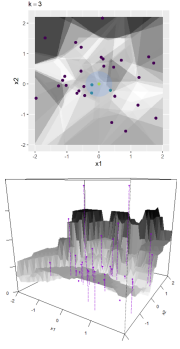
Introduction to Machine Learning

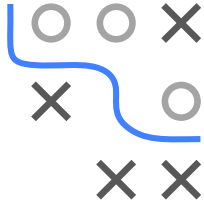
k-Nearest Neighbors



Learning goals

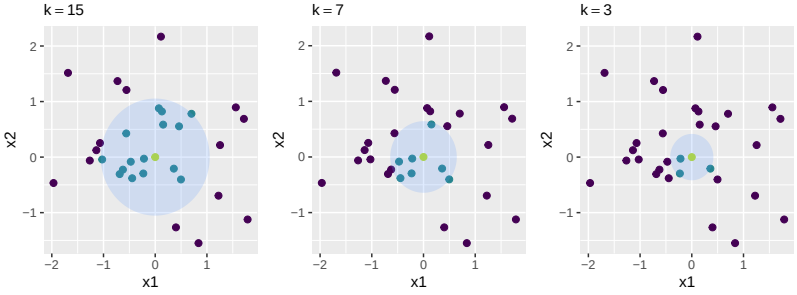
- Understand the basic idea of *k*-NN for regression and classification
- Understand that *k*-NN is a non-parametric, local model
- Know different distance measures for different scales of feature variables

K-NEAREST-NEIGHBORS

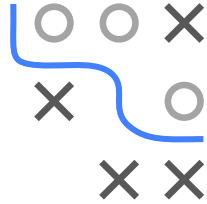


- k-**NN** can be used for regression and classification.
- Generates "similar" predictions for $\mathbf{x}$ to its k closest neighbors.
- "Closeness" requires a distance or similarity measure.
- The subset of $\mathcal{D}_{\text{train}}$ that is at least as close to $\mathbf{x}$ as its k-th closest neighbor $\mathbf{x}^{(k)}$ in $\mathcal{D}_{\text{train}}$ is called the k-**neighborhood** $N_k(\mathbf{x})$ of $\mathbf{x}$:

$$N_k(\mathbf{x}) = \{\mathbf{x}^{(i)} \in \mathcal{D}_{\text{train}} \mid d(\mathbf{x}^{(i)}, \mathbf{x}) \leq d(\mathbf{x}^{(k)}, \mathbf{x})\}$$



DISTANCE MEASURES



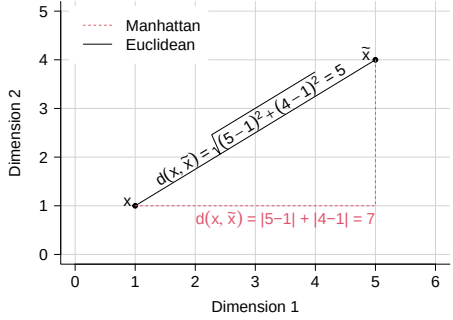
- Popular for numerical features: **Minkowski** distances of the form

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_q = \left(\sum_{j=1}^{p} |x_j - \tilde{x}_j|^q \right)^{\frac{1}{q}} \quad \text{for } \mathbf{x}, \tilde{\mathbf{x}} \in \mathcal{X} \text{ with } p \text{ numeric features}$$

- Especially, **Manhattan** ($q = 1$) and **Euclidean** ($q = 2$) distance

$$d_{Manhattan}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|_1 = \sum_{j=1}^{p} |x_j - \tilde{x}_j|$$

$$d_{Euclidean}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|_2 = \sqrt{\sum_{j=1}^{p} (x_j - \tilde{x}_j)^2}$$

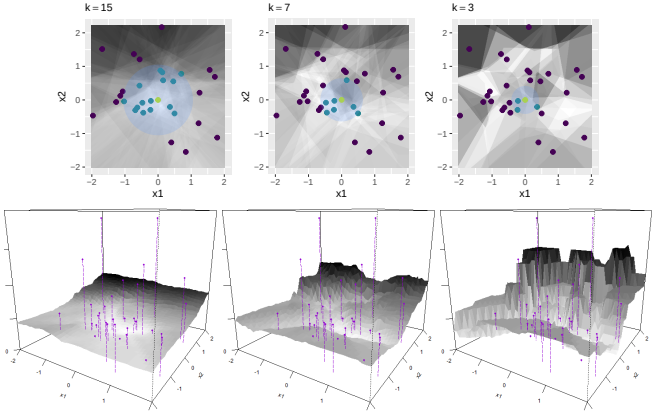


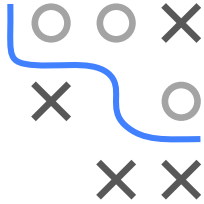
PREDICTION - REGRESSION

Compute for each point the average output y of the k-nearest neighbours in $N_k(\mathbf{x})$:

$$\hat{f}(\mathbf{x}) = \frac{1}{k} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} y^{(i)} \text{ or } \hat{f}(\mathbf{x}) = \frac{1}{\sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} w^{(i)}} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} w^{(i)} y^{(i)}$$

with neighbors weighted based on their distance to $\mathbf{x}$: $w^{(i)} = \frac{1}{d(\mathbf{x}^{(i)}, \mathbf{x})}$





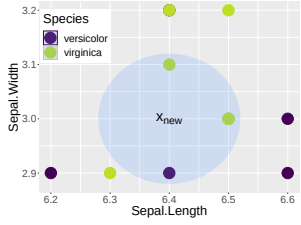
PREDICTION - CLASSIFICATION

For classification in g groups, a majority vote is used:

$$\hat{h}(\mathbf{x}) = \underset{\ell \in \{1,\dots,g\}}{\arg\max} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$$

And posterior probabilities can be estimated with:

$$\hat{\pi}_\ell(\mathbf{x}) = \frac{1}{k} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$$



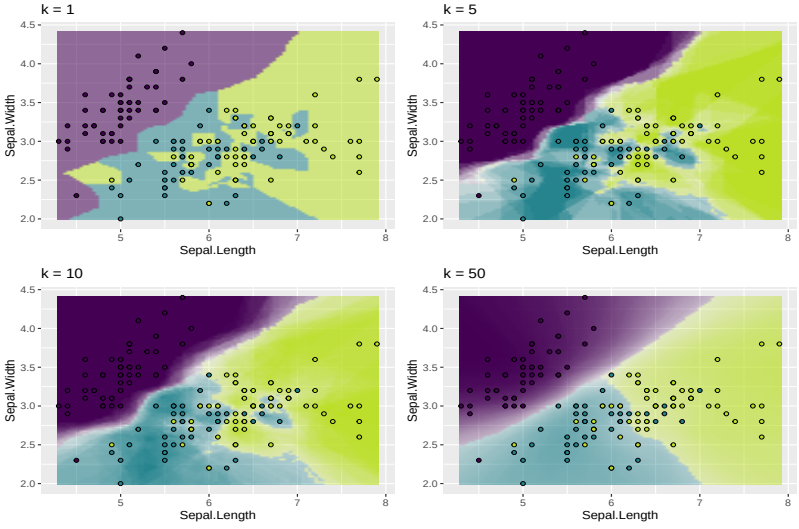
	SL	SW	Species	dist
52	6.4	3.2	versicolor	0.200
59	6.6	2.9	versicolor	0.224
75	**6.4**	**2.9**	**versicolor**	**0.100**
76	6.6	3.0	versicolor	0.200
98	6.2	2.9	versicolor	0.224
104	6.3	2.9	virginica	0.141
105	**6.5**	**3.0**	**virginica**	**0.100**
111	6.5	3.2	virginica	0.224
116	6.4	3.2	virginica	0.200
117	**6.5**	**3.0**	**virginica**	**0.100**
138	6.4	3.1	virginica	0.100
148	6.5	3.0	virginica	0.100

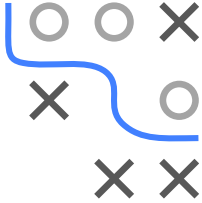
Example with subset of iris data ($k = 3$)

$\hat{\pi}_{setosa}(\mathbf{x}_{new}) = \frac{0}{3} = 0\%$, $\hat{\pi}_{versicolor}(\mathbf{x}_{new}) = \frac{1}{3} = 33\%$, $\hat{\pi}_{virginica}(\mathbf{x}_{new}) = \frac{2}{3} = 67\%$,

$\hat{h}(\mathbf{x}_{new}) = virginica$

K-NN: FROM SMALL TO LARGE K

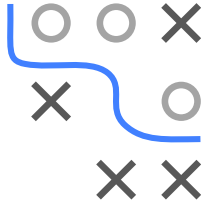




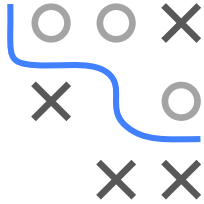
Complex, local model vs smoother, more global model

K-NN SUMMARY

- k-NN is a lazy classifier, it has no real training step, it simply stores the complete data - which are needed during prediction.
- Hence, its parameters are the training data, there is no real compression of information.
- As the number of parameters grows with the number of training points, we call k-NN a non-parametric model
- k-NN is not based on any distributional or functional assumption, and can, in theory, model data situations of arbitrary complexity.
- The smaller k, the less stable, less smooth and more “wiggly” the decision boundary becomes.
- Accuracy of k-NN can be severely degraded by the presence of noisy or irrelevant features, or when the feature scales are not consistent with their importance.



STANDARDIZATION AND WEIGHTS

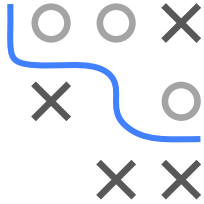


- **Standardization:** Features in k-NN are usually standardized or normalized. If two features have values on a very different range, most distances would place a higher importance on the one with a larger range, leading to an imbalanced influence of that feature.
- **Importance:** Sometimes one feature has a higher importance (maybe we know this via domain knowledge). It can now manually be upweighted to reflect this.

$$d_{Euclidean}^{weighted}(\mathbf{x}, \tilde{\mathbf{x}}) = \sqrt{\sum_{j=1}^{p} w_j (x_j - \tilde{x}_j)^2}$$

- If these weights would have to be learned in a data-driven manner, we could only do this by hyperparameter tuning in k-NN. This is inconvenient, and Gaussian processes handle this much better.

GOWER DISTANCE



- A weighted mean of univ. distances in the j-th feature.
- It can handle categoricals, missings, and different ranges.

$$d_{gower}(\mathbf{x}, \tilde{\mathbf{x}}) = \frac{\sum_{j=1}^{p} \delta_{x_j,\tilde{x}_j} \cdot d_{gower}(x_j, \tilde{x}_j)}{\sum_{j=1}^{p} \delta_{x_j,\tilde{x}_j}}.$$

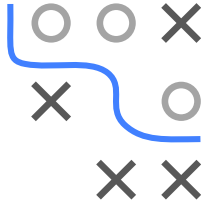
- $\delta_{x_j,\tilde{x}_j}$ is 0 or 1. It's 0 if *j*-th feature is *missing* in at least one observation, or when the feature is asymmetric binary (where "1" is more important than "0") and both values are zero. Otherwise 1.
- $d_{gower}(x_j, \tilde{x}_j)$: For nominals it's 0 if both values are equal and 1 otherwise. For integers and reals, it's the absolute difference, divided by range.

GOWER DISTANCE / 2

Example of Gower distance with data on sex and income:

index	sex	salary
1	m	2340
2	w	2100
3	NA	2680

$$d_{gower}(\mathbf{x}, \tilde{\mathbf{x}}) = \frac{\sum_{j=1}^{p} \delta_{x_j, \tilde{x}_j} \cdot d_{gower}(x_j, \tilde{x}_j)}{\sum_{j=1}^{p} \delta_{x_j, \tilde{x}_j}}$$



$$d_{gower}(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}) = \frac{1 \cdot 1 + 1 \cdot \frac{|2340-2100|}{|2680-2100|}}{1+1} = \frac{1+\frac{240}{580}}{2} = \frac{1+0.414}{2} = 0.707$$

$$d_{gower}(\mathbf{x}^{(1)}, \mathbf{x}^{(3)}) = \frac{0 \cdot 1 + 1 \cdot \frac{|2340-2680|}{|2680-2100|}}{0+1} = \frac{0+\frac{340}{580}}{1} = \frac{0+0.586}{1} = 0.586$$

$$d_{gower}(\mathbf{x}^{(2)}, \mathbf{x}^{(3)}) = \frac{0 \cdot 1 + 1 \cdot \frac{|2100-2680|}{|2680-2100|}}{0+1} = \frac{0+\frac{580}{580}}{1} = \frac{0+1.000}{1} = 1$$