# Machine Learning

## FIB, Master in Data Science

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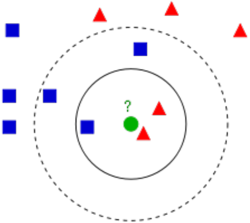
**Nearest neighbors**

# Nearest neighbor prediction

The **nearest neighbor** predictor uses the **local** neighborhood to compute a prediction

- 1-NN predicts using same target as the **closest** training example
- $k$-NN predicts using combination of targets from $k$ **closest** training examples



# Nearest neighbor pseudocode

- **Training:**
  1. store all examples

- **Prediction:** given new example $\mathbf{x}$:
  1. Compute distance/similarity with all examples in training set
  2. Locate $k$ closest
  3. Emit prediction by combining labels of $k$ closest

There are three things to decide when applying $k$-NN:

1. Distance/similarity function
2. How many neighbors $k$ to choose
3. How to combine labels of $k$ neighbors to emit final prediction

# Locality: similarities and distances

## What does "closest" neighbor mean?

A crucial aspect of nearest neighbor prediction is the notion of **distance/similarity** since it affects very directly the predictions made

Let $a, b, c$ be examples in some feature space. Then a **distance function** should satisfy:

1. $d(a, b) \geq 0$
2. $d(a, b) = 0$ iff $a = b$
3. $d(a, b) = d(b, a)$ (symmetry)
4. $d(a, b) \leq d(a, c) + d(c, b)$ (triangle inequality)

If using a **similarty function**, it should satisfy:

1. $-1 \geq s(a, b) \geq 1$ or $0 \geq s(a, b) \geq 1$
2. $s(a, b) = 1$ iff $a = b$
3. $s(a, b) = s(b, a)$ (symmetry)

# Examples of distance functions for continuous data in $\mathbb{R}^d$

- The most common is the **Minkownski distance** family; typically Euclidean ($p = 2$) or Manhattan ($p = 1$):

$$d(\mathbf{a}, \mathbf{b}) = \|\mathbf{a} - \mathbf{b}\|_p = \left( \sum_{j=1}^{d} |a_j - b_j|^p \right)^{\frac{1}{p}}$$

- Another choice is to use the **Mahalanobis distance** if we want to take into account covariances $\Sigma$ among features:

$$d(\mathbf{a}, \mathbf{b}) = (\mathbf{a} - \mathbf{b})^T \Sigma^{-1} (\mathbf{a} - \mathbf{b})$$

# Examples of similarity functions for continuous data in $\mathbb{R}^d$

- **Cosine similarity**

$$s(\mathbf{a}, \mathbf{b}) = \frac{\mathbf{a}^T \mathbf{b}}{\|\mathbf{a}\|_2 \|\mathbf{b}\|_2}$$

- The **Pearson correlation measure** is similar to cosine similarity but centers data ($\mu$ is the **mean** of all training points):

$$s(\mathbf{a}, \mathbf{b}) = \frac{(\mathbf{a} - \mu)^T (\mathbf{b} - \mu)}{\|\mathbf{a} - \mu\|_2 \|\mathbf{b} - \mu\|_2}$$

# Examples of similarities for binary data

- **Hamming distance**: proportion of common “bits”
- **Jaccard coefficient**

$$s(\mathbf{a},\mathbf{b}) = \frac{\sum_j [a_j = b_j = 1]}{\sum_j [a_j = 1 \text{ or } b_j = 1]}$$

Example:

$$\begin{aligned}\mathbf{a} &= + - - + - - - - + + - - - - \\ \mathbf{b} &= + + - - - - - + + - - - - +\end{aligned}$$

Here, $s_{Jaccard}(\mathbf{a},\mathbf{b}) = \frac{2}{7} \approx 0.3$ and $s_{Hamming}(\mathbf{a},\mathbf{b}) = \frac{9}{14} \approx 0.6$.

# Choosing $k$

Nearest neighbor is very sensitive to different values of $k$

- if $k$ is too **low**, then we can easilily overfit
- if $k$ is too **large**, then we can underfit

So, it is important to select an appropriate $k$, which will depend on the dataset. Typically we use **cross-validation** or other resampling methods.

$k$ can be seen as a hyper-parameter that trades-off bias and variance of the resulting classifier.

# On combining labels to make predictions

For **classification**:

- Majority vote (ties broken randomly)
- Distance-weighted vote: choose weights that are higher for closer points
  - e.g. inverse of the distance or inverse of the squared distance

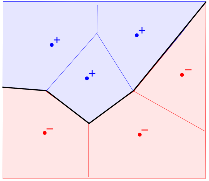
For **regression**:

- Use the **average** of targets of $k$ nearest neighbors
- Use **weighted average** of targets of $k$ nearest neighbors
  - e.g. use inverse distance as weight, or squared of inverse distance
  - *kernel smoothing*

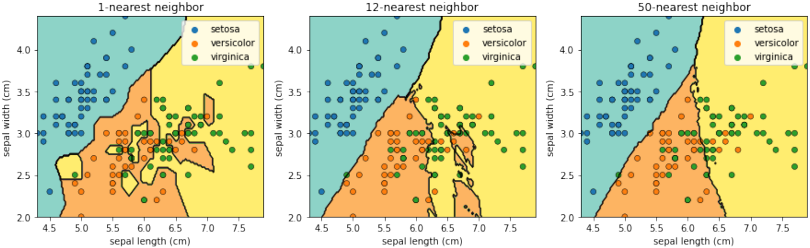
Once we use weights for the prediction, we can relax the constraint of using only $k$ examples and use the whole training set instead.

# Decision boundaries for nearest neighbors classifier

In 1-nearest neighbor, the decision regions correspond to the union of each example's *Voronoi* cell, with appropriate "class"



The decision boundaries and regions are highly non-linear, but get smoother as we increase $k$



# Considerations with $k$-NN

- Making prediction can be **slow** especially if we have a large training set
  - data structures like *kd* trees used to speed up neighbor retrieval, only good for moderate nr. of features
  - use *prototypes*
  - use approximate neighbors; e.g. with *locality sensitive hashing*

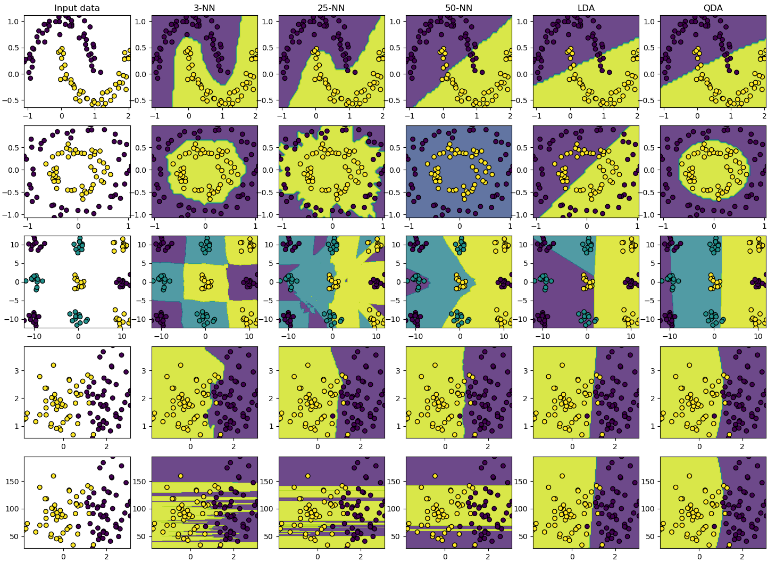
- Prone to **overfitting**
  - remove "noisy" examples from training (e.g. examples with nearest neighbor of different class)
  - use *prototypes*
  - set $k$ to appropriate value

- Suffers from **curse of dimensionality**: as dimensionality increases, everything seems to be close

- Suffers from presence of **irrelevant** features

- **Standarization** of features is crucial to avoid domination of features with larger (absolute) values

# Comparison with toy datasets


Input data
3-NN
25-NN
50-NN
LDA
QDA