Machine Learning

Lecture 2: k-Nearest Neighbors

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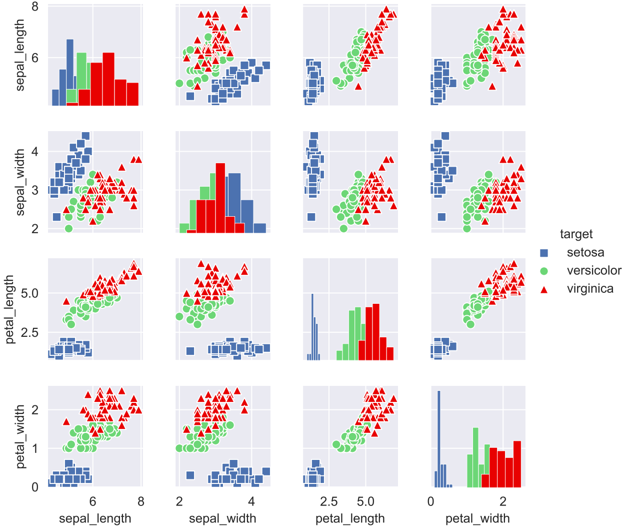
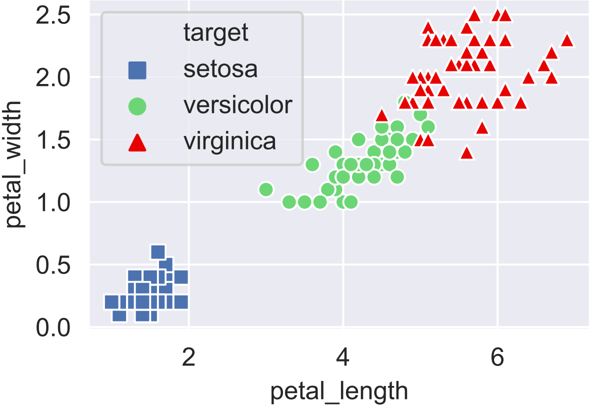
Winter term 2023/2024

Iris dataset



Iris dataset: 2 features



How do we intuitively label new samples by hand?
Look at the *surrounding* points. Do as your neighbor does.

1-NN algorithm

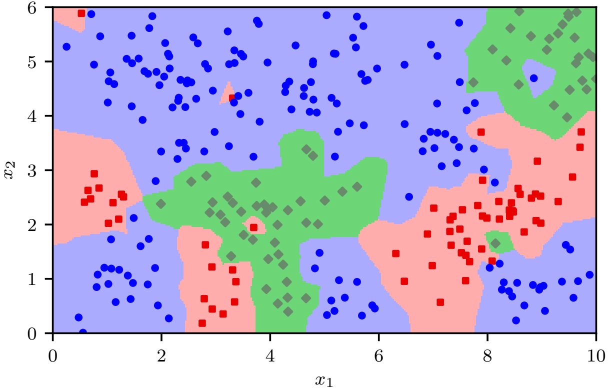
Given a training dataset $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{N}$
where $\boldsymbol{x}_i \in \mathbb{R}^D$ are features and $y_i \in \{1, \ldots, C\}$ are class labels

To classify new observations:

- define a distance measure (e.g. Euclidean distance)
- compute the nearest neighbor for all new data points
- and label them with the label of their nearest neighbor

This works for both *classification* and *regression*.

1-NN



https://zh.wikipedia.org/wiki/%E6%B2%83%E7%BD%97%E8%AF%BA%E4%BC%8A%E5%9B%BE

This corresponds to a Voronoi tesselation.
And results in poor generalization...

k-Nearest Neighbor classification

More *robust* against errors in the training set:

Look at multiple nearest neighbors and pick the majority label.

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Let $\mathcal{N}_k(\boldsymbol{x})$ be the k nearest neighbors of a vector $\boldsymbol{x}$, then in classification tasks:

$$p(y = c \mid \boldsymbol{x}, k) = \frac{1}{k} \sum_{i \in \mathcal{N}_k(\boldsymbol{x})} \mathbb{I}(y_i = c),$$

$$\hat{y} = \arg\max_c p(y = c \mid \boldsymbol{x}, k)$$

with the *indicator variable* $\mathbb{I}(e)$ is defined as:

$$\mathbb{I}(e) = \begin{cases} 1 \text{ if } e \text{ is true} \\ 0 \text{ if } e \text{ is false.} \end{cases}$$

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i.e., the vector will be labeled by the mode of its neighbors' labels.

Refresher: discrete probability theory

Given a jar that contains different colored balls $\{\mathbf{4}, \mathbf{10}, \mathbf{6}\}$. What is the probability of randomly drawing a ball with a particular color (e.g. red)?

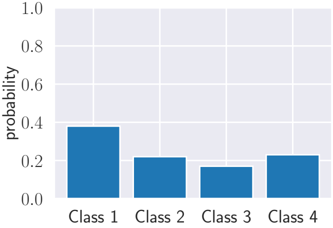
Intuitively: $p(\text{ball} = \textbf{red}) = \frac{\text{number of } \textbf{red} \text{ balls}}{\text{total number of balls}} = \frac{\mathbf{4}}{\mathbf{4}+\mathbf{10}+\mathbf{6}} = \frac{4}{20} = 0.2$

Similarly: $p(\text{ball} = \textbf{green}) = 0.5, \quad p(\text{ball} = \textbf{blue}) = 0.3$

The probability mass function p assigns value to each possible outcome.

In general it has to hold:

- $\forall x,\ p(X = x) \geq 0$
- $\sum_x p(X = x) = 1$



k-Nearest Neighbor classification: weighted

Look at multiple nearest neighbors and pick the weighted majority label.

k-Nearest Neighbor classification: weighted

Look at multiple nearest neighbors and pick the weighted majority label. The weight is inversely proportional to the distance.

Let $\mathcal{N}_k(\boldsymbol{x})$ be the k nearest neighbors of a vector $\boldsymbol{x}$, then in classification tasks:

$$p(y = c \mid \boldsymbol{x}, k) = \frac{1}{Z} \sum_{i \in \mathcal{N}_k(\boldsymbol{x})} \frac{1}{\mathrm{d}(\boldsymbol{x}, \boldsymbol{x}_i)} \mathbb{I}(y_i = c),$$

$$\hat{y} = \arg\max_c p(y = c \mid \boldsymbol{x}, k)$$

with $Z = \sum_{i \in \mathcal{N}_k(x)} \frac{1}{\mathrm{d}(\boldsymbol{x}, \boldsymbol{x}_i)}$ the normalization constant and $\mathrm{d}(\boldsymbol{x}, \boldsymbol{x}_i)$ being a distance measure between $\boldsymbol{x}$ and $\boldsymbol{x}_i$.

k-Nearest-Neighbor regression

Regression is similar:

Let $\mathcal{N}_k(\boldsymbol{x})$ be the k nearest neighbors of a vector $\boldsymbol{x}$, then for regression:

$$\hat{y} = \frac{1}{Z} \sum_{i \in \mathcal{N}_k(\boldsymbol{x})} \frac{1}{\mathrm{d}(\boldsymbol{x}, \boldsymbol{x}_i)} \, y_i,$$

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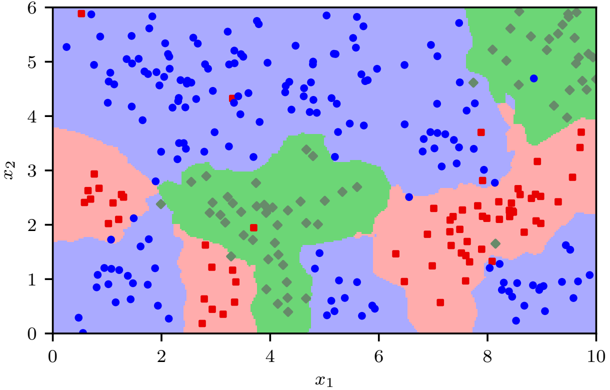
i.e., the vector will be labeled by a weighted mean of its neighbors' values.

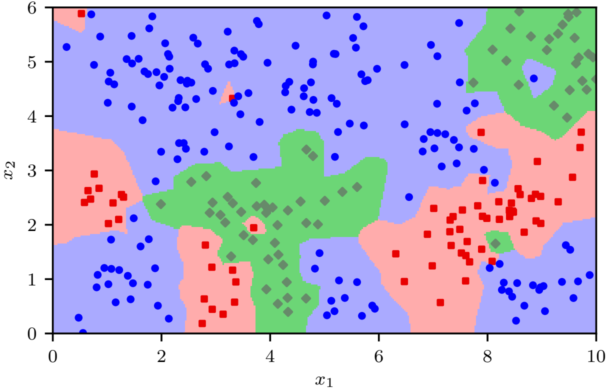
Note: y_i is a real number here (rather then categorical label).

3-NN



So, how many neighbors are best?

1-NN

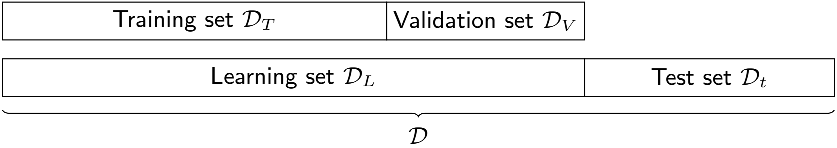


Compare the decision boundaries of 1-NN and 3-NN

Choosing k

Goal is generalization: pick k (called a *hyper-parameter*) that performs best[1] on unseen (future) data.

Unfortunately, no access to future data, so split the dataset $\mathcal{D}$:



Training set $\mathcal{D}_T$

Validation set $\mathcal{D}_V$

Learning set $\mathcal{D}_L$

Test set $\mathcal{D}_t$

$\mathcal{D}$

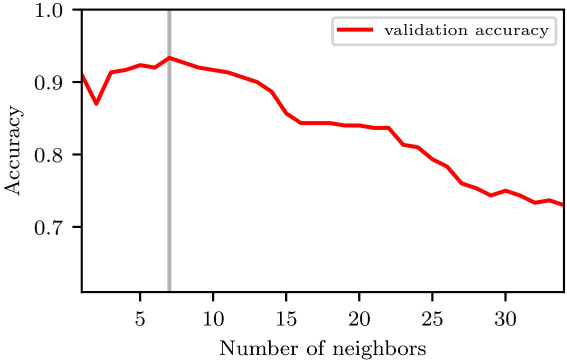
Hyper-parameter tuning procedure

- Learn the model using the training set
- Evaluate performance with different k on the *validation set* picking the best k
- Report final performance on the test set.[2]

[1] In terms of some predefined metric, e.g., accuracy

[2] Good data science practices: See slides on Decision Trees

Using validation set to choose k



We choose $k = 7$.

Measuring classification performance

How can we assess the performance of a (binary) classification algorithm?

⇒ Confusion table

	True condition	
Predicted	$y = 1$	$y = 0$
$y = 1$	TP	FP
$y = 0$	FN	TN

$$\left.\begin{array}{ll} TP & = \text{true positive} \\ TN & = \text{true negative} \end{array}\right\} \text{correct predictions}$$

$$\left.\begin{array}{ll} FP & = \text{false positive} \\ FN & = \text{false negative} \end{array}\right\} \text{wrong predictions}$$

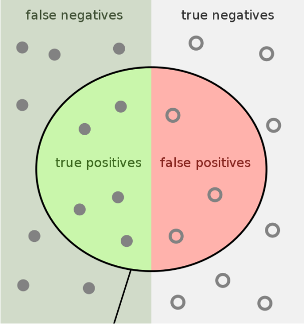


Image source: `https://en.wikipedia.org/wiki/Precision_and_recall`

Measuring classification performance

Accuracy:	$\mathrm{acc} = \frac{TP + TN}{TP + TN + FP + FN}$
Precision:	$\mathrm{prec} = \frac{TP}{TP + FP}$
Sensitivty/Recall:	$\mathrm{rec} = \frac{TP}{TP + FN}$
Specificity:	$\mathrm{tnr} = \frac{TN}{FP + TN}$
False Negative Rate:	$\mathrm{fnr} = \frac{FN}{TP + FN}$
False Positive Rate:	$\mathrm{fpr} = \frac{FP}{FP + TN}$
F1 Score:	$f1 = \frac{2 \cdot \mathrm{prec} \cdot \mathrm{rec}}{\mathrm{prec} + \mathrm{rec}}$

$\Rightarrow$ Trade-off between precision and recall: increasing one (most often) leads to decreasing the other

General note: Be careful when you have imbalanced classes!

Distance measures

- K-NN can be used with various distance measures → highly flexible
- Euclidean distance (L_2 norm): $\sqrt{\sum_i (u_i - v_i)^2}$

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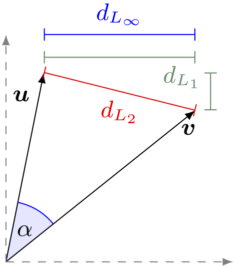
- Angle:

$$\cos\alpha = \frac{\boldsymbol{u}^T \boldsymbol{v}}{\|\boldsymbol{u}\| \|\boldsymbol{v}\|}$$



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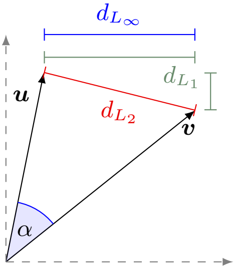
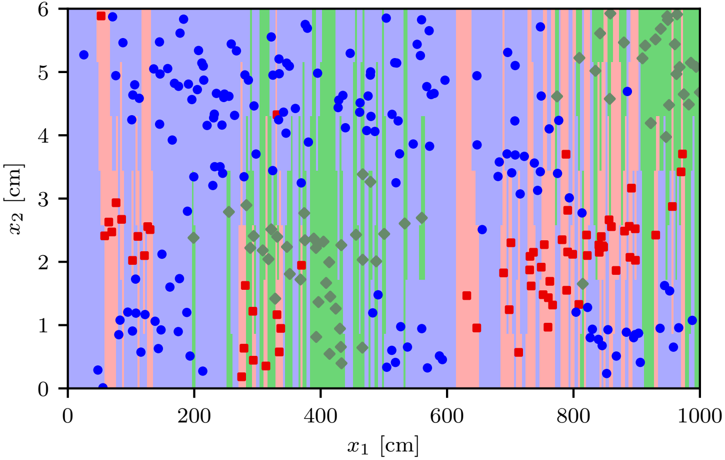


- *Mahalanobis distance* ($\boldsymbol{\Sigma}$ is *positive (semi) definite* and *symmetric*):

$$\sqrt{(\boldsymbol{u} - \boldsymbol{v})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{u} - \boldsymbol{v})}$$

- Hamming distance, Edit distance, . . .

Scaling issues



The same old example but one of our features is in the order of meters, the other in the order of centimeters. $(k = 1)$

Circumventing scaling issues

- Data *standardization*
  Scale each feature to zero mean and unit variance.

$$x_{i,\text{std}} = \frac{x_i - \mu_i}{\sigma_i}$$

(This is a standard procedure in machine learning. Many models are sensitive to differences in scale.)

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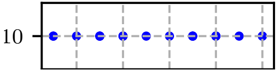
  $$x_{i,\text{std}} = \frac{x_i - \mu_i}{\sigma_i}$$

  (This is a standard procedure in machine learning. Many models are sensitive to differences in scale.)
- Use the Mahalanobis distance.

  $$\text{mahalanobis}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sqrt{(\boldsymbol{x}_1 - \boldsymbol{x}_2)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}_1 - \boldsymbol{x}_2)}$$

  $\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \cdots & 0 \\ 0 & 0 & \sigma_n^2 \end{bmatrix}$ is equal to Euclidean distance on normalized data

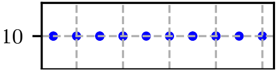
The curse of dimensionality



Given a discrete one-dimensional input space $x \in \{1, 2, \ldots, 10\}$

For $N = 20$ uniformly distributed samples the data covers 100% of the input space.

The curse of dimensionality



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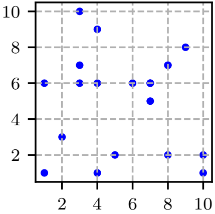
Add a second dimension (now $\boldsymbol{x} \in \{1, \ldots, 10\}^2$) and your data only covers 18% of the input space.



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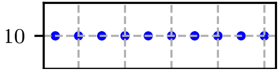

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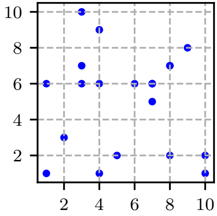

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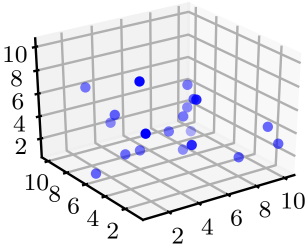
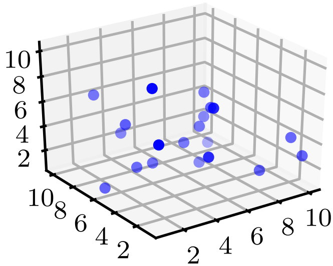


Once you add a third dimension you only cover 2%.

The curse of dimensionality

- The nearest neighbor will now be pretty far away..
- N has to grow exponentially with the number of features. Consider this when using k-NN on high-dimensional data.

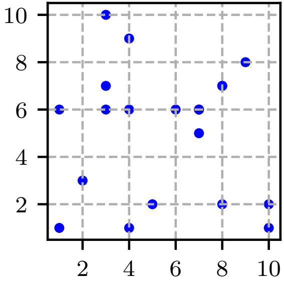


Practical considerations

Expensive: memory and naive inference are both $O(N)$:

we need to store the entire training data and compare with all training instances to find the nearest neighbor

Solution: use tree-based search structures (e.g. k-d tree) for efficient (approximate) NN [3]



[3] At the expense of an additional computation performed only once

What we learned

- k-NN Algorithm
- Train-validation-test split
- Measuring classification performance
- Distance metrics
- Curse of dimensionality

Reading material

Main reading

- "Machine Learning: A Probabilistic Perspective" by Murphy [ch. 1.4.1 - 1.4.3]

Extra reading

- "Bayesian Reasoning and Machine Learning" by Barber [ch. 14]

Slides adapted from previous versions by W. Koepp & D. Korhammer