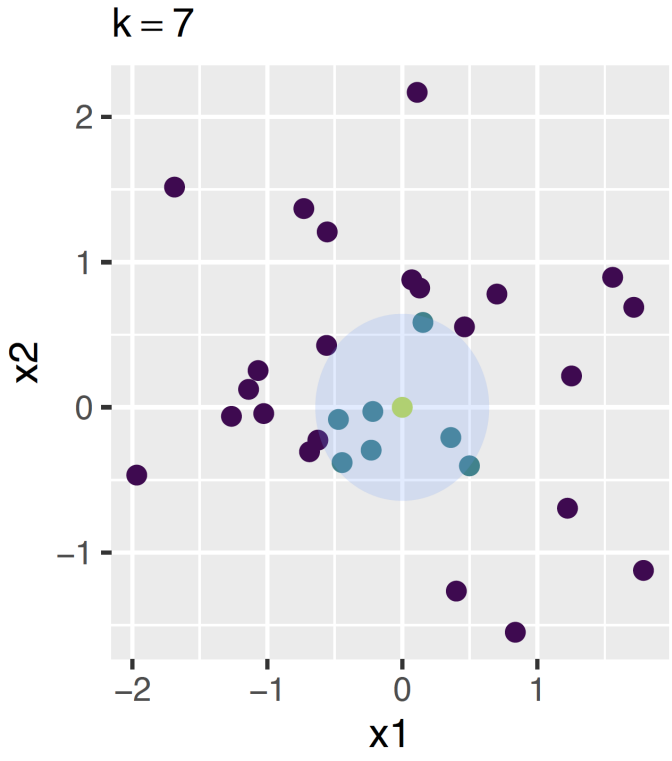
Introduction to Machine Learning

k-Nearest Neighbors

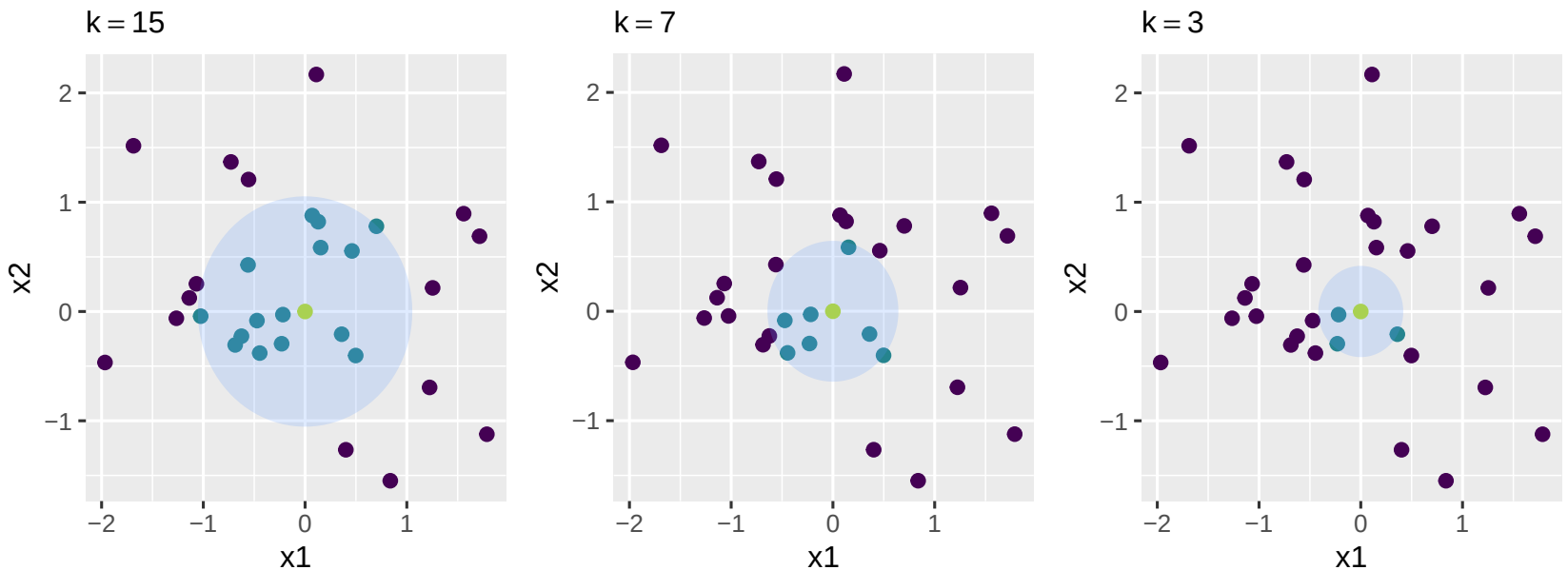


Learning goals

- Understand the basic idea of k-NN
- Know different distance measures for different scales of feature variables
- Understand that k-NN has no optimization step

K-NEAREST-NEIGHBORS

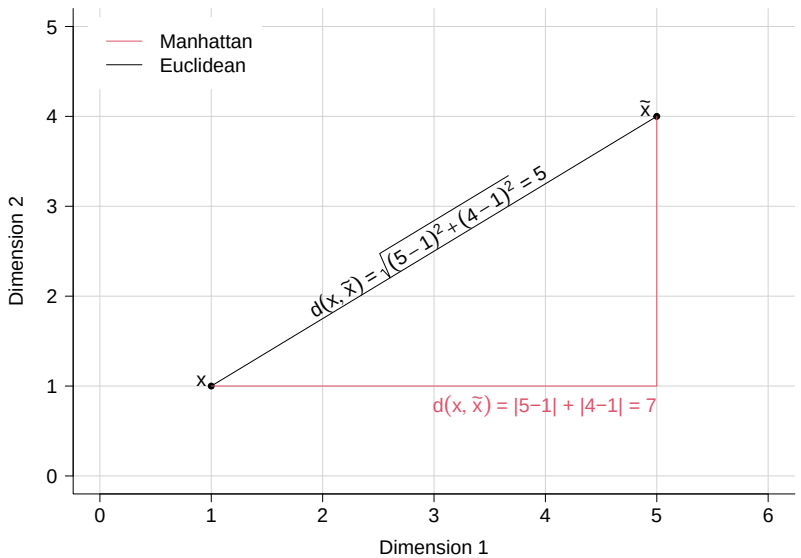
- k-**NN** can be used for regression and classification
- It generates predictions $\hat{y}$ for a given $\mathbf{x}$ by comparing the k observations that are closest to $\mathbf{x}$
- "Closeness" requires a distance or similarity measure (usually: Euclidean).
- The set containing the k closest points $\mathbf{x}^{(i)}$ to $\mathbf{x}$ in the training data is called the k-**neighborhood** $N_k(\mathbf{x})$ of $\mathbf{x}$.



DISTANCE MEASURES

How to calculate distances?

- Most popular distance measure for numerical features: **Euclidean distance**
- For two data points $\mathbf{x}$ and $\tilde{\mathbf{x}}$ with p features $\in \mathbb{R}$
  - the Euclidean distance is $d_{Euclidean}(\mathbf{x}, \tilde{\mathbf{x}}) = \sqrt{\sum_{j=1}^{p}(x_j - \tilde{x}_j)^2}$.
  - the Manhattan distance is $d_{manhattan}(\mathbf{x}, \tilde{\mathbf{x}}) = \sum_{j=1}^{p}|x_j - \tilde{x}_j|$.

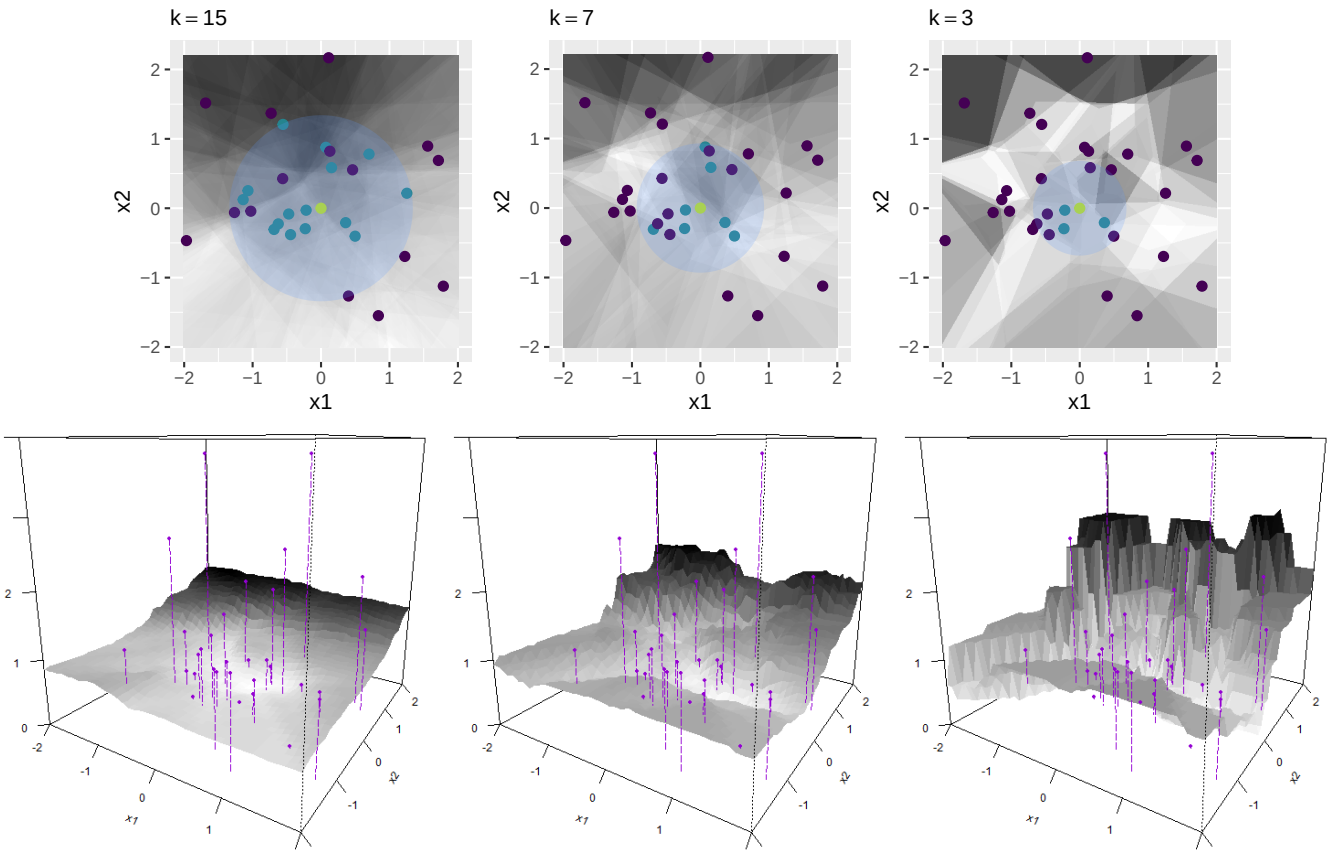


PREDICTION - REGRESSION

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:

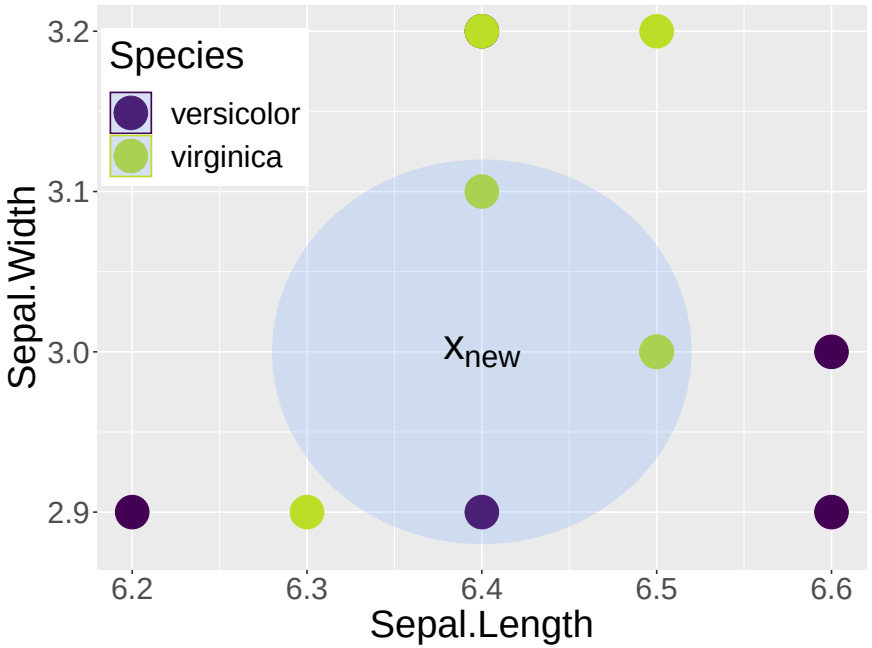
$$\hat{h}(\mathbf{x}) = \underset{\ell \in \{1,\ldots,g\}}{\arg\max} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$$

And posterior probabilities can be estimated with:

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

PREDICTION - CLASSIFICATION

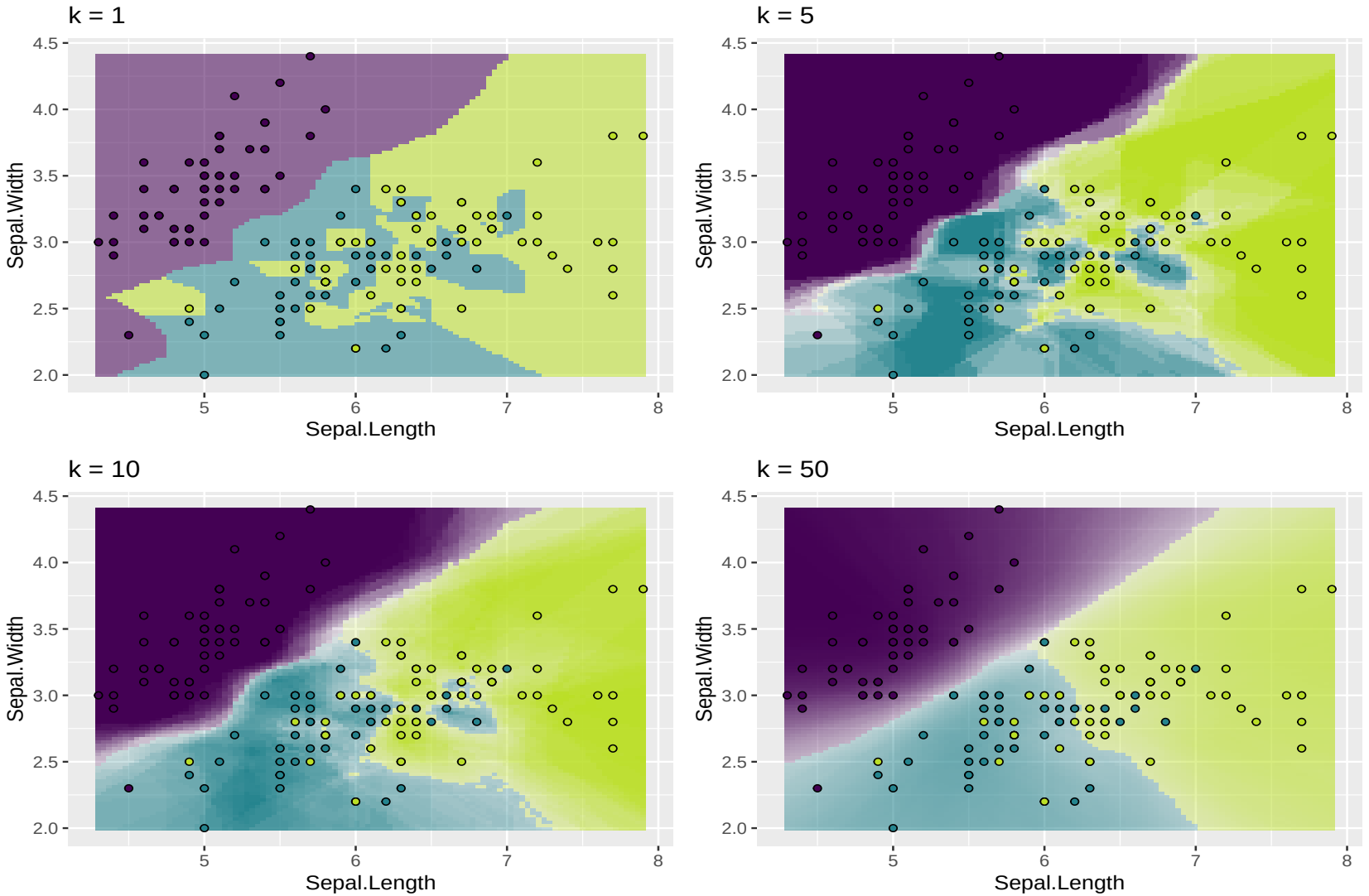
Example with subset of iris data ($k = 3$):



	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

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

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
- Hence, k-NN is not based on any distributional or strong functional assumption, and can, in theory, model data situations of arbitrary complexity.
- k-NN has no optimization step and is a very local model.
- We cannot simply use least-squares loss on the training data for picking k, because we would always pick $k = 1$. 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.

DISTANCE MEASURES - EXTENSIONS

Categorical variables, missing data and mixed space:
The Gower distance $d_{gower}(\mathbf{x}, \tilde{\mathbf{x}})$ is a weighted mean of $d_{gower}(x_j, \tilde{x}_j)$:

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

- $\delta_{x_j, \tilde{x}_j}$ is 0 or 1. It becomes 0 when the j-th variable is ***missing*** in at least one of the observations ($\mathbf{x}$ or $\tilde{\mathbf{x}}$), or when the variable is asymmetric binary (where "1" is more important/distinctive than "0", e. g., "1" means "color-blind") and both values are zero. Otherwise it is 1.

DISTANCE MEASURES - EXTENSIONS

- $d_{gower}(x_j, \tilde{x}_j)$, the j-th variable contribution to the total distance, is a distance between the values of x_j and $\tilde{x}_j$. For nominal variables the distance is 0 if both values are equal and 1 otherwise. The contribution of other variables is the absolute difference of both values, divided by the total range of that variable.

DISTANCE MEASURES - EXTENSIONS

Example of Gower distance with data on sex and income:

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

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

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

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

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

DISTANCE MEASURES - EXTENSIONS

Weights:

Weights can be used to address two problems in distance calculation:

- **Standardization:** Two features may have values with a different scale. Many distance formulas (not Gower) would place a higher importance on a feature with higher values, leading to an imbalance. Assigning a higher weight to the lower-valued feature can combat this effect.
- **Importance:** Sometimes one feature has a higher importance (e. g., more recent measurement). Assigning weights according to the importance of the feature can align the distance measure with known feature importance.

For example:

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