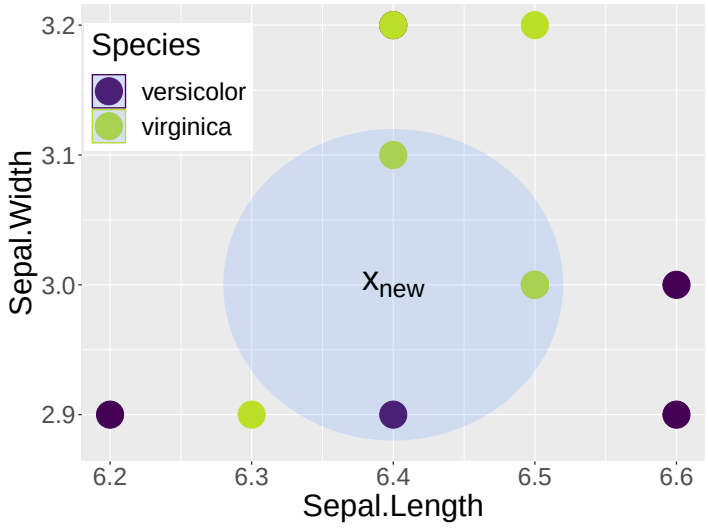
Introduction to Machine Learning

Classification: K-Nearest Neighbors



Learning goals

- Understand the idea of k-NN classification
- Know how the hyperparameter k affects the results of k-NN classification

K-NEAREST NEIGHBORS

For each point to predict:

- Compute k-nearest neighbours in training data $N_k(\mathbf{x})$
- Average output y of these k neighbors
- For regression:

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

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

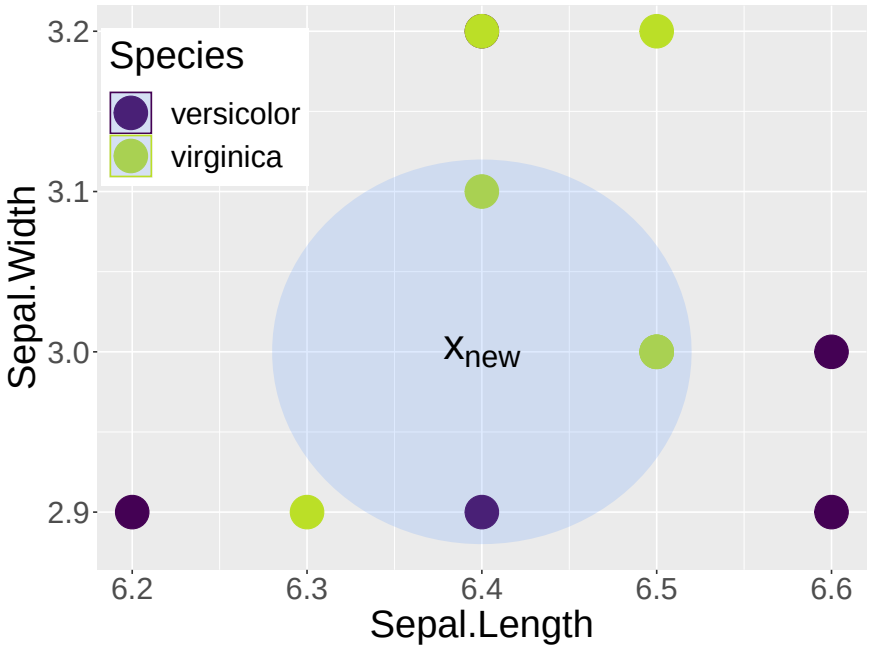
$$\hat{h}(\mathbf{x}) = \underset{\ell \in \{1,\ldots,g\}}{\arg\max} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$$

  And posterior probabilities can be estimated with:

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

K-NEAREST NEIGHBORS

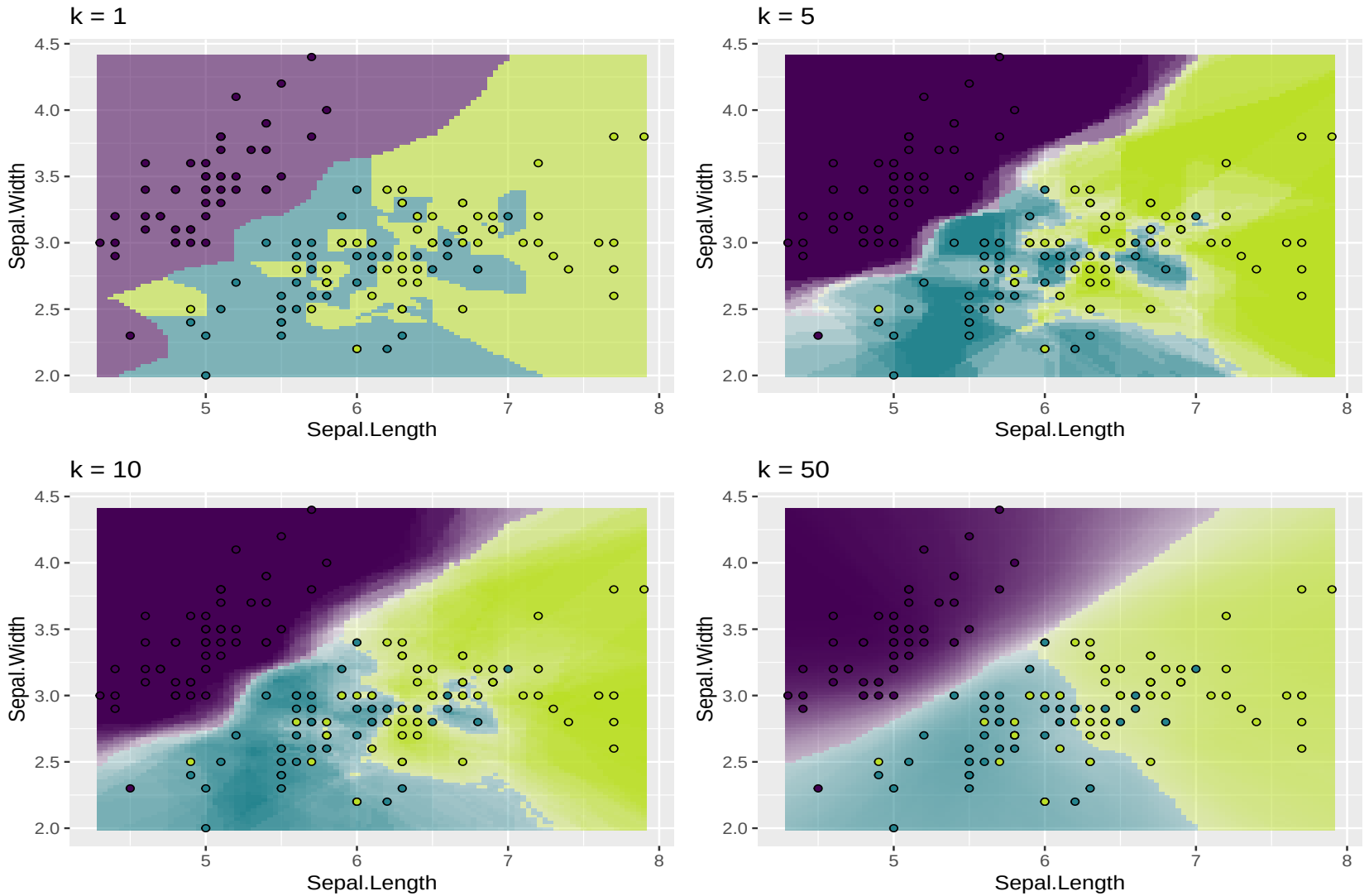
Example with subset of iris data ($k = 3$):



	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 AS NON-PARAMETRIC MODEL

- 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