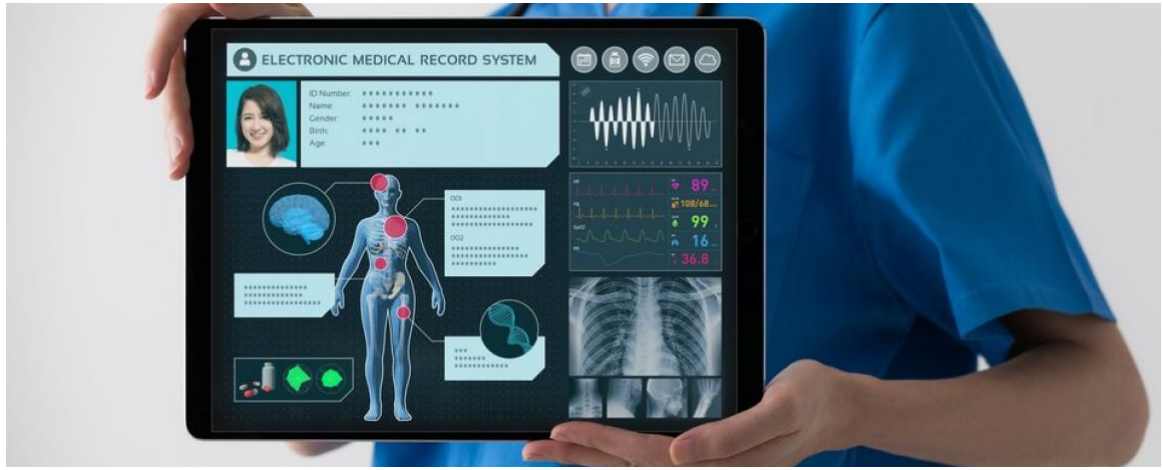
100->011 has distance 3 (red path)
010->111 has distance 2 (blue path)



Mixed data

- A data space can be composed by **non-iid numeric variables**
  - iid stands for **i**ndependent and **i**dentically **d**istributed
  - two numeric variables may be correlated, i.e. not independent
  - two numeric variables may have distinct distributions (e.g. $U(0,100)$ and $N(3,5)$), i.e. non-identically distributed
- A dataset can be composed of numeric variables (continuous and discrete), nominal and ordinal variables
  - we informally term such data as **mixed data**
  - examples?



Distances for mixed data

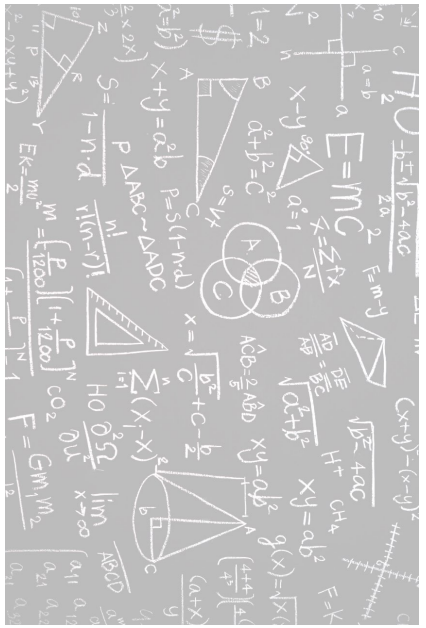
- First concern: two non-identically distributed variables – e.g. $Y_1 \sim U(0,1)$ and $Y_2 \sim U(0,100)$
  - *Problem*? In the given example, distances are most affected by variable Y_2
    - yet why should this variable have higher weight than Y_1!
  - *Solution*? Normalize variable features
    - do not confuse variable normalization with the normalization of a data instance/observation!
    - in the given example, $Y_2 \sim U'(0,1)$ by applying for instance min-max scaling

- Second concern: how to deal with simultaneous categoric and numeric variables?
  - distance can be a composition: $d(\mathbf{x}_1, \mathbf{x}_2) = \alpha\, d_{numeric}(\mathbf{x}_1, \mathbf{x}_2) + \beta\, d_{categoric}(\mathbf{x}_1, \mathbf{x}_2)$
    - where α and β are parameters that reveal the importance of each component, generally $\alpha + \beta = 1$
      - parameters can be fixed based on the number of variables or based on available domain knowledge

Algebra

- We had a first glimpse on few algebraic foundations on high-dimensional spaces
  - vector representations and distances in distinct spaces

- More to come in the upcoming lectures…
  - *multivariate Bayesian* and *neural network learning*
    - high-order **matrix operations**: product, determinant, inverse
  - *kernel methods*
    - high-order **data space transformations**
  - *dimensionality reduction*
    - orthogonal projections (eigenvectors and eigenvalues)



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  - **challenges: non-iid variables and dimensionality**

Parametric models

- We select a hypothesis and learn a fixed set of parameters
  - example: linear regression to describe a real-valued feature changing along time
    - parameters? two: slope and intercept
    - *predictive modeling:* what are the expected values for upcoming points in time?
    - *descriptive modeling*: how the values change along time?
- We assume that the parameters $\Phi = \{\phi_1, \ldots, \phi_K\}$ summarize the (training) data
  - compression

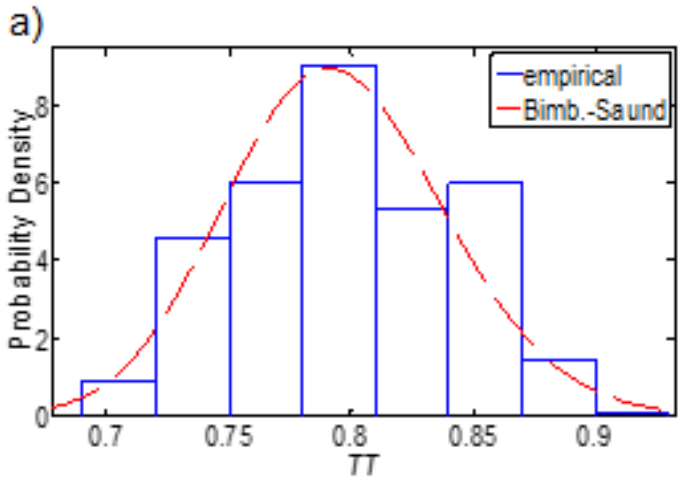
- These methods are called **parametric models**
  - examples: Bayesian models, neural networks (to come!)
  - when we have a small amount of data: models are simpler, need less parameters
  - when we have a large quantity of data: models can be more complex

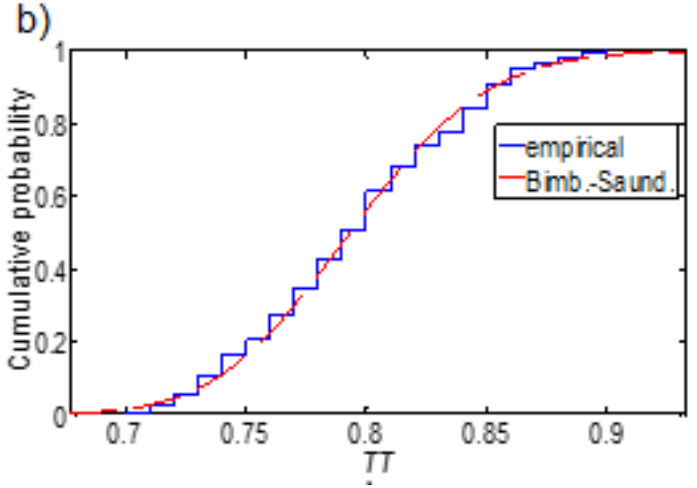
Non parametric Learning

- A **non-parametric model** is one that is not characterized by a well-defined set of parameters
- A family of non-parametric models is **instance-based learning**
  - instance-based learning is based on data memorization
  - there is not a model associated with the learned concepts
    - predictive and descriptive tasks are obtained by looking into the memorized examples
    - … and inspecting the set of similar-related instances in memory
- Yet.. to assess similarity we need to have a (dis)similarity measure! Isn't this a parameter?
  - ***parameters*** in classic stances are learned to describe the predictive/descriptive function
  - similarity criterion is not something that is learned but an *a priori* decision on the target function
    - ***hyperparameters*** are more appropriate term

(Non-)parametric univariate modeling

- Theoretical probability density/mass functions are parametric
  - e.g. univariate normal and uniform distributions have 2 parameters, Poisson has 1 parameter
- Empirical probability functions are non-parametric
  - observations can be sorted and probabilities indexed based on values or percentiles
  - there is no need to learn parameters





Instance-based learning

- When?
  - **Predictive modeling**, $M: X \rightarrow Z$
    - approximating real-valued ($Z = \mathbb{R}$) or discrete-valued ($Z = \Sigma$) target functions
  - **Descriptive modeling**, e.g. clustering, $M: X \rightarrow \{X_1 .. X_K\}$ with $X_k \subseteq X$
- Learning principles
  - store available (training) data
  - identify the most similar instances
    - in predictive modeling: given new instance, retrieve most similar training observations
    - in clustering: group instances above\below a similarity\dissimilarity threshold
- Let us now focus on *predictive modeling*

Instance-based learning

- **Neighborhood** of an instance: most similar instances
  - which strategies of (dis)similarity have we covered?
- Local approximation of the target function using the *neighborhood* of a given instance
    - instance-based learning also known as **local learning**
- In supervised learning, the training cost is *0*, all the cost is in the computation of the prediction
    - this kind learning is also known as *lazy learning*
- *Claim*: never construct an approximation designed to perform well over the entire instance space! Why?
- Disadvantage:
  - *testing efficiency*
    - pairwise distances to test new instance against all training instances
    - nearly all computation takes place at classification time rather than learning time
  - *memory efficiency*: need to store available training data

k-Nearest Neighbor

- Nearest-neighbor learning is a specific instance-based learning
- In **predictive modeling**, the target of a new observation is estimated in two steps:
  - the *k* nearest observations (neighborhood) are retrieved
  - a estimator is applied over the targets of the training observations in the neighborhood
    - classification (discrete output variable):
      - mode estimator
    - regression (numeric output variable)
      - mean or median estimator
- In **clustering**
  - observations are grouped when at least *k* neighbors are below a given distance threshold
  - let us leave this for later in the course

*k*NN classifier

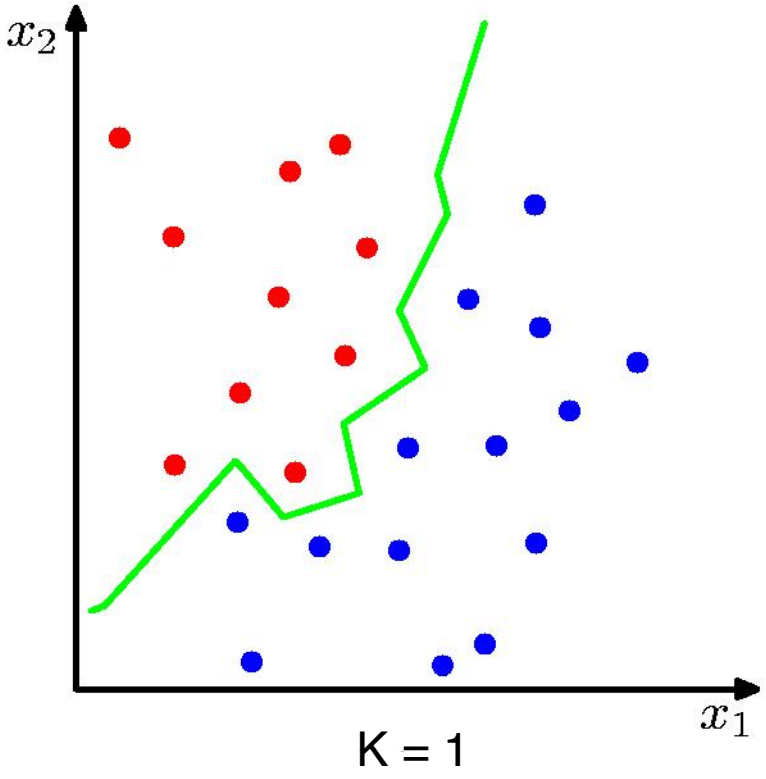
- Data $= \left\{ \left(\mathbf{x}_1, z_1\right), \left(\mathbf{x}_2, z_2\right) \ldots, \left(\mathbf{x}_n, z_n\right) \right\}$
- Goal: given data, learn classifier f to label new observations, $z_{new} = f(\mathbf{x}_{new})$
- kNN **training** algorithm
  - for each training pair observation-target $\left(\mathbf{x}_i, z_i\right)$, add the example to the list
- kNN **testing**/classification algorithm
  - given a query instance $\mathbf{x}_{new}$
    - find the k nearest neighbors to $\mathbf{x}_{new}$
    - let $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$ be the $\mathbf{x}_{new}$ neighborhood

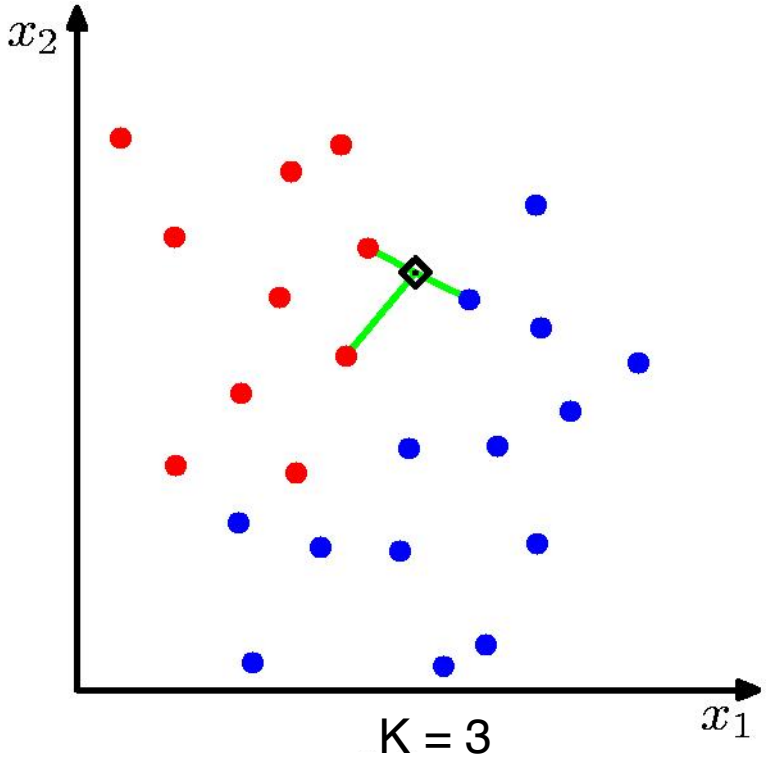
$$f(\mathbf{x}_{new}) \longleftarrow \underset{c \in Z}{argmax} \; \Sigma_{i=1}^{k} \delta(c, f(\mathbf{x}_i))$$

where $\delta(c, z) = 1$ if $z = c$, otherwise $\delta(c, z) = 0$ (**Kronecker** function)

*k*NN classifier

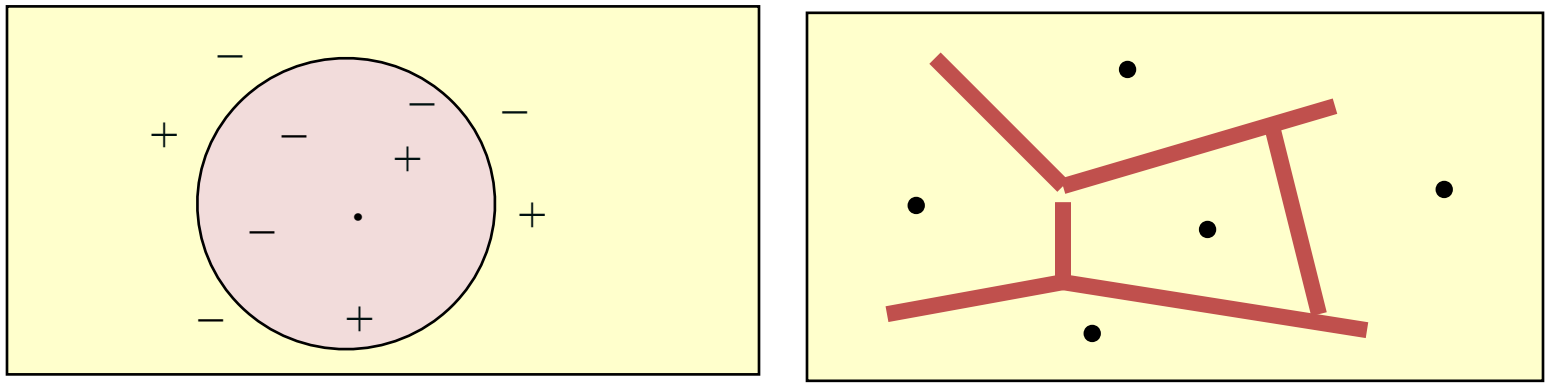
- Exercise: draw the kNN boundary for the following data assuming Euclidean distance and k=3





Inspecting *k*NN boundaries

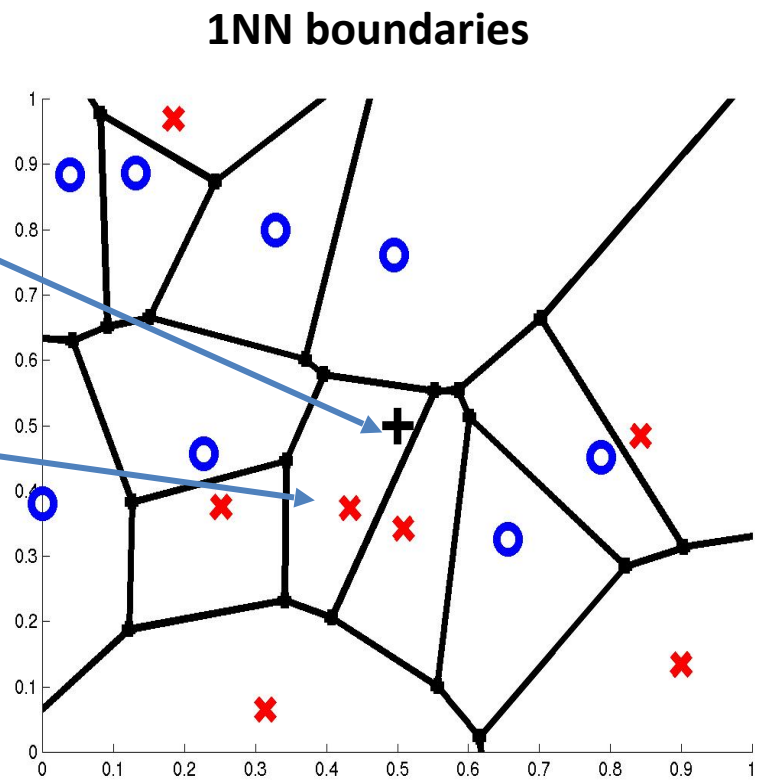
- Let us look to classification
  - kNN rule leads to partition of the space into cells (**Voronoi cells**) enclosing the training points labelled as belonging to the same class
  - the **decision boundary** in a Voronoi tessellation of the feature space resembles the surface of a crystal

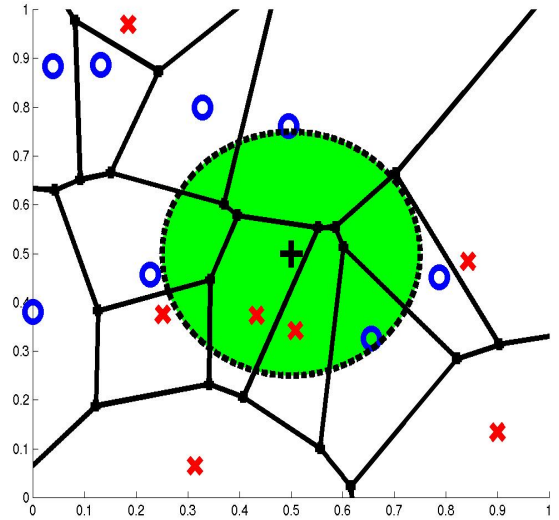


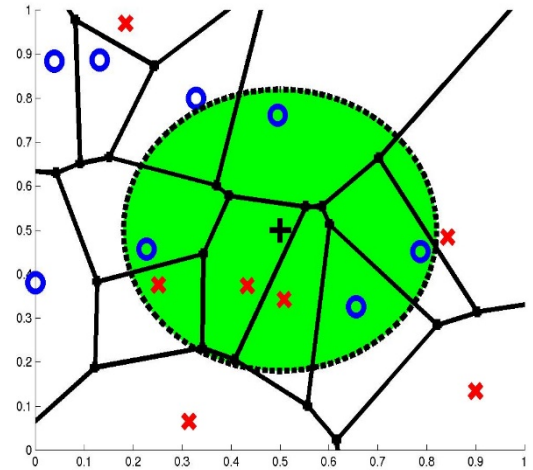
Inspecting *k*NN boundaries

query observation $\mathbf{x}_{new}$

nearest neighbor $\mathbf{x}_i$



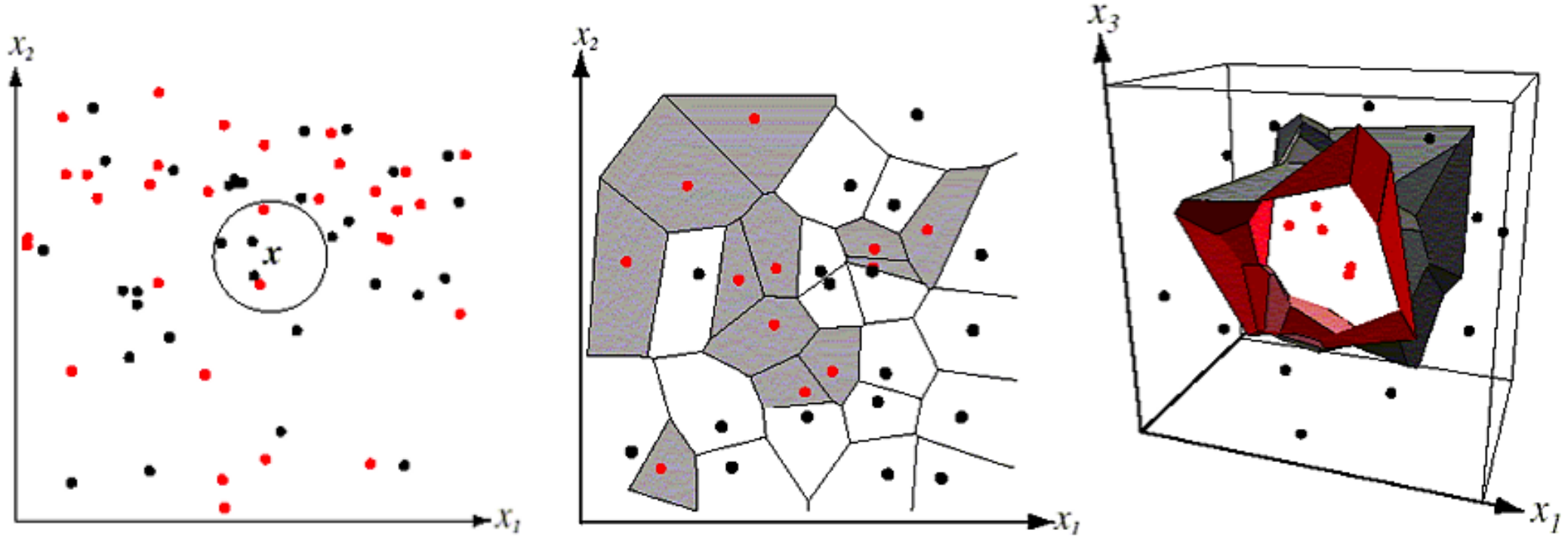




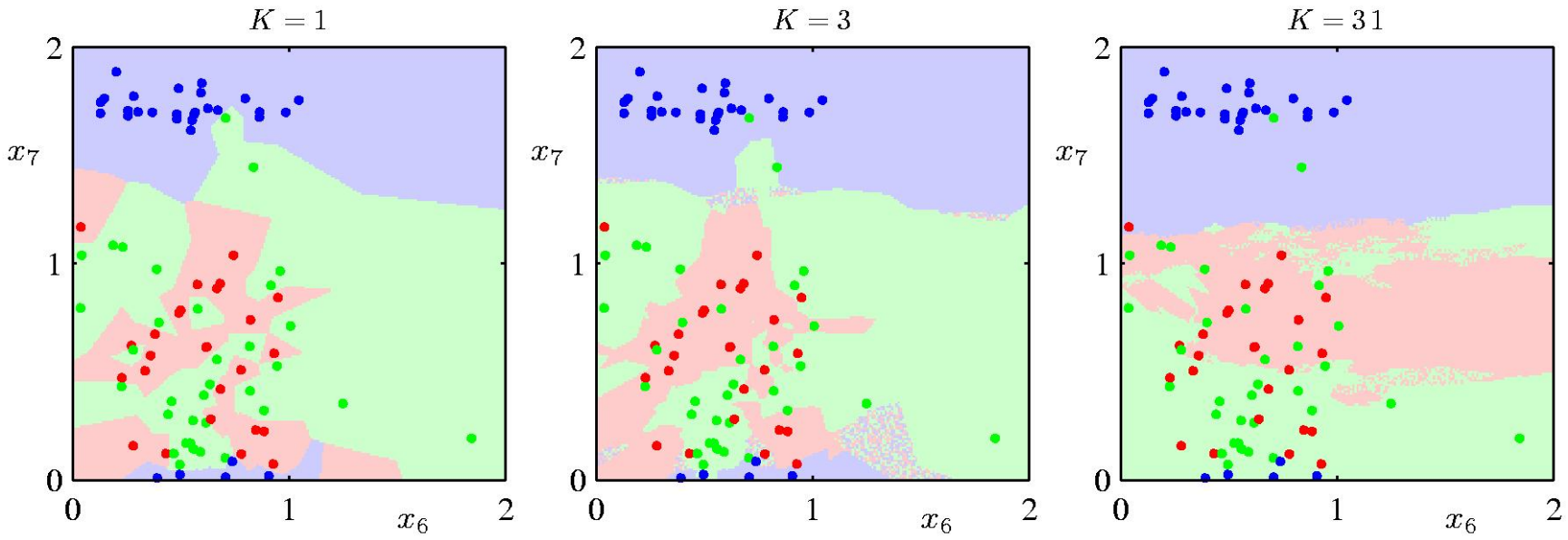
Boundaries preserved in **3NN**? And **7NN**?

Inspecting *k*NN boundaries

- Going into higher-dimensional spaces



*k*NN classifier: *k* and smoothing



- *k* acts as a smother
- For $n \longrightarrow \infty$, the error rate of the 1-nearest-neighbour classifier is never more than twice the optimal error (obtained from the true conditional class distributions)

How to determine *k*?

- Determined experimentally
  - use a test set to validate the error rate of the classifier
  - start with $k = 1$ and assess the error rate
  - repeat with $k = k + 2$
  - choose the value of k for which the error rate is minimum

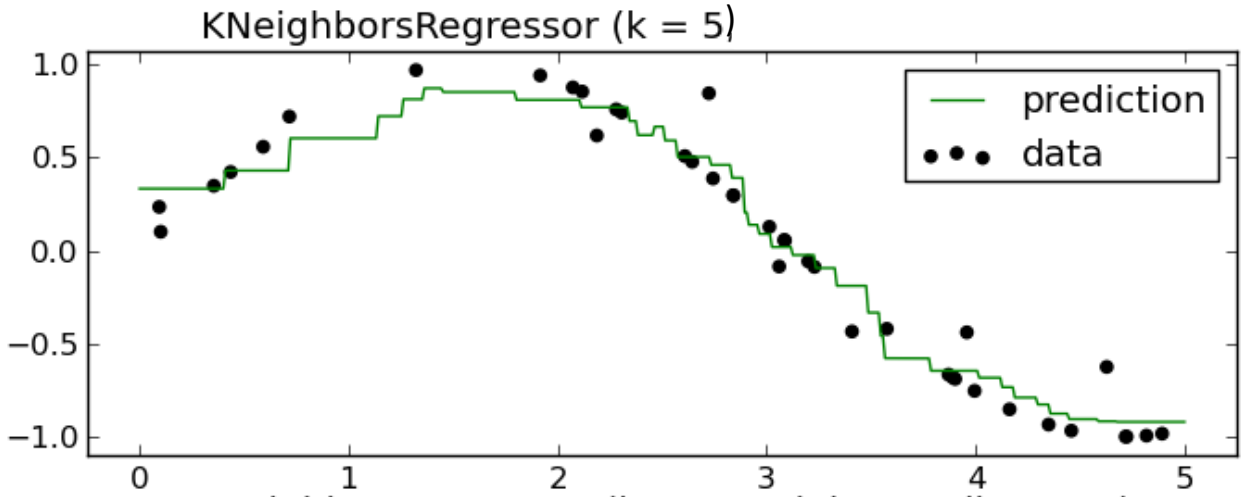
- Note: k should be odd number to avoid ties
- More to come on
  - simple error rate = number of observations incorrectly classified. Better alternatives?
  - training *versus* testing error rates?

*k*NN regressor

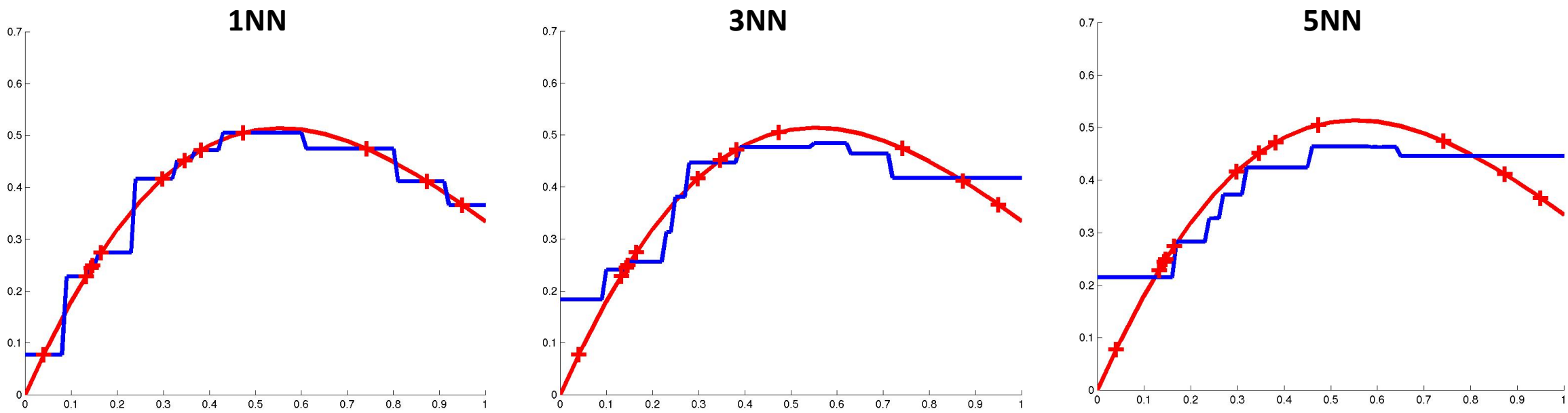
- *k*NN can alternatively approximate continuous-valued target functions
  - … by calculating the mean or median value of the *k* nearest training examples

$$f: X \rightarrow \mathbb{R}$$

$$f(\mathbf{x}_{new}) \longleftarrow \frac{\sum_{i=1}^{k} f(\mathbf{x}_i)}{k}$$



*k*NN regressor



- in **red**: samples of a well-defined signal
- in **blue**: kNN regression function

*k*NN in numeric, categorical and mixed data spaces

- kNN can be parameterized with different similarity criteria
  - *numeric data spaces*
    - **Manhattan** and **Euclidean** distances are common choices
    - recall: when are **Chebyshev** distance, **cosine** similarity and **correlation** coefficient desirable?
  - *categorical data*
    - **encodings** for ordinal variables
    - **Hamming** for nominal variables
    - what is the problem with discrete variables with different cardinalities?
      - solutions?
  - *mixed data*
    - weighted similarity contributions from numeric, ordinal and nominal variables
- kNN can therefore be applied on vector and symbolic spaces

Distance weighted kNN

- Until now we assumed that the weights of the contributions of each *k* neighbor is **uniform**
  - i.e. every neighbor in the neighborhood has the same weight to the final decision
- However, some neighbors may be closer to the target observation than others!
- *k*NN can be refined by considering non-uniform weights
  - How to set **weights**? According to the distance to the query point $\mathbf{x}_{new}$
    - greater weight to closer neighbors
  - For discrete target functions (**classification**)

$$f(\mathbf{x}_{new}) \longleftarrow \underset{c \in Z}{argmax} \; \Sigma_{i=1}^{k} w_i \cdot \delta(c, f(\mathbf{x}_i))$$

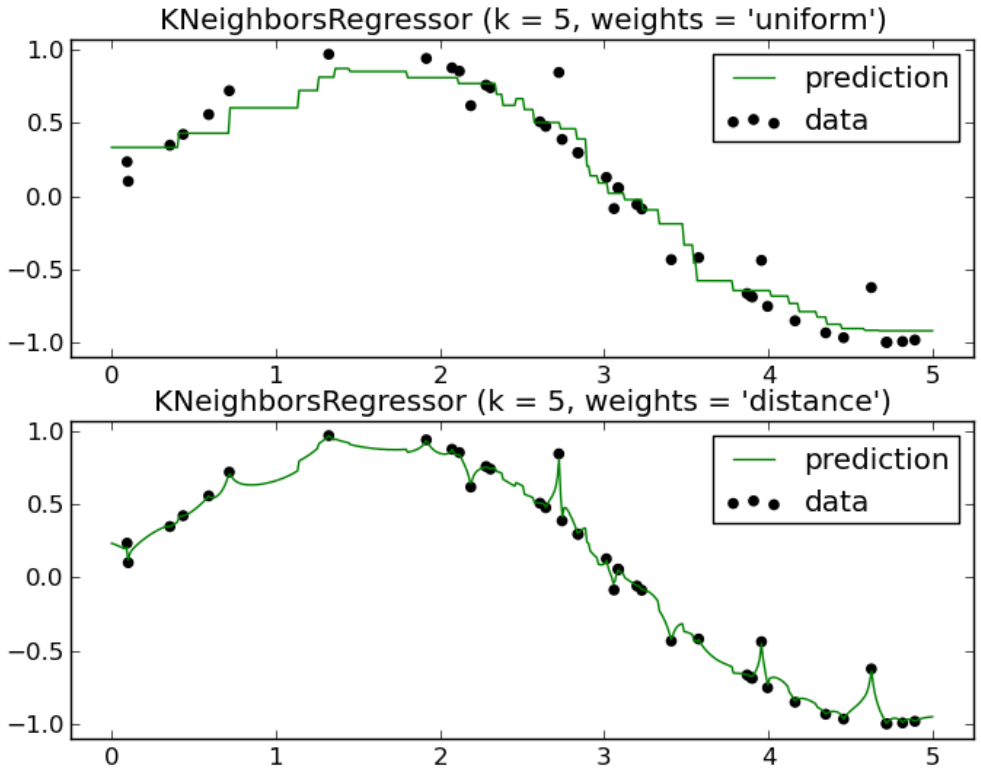
$$w_i = \begin{cases} \frac{1}{d(\mathbf{x}_{new}, \mathbf{x}_i)} & \text{if } \mathbf{x}_{new} \neq \mathbf{x}_i \\ 1 & \text{else} \end{cases}$$

Distance weighted kNN

- In **regression** (numeric targets):

$$f(\mathbf{x}_{new}) \longleftarrow \frac{\sum_{i=1}^{k} w_i f(\mathbf{x}_i)}{\sum_{i=1}^{k} w_i}$$

$$w_i = \begin{cases} \frac{1}{d(\mathbf{x}_{new}, \mathbf{x}_i)} & \text{if } \mathbf{x}_{new} \neq \mathbf{x}_i \\ 1 & \text{else} \end{cases}$$



*k*NN challenges and solutions

- Let us assume we have three numeric variables, $y_1 \in [0,1], y_2 \in [0,1]$ and $y_3 \in [0,100]$
  - ***Problem*** in the Euclidean space?
    - variables with wider range of values have higher importance when measuring distances
  - **Solution**: variable **normalization**

- Let us assume we have two variables, $y_1 \in \{0,1\}$ and $y_2 \in [0,1]$
  - Comparable problem? Solution?

- Let us assume we have hundreds of variables
  - ***Problem*** in the Euclidean space?
    - contributions from an important subset of variables will get lost amidst all variables!
  - **Solution**: **dimensionality reduction**, e.g. feature selection

Outline

- **Learning in the vector space**
  - from univariate to multivariate data spaces
  - Minkowski distances
  - norm and cosine similarity
  - encodings for categoric variables and mixed data
- **Instance-based learning**
  - parametric vs non-parametric models
  - k-nearest neighbor classifier
  - k-nearest neighbor regressor
  - distance-based kNN
  - challenges: non-iid variables and dimensionality

Thank You

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