

# Classifiers: Naïve Bayes, k-NN, evaluation

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## Bayes optimal strategy

- ▶ The **Bayes optimal strategy** : one minimizing mean risk.  $\delta^* = \arg \min_{\delta} r(\delta)$
- ▶  $s$  states,  $x$  possible measurements,  $P(s, x)$  joint probabilities

$$\begin{aligned} r(\delta) &= \sum_x \sum_s \ell(s, \delta(x)) P(x, s) = \sum_s \sum_x \ell(s, \delta(x)) P(s|x) P(x) \\ &= \sum_x P(x) \underbrace{\sum_s \ell(s, \delta(x)) P(s|x)}_{\text{Conditional risk}} \end{aligned}$$

Risk of a strategy is a weighted sum of conditional risks (conditioned by  $x$ )

- ▶ The optimal strategy is obtained by minimizing the conditional risk *separately* for each  $x$ :

$$\delta^*(x) = \arg \min_d \sum_s \ell(s, d) P(s|x)$$

## A special case - Bayesian *classification*

- ▶ Attribute vector  $\vec{x} = (x_1, x_2, \dots)$ : pixels 1, 2,  $\dots$
- ▶ **State set  $\mathcal{S}$  = decision set  $\mathcal{D} = \{0, 1, \dots, 9\}$ .**
- ▶ **State = actual class, Decision = recognized class**
- ▶ **Loss function :**

$$\ell(s, d) = \begin{cases} 0, & d = s \\ 1, & d \neq s \end{cases}$$

Optimal decision strategy:

$$\delta^*(\vec{x}) = \arg \min_d \sum_s \underbrace{\ell(s, d)}_{0 \text{ if } d=s} P(s|\vec{x}) = \arg \min_d \sum_{s \neq d} P(s|\vec{x})$$

Obviously  $\sum_s P(s|\vec{x}) = 1$ , then:

$$P(d|\vec{x}) + \sum_{s \neq d} P(s|\vec{x}) = 1$$

Inserting into above:

$$\delta^*(\vec{x}) = \arg \min_d [1 - P(d|\vec{x})] = \arg \max_d P(d|\vec{x})$$

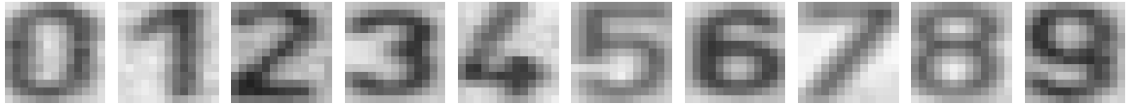
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### Notes

We are using different word – *classification* instead of *decision* but the reasoning and methods can be well applied in both. In classification problem we usually treat all mistakes – wrong classifications – equally painful, contrary to decision problem – remember “What to cook for dinner” problem?

## Example: Digit recognition/classification



- ▶ **Input:** 8-bit image  $13 \times 13$ , pixel intensities 0 – 255. (0 means black, 255 means white)
- ▶ **Output:** Digit 0 – 9. Decision about the class, classification.
- ▶ **Features:** Pixel intensities ...

**Decision/classification problem** : What cipher is in the (query) image?



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### Notes

Digit recognition is a very classical example of classification problem. It has been used for decades, and it is used till today, see e.g. [MNIST demo at PyTorch](#)

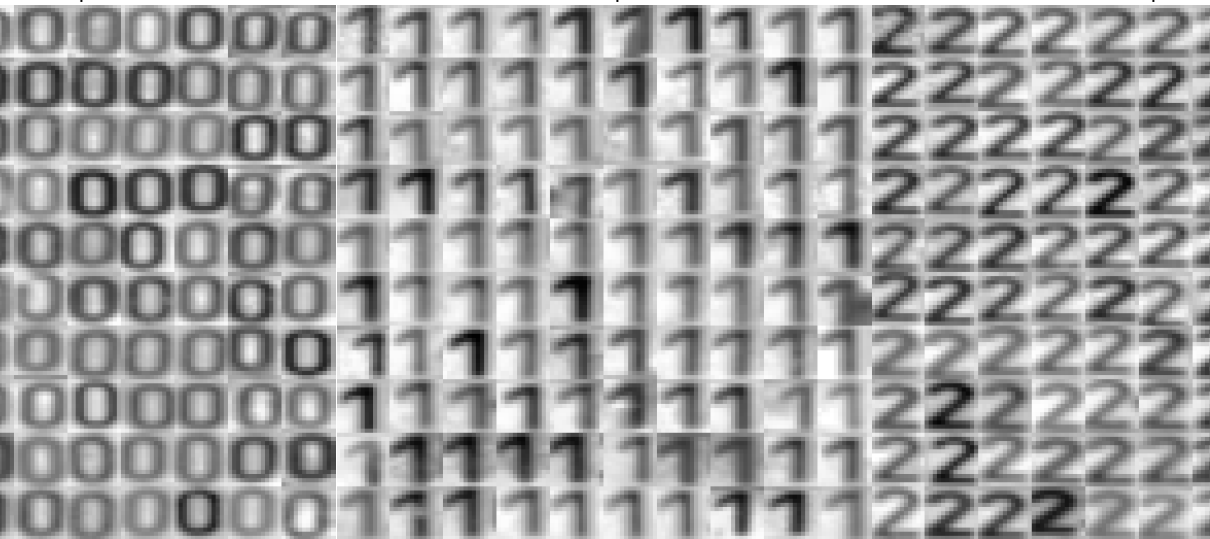
$$\delta^*(\text{img}) = \arg \max_d P(d | \text{img})$$

# Machine Learning: Prepare training data, let (an) algorithm learn itself

data for cipher 0

data for cipher 1

data for cipher 2



Training samples:  $(\vec{x}_i, s = 0)$  Training samples:  $(\vec{x}_i, s = 1)$  Training samples:  $(\vec{x}_i, s = 2)$

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## Notes

# Bayes classification in practice; $P(s|\vec{x}) = ?$

- ▶ Usually, we are not given  $P(s|\vec{x})$
- ▶ It has to be estimated from already classified examples – training data
- ▶ For discrete  $\vec{x}$ , training examples  $(\vec{x}_1, s_1), (\vec{x}_2, s_2), \dots, (\vec{x}_I, s_I)$ 
  - ▶ every  $(\vec{x}_i, s_i)$  is drawn independently from  $P(\vec{x}, s)$ , i.e. sample  $i$  does not depend on  $1, \dots, i-1$
  - ▶ so-called i.i.d (independent, identically distributed) multiset
- ▶ Without knowing anything about the distribution, a non-parametric estimate:

$$P(s|\vec{x}) = \frac{P(\vec{x}, s)}{P(\vec{x})} \approx \frac{\# \text{ examples where } \vec{x}_i = \vec{x} \text{ and } s_i = s}{\# \text{ examples where } \vec{x}_i = \vec{x}}$$

- ▶ Hard in practice:

- ▶ To reliably estimate  $P(s|\vec{x})$ , the number of examples grows exponentially with the number of elements of  $\vec{x}$ .
  - ▶ e.g. with the number of pixels in images
  - ▶ curse of dimensionality
  - ▶ denominator often 0



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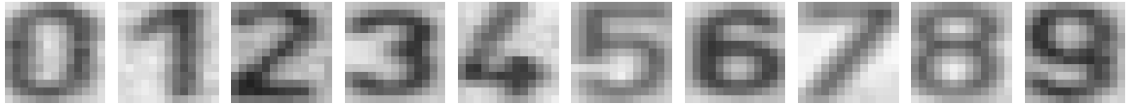
## Notes

Why hard? Way too many various  $\vec{x}$ .

What is the difference between set and multiset?

Reminder about math notation. In literature, vectors are mostly denoted by bold lower case  $\mathbf{x}$ . In lectures, we use  $\vec{x}$  to match notation used on blackboard. It is difficult to write bold with a chalk.

## How many images?



8-bit image  $13 \times 13$ , pixel intensities 0 – 255. (0 means black, 255 means white)

- A:  $169^{256}$
- B:  $256^{169}$
- C:  $13^{13}$
- D:  $169 \times 256$
- E: different quantity

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### Notes

Think about simple binary  $10 \times 10$  image -  $\vec{x}$  contains 0, 1, position matters. What is the total number of unique images? Think binary,  $1 \times 8$  binary image? Hence:  $B=256^{169}$  is the answer.

And a minimal dataset would contain each possible image at least once! We must be ready for any image (like for any state).



# Naïve Bayes classification

- ▶ For efficient classification we must thus rely on additional assumptions.
- ▶ In the exceptional case of **statistical independence** between components of  $\vec{x}$  for each class  $s$  it holds

$$P(\vec{x}|s) = P(x[1]|s) \cdot P(x[2]|s) \cdot \dots$$

- ▶ Use simple Bayes law and maximize:

$$P(s|\vec{x}) = \frac{P(\vec{x}|s)P(s)}{P(\vec{x})} = \frac{P(s)}{P(\vec{x})} P(x[1]|s) \cdot P(x[2]|s) \cdot \dots =$$

- ▶ No combinatorial curse in estimating  $P(s)$  and  $P(x[i]|s)$  separately for each  $i$  and  $s$ .
- ▶ No need to estimate  $P(\vec{x})$ . (Why?)
- ▶  $P(s)$  may be provided apriori.
- ▶ **naïve** = when used despite statistical dependence

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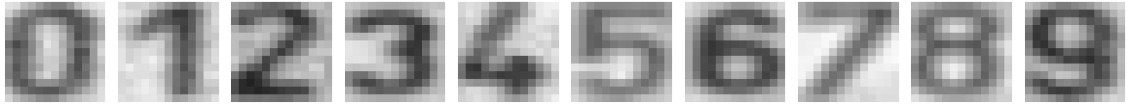
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## Notes

Why naïve at all? Consider  $N$ -dimensional feature space and 8-bit values. Instead of considering  $8^N$  combinations (joint prob. distribution), we can consider only  $N \times 8$ —treating every feature separately.

Think about statistical independence. Example1: person's weight and height. Are they independent? Example2: pixel values in images.

## Example: Digit recognition/classification



- ▶ **Input:** 8-bit image  $13 \times 13$ , pixel intensities 0 – 255. (0 means black, 255 means white)
- ▶ **Output:** Digit 0 – 9. Decision about the class, classification.
- ▶ **Features:** Pixel intensities ...

Collect **data** , ...

- ▶  $P(\vec{x})$ . What is the dimension of  $\vec{x}$ ? How many possible images?
- ▶ Learn  $P(\vec{x}|s)$  per each class (digit).
- ▶ Classify  $s^* = \operatorname{argmax}_s P(s|\vec{x})$ .

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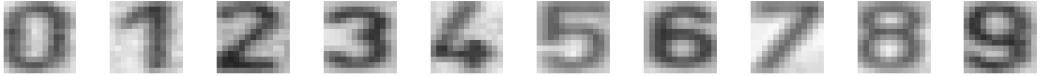
### Notes

We can create many more features than just pixel intensities. But first things first.

We are assuming all errors are equally important - minimizing the number of wrong decisions.

Dimension of  $\vec{x}$  is  $13 \times 13 = 169$ . There are  $256^{169}$  possible images. (we already know)

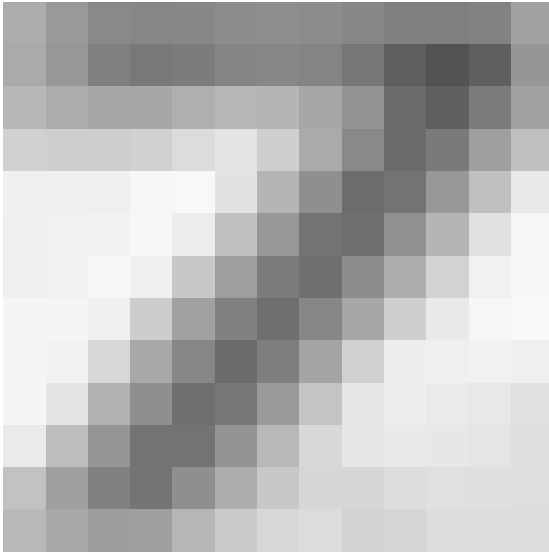
From images to  $\vec{x}$



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Notes

# Conditional probabilities, likelihoods



- ▶ Apriori digit probabilities  $P(s_k)$
- ▶ Likelihoods for pixels.  $P(x_{r,c} = I_i | s_k)$

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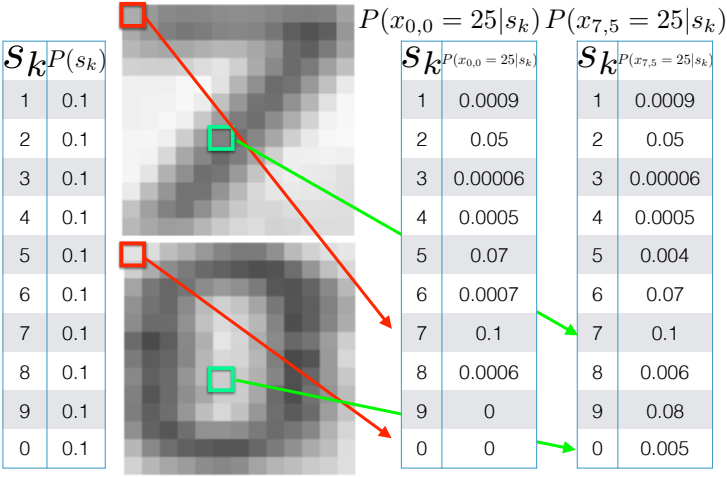
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## Notes

A lexical note, especially for Czech speakers. *probability* as well as *likelihood* can be translated as *pravděpodobnost*. I suggest the following mental model than can work for our purposes.

- **Probability** is related to the future events (unknown outcome). E.g. what is the probability of selecting blue box? What is the probability that a random ZIP Code number begins with 7?
- **Likelihood** refers to past events (known outcome). In my data, how many images of 7 have dark pixel in top right corner? We can think about relative frequency (relativní četnost). Or, we can think: what is the probability that an observation of a dark pixel in the top right corner was generated by an image of 7. Jak věrohodné to je?

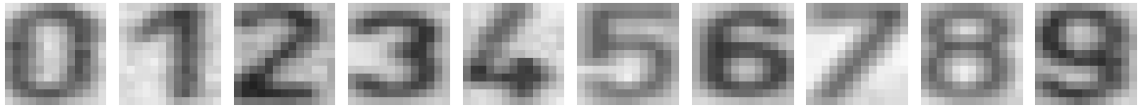
# Conditional likelihoods



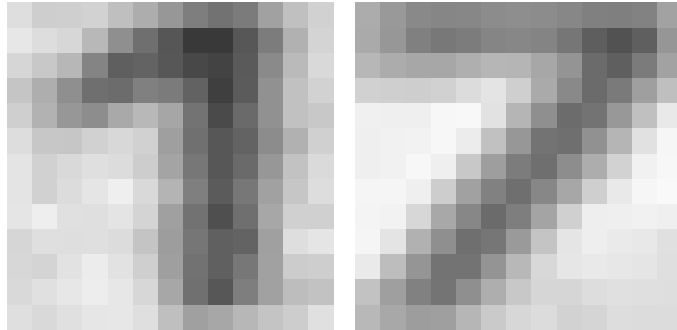
## Notes

For each pixel (position) and possible intensity (image/pixel value) we create such a table.

# Unseen events



Images  $13 \times 13$ , intensities 0 – 255, 100 exemplars per each class.



$$\begin{aligned} \vdots &= \vdots \\ P(x_{0,0} = 100 \mid s = 7) &= 0.05 \\ P(x_{0,0} = 101 \mid s = 7) &= 0 \\ P(x_{0,0} = 102 \mid s = 7) &= 0.06 \\ \vdots &= \vdots \end{aligned}$$

A new (not in training) query image with  $x_{0,0} = 101$ . How would you classify?

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## Notes

Think about the problem of classifying numerals. Some  $P(x_{r,c} = l \mid s) = 0$ . What about an example:

$$\begin{aligned} \vdots &= \vdots \\ P(x_{0,0} = 100 \mid s = 7) &= 0.05 \\ P(x_{0,0} = 101 \mid s = 7) &= 0 \\ P(x_{0,0} = 102 \mid s = 7) &= 0.06 \\ \vdots &= \vdots \end{aligned}$$

A new (not in training) query image with  $x_{0,0} = 101$ . How would you classify?

## Unseen event, how to decide?

A new (not in training) query image with  $x_{0,0} = 101$ . How would you classify?

$$P(x_{0,0} = 101 | s_j) = 0, \text{ for all classes}$$

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Notes

# Laplace smoothing (“additive smoothing”)

Think about a particular pixel with intensity  $x$

$$P(x) = \frac{\text{count}(x)}{\text{total samples}}$$

Problem:  $\text{count}(x) = 0$

Pretend you see the (any) sample one more time.

$$P_{\text{LAP}}(x) = \frac{c(x) + 1}{\sum_x [c(x) + 1]}$$

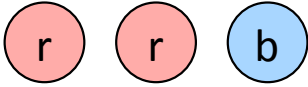
$$P_{\text{LAP}}(x) = \frac{c(x) + 1}{N + |X|}$$

where  $N$  is the number of (total) observations;  $|X|$  is the number of possible values  $X$  can take (cardinality).



$$P_{LAP}(x) = \frac{c(x)+1}{\sum_x [c(x)+1]} = \frac{c(x)+1}{N+|X|} = ?$$

Observation:



What is  $P_{LAP}(X = \text{red})$  and  $P_{LAP}(X = \text{blue})$ ?

A:  $P_{LAP}(X = \text{red}) = 7/10$ ,  $P_{LAP}(X = \text{blue}) = 3/10$

B:  $P_{LAP}(X = \text{red}) = 2/3$ ,  $P_{LAP}(X = \text{blue}) = 1/3$

C:  $P_{LAP}(X = \text{red}) = 3/5$ ,  $P_{LAP}(X = \text{blue}) = 2/5$

D: None of the above.

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### Notes



$$P_{ML}(X) =$$

$$P_{LAP}(X) =$$

originally:

- $P(\text{red}) = 2/3$
- $P(\text{blue}) = 1/3$

after Laplace smoothing – adding one red ball and blue ball to the actual observations:

- $P_{LAP}(\text{red}) = (2 + 1)/(2 + 1 + 1 + 1) = 3/5$
- $P_{LAP}(\text{blue}) = (1 + 1)/(2 + 1 + 1 + 1) = 2/5$

# Laplace smoothing - as a hyperparameter $k$

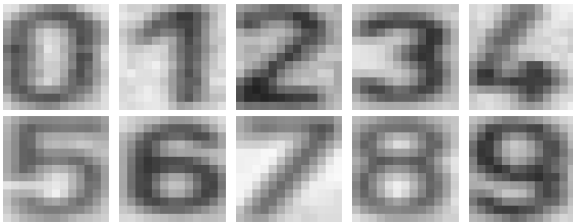
Pretend you see every sample  $k$  extra times:

$$P_{\text{LAP}}(x) = \frac{c(x) + k}{\sum_x [c(x) + k]}$$

$$P_{\text{LAP}}(x) = \frac{c(x) + k}{N + k|X|}$$

For conditional, smooth each condition independently

$$P_{\text{LAP}}(x|s) = \frac{c(x, s) + k}{c(s) + k|X|}$$



What is  $|X|$  equal to?

- A: 10
- B: 2
- C: 256
- D: None of the above

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## Notes

Hyperparameter would be tuned along with your classifier

For  $k = 100$  and blue and red, you would get:

- $P_{\text{LAP}}(\text{red}) = (2 + 100)/(3 + 100 * 2) = 102/203$
- $P_{\text{LAP}}(\text{blue}) = (1 + 100)/(3 + 100 * 2) = 101/203$

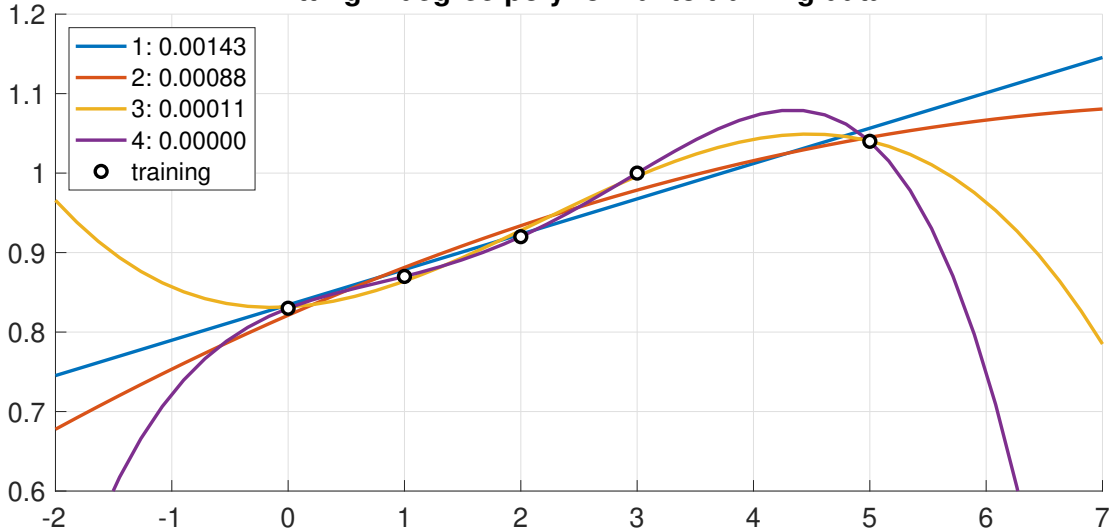
In this case, smoothing ("prior") would dominate over the observations - shifting estimate from empirical to uniform.

In the digit recognition from pixels example: 256 intensity values;  $13 \times 13 = 169$  pixels: Applying Laplace smoothing with  $k = 1$  to  $P(x)$  (prior probability of a particular pixel will take an intensity value  $i$ ):  $P(x_{r,c} = i) = (c(x) + 1)/(N + 256)$

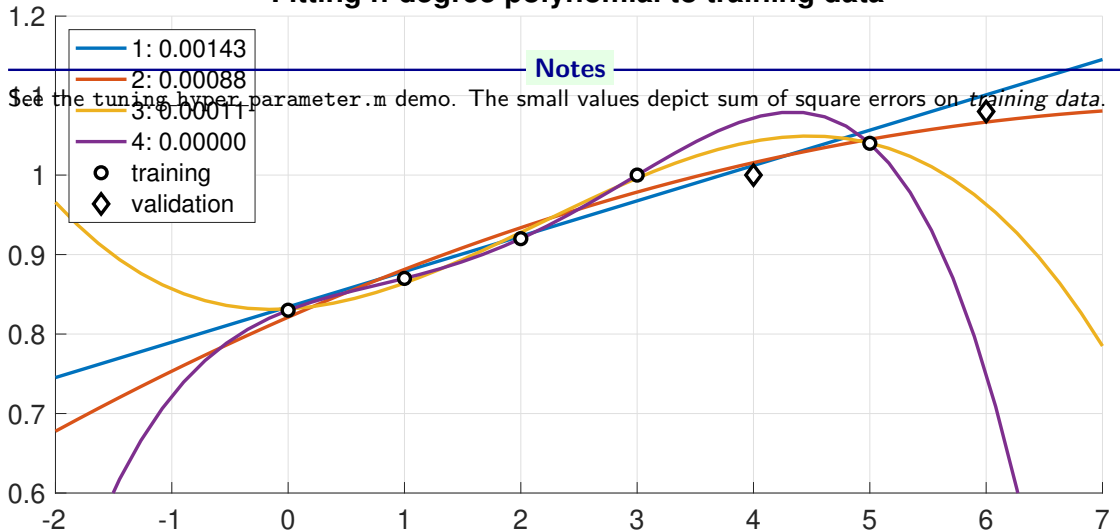
Conditional: relevant for the Naïve Bayes case.

# What is the right degree of polynomial (hyperparameter of a regressor)

## Fitting n-degree polynomial to training data

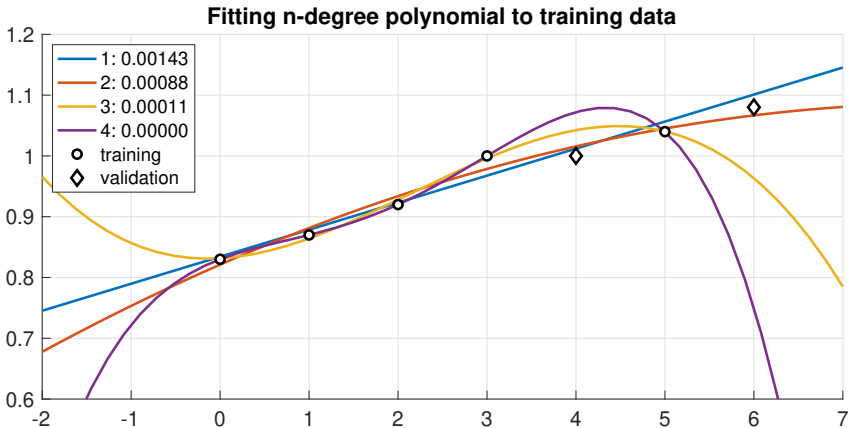


## Fitting n-degree polynomial to training data



# Generalization and overfitting

- ▶ **Data: training, validating, testing** . Wanted classifier performs well on what data?
- ▶ Overfitting: too close to training, poor on testing.



# Training and testing

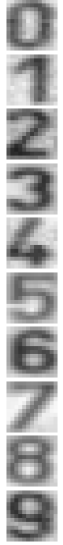
**Data** labeled instances.

- ▶ Training set
- ▶ Held-out (validation) set
- ▶ Testing set.

**Features** : Attribute-value pairs.

**Learning cycle:**

- ▶ **Learn** parameters (e.g. probabilities) on training set.
- ▶ **Tune** hyperparameters on held-out (validation) set.
- ▶ **Evaluate** performance on testing set.



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## Notes

Training set - biggest part.

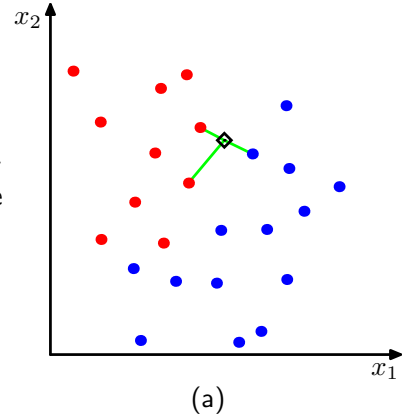
# $K$ – Nearest Neighbor and Bayes $j^* = \operatorname{argmax}_j P(s_j | \vec{x})$

Assume data:

- ▶  $N$  samples  $\vec{x}$  in total.
- ▶  $N_j$  samples in  $s_j$  class. Hence,  $\sum_j N_j = N$ .

We want classify to  $\vec{x}$ . We draw a circle (hyper-sphere) centered at  $\vec{x}$  containing  $K$  points irrespective of class.  $V$  is the volume of this sphere.  $P(s_j | \vec{x}) = ?$

$$P(s_j | \vec{x}) = \frac{P(\vec{x} | s_j) P(s_j)}{P(\vec{x})}$$

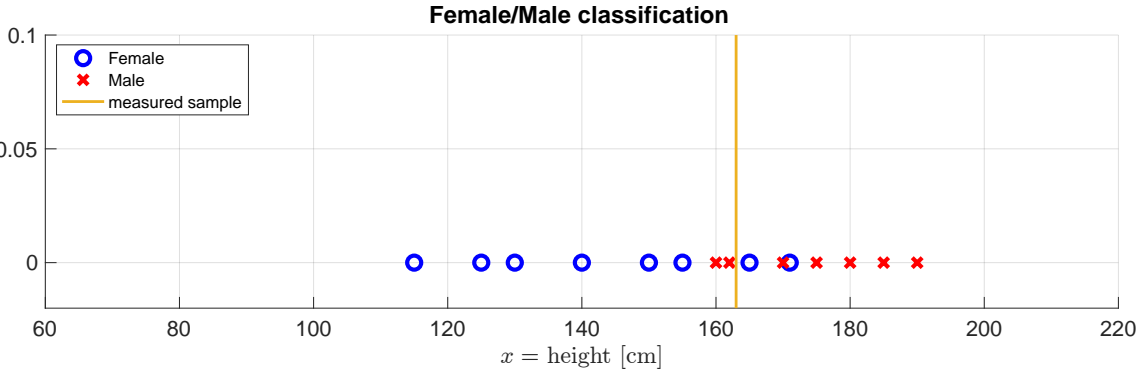


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## Notes

$$\begin{aligned} P(s_j) &= \frac{N_j}{N} \\ P(\vec{x}) &= \frac{K}{NV} \\ P(\vec{x} | s_j) &= \frac{K_j}{N_j V} \\ P(s_j | \vec{x}) &= \frac{P(\vec{x} | s_j) P(s_j)}{P(\vec{x})} = \frac{K_j}{K} \end{aligned}$$

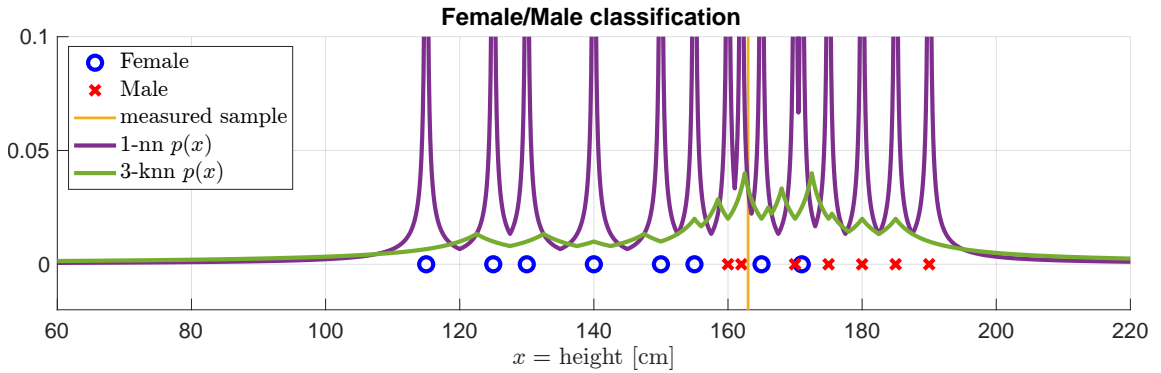
# Female/male classification based on height. $N$ data points available.



Ignore the  $y$  axis. A new measurement comes,  $x = 163$  cm. Female or male?

Notes

# $K$ -NN $p(x)$ estimate

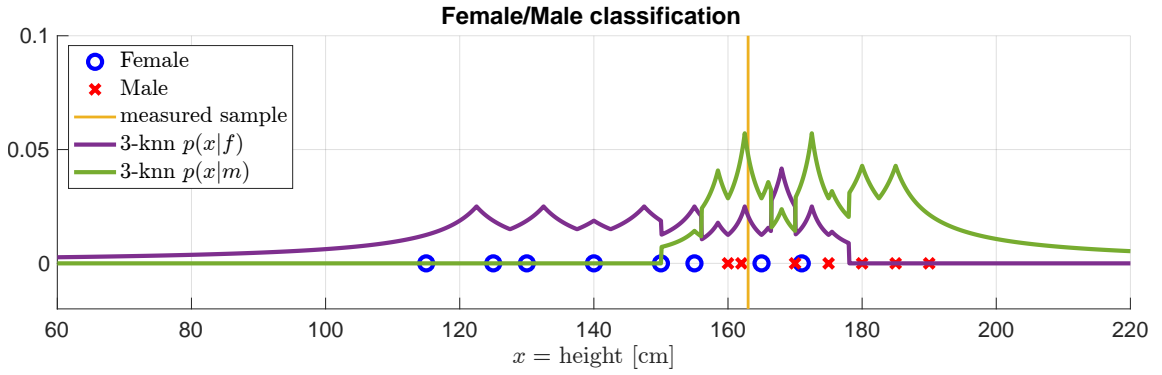


$$p(x) = \frac{K}{NV}$$

$V = 2r_k(x)$ , where  $r_k(x)$  is the distance of  $k$ -th nearest data point to  $x$

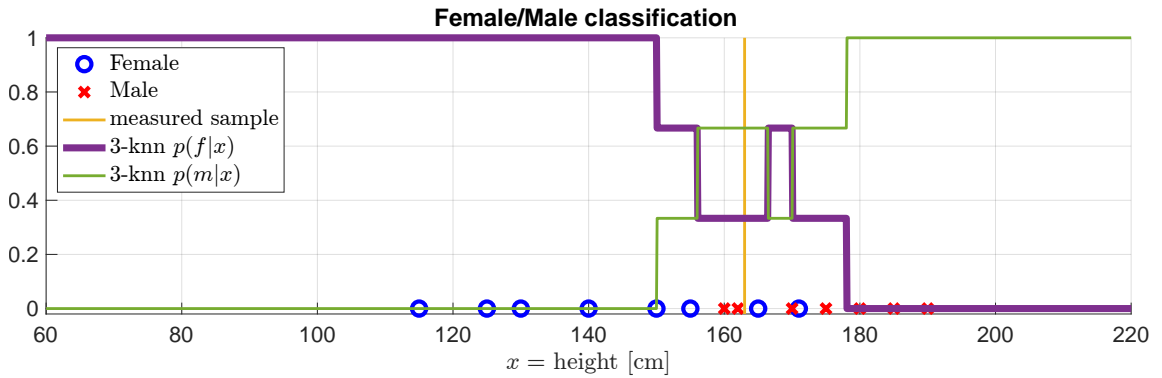


# $K$ -NN $p(x|s_j)$ estimates



$$p(x|s_j) = \frac{K_j}{N_j V}$$

# $K$ -NN $p(s_j|x)$ posteriors



$$p(s_j|x) = \frac{p(x|s_j)p(s_j)}{p(x)}$$

## Notes

On the first sight it looks suspiciously regular but it is all true:

$$p(s_j|x) = \frac{\frac{K_j}{N_j V} \frac{N_j}{N}}{\frac{K}{NV}} = \frac{K_j}{K}$$

# Volume in $k - NN$ in higher dimensions

Complement slide, for the sake of completeness. The decision rule  $P(s_j|x) = N_j/N$  is the same for all dimensions.

$$P(\vec{x}) = \frac{K}{NV}$$

$$V = V_d R_k^d(\vec{x})$$

$R_k(\vec{x})$  - distance from  $\vec{x}$  to its  $k$ -th nearest neighbour point (radius)

$$V_d = \frac{\pi^{d/2}}{\Gamma(d/2 + 1)}$$

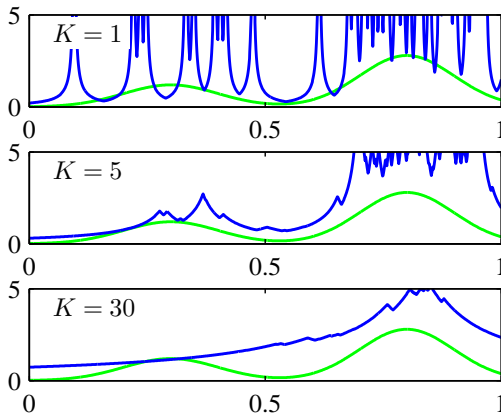
volume of unit  $d$ -dimensional sphere,

$\Gamma$  denotes gamma function.

$$V_1 = 2, V_2 = \pi, V_3 = \frac{4}{3}\pi$$

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## Notes



More details, including a computational example, in [2].

A  $K$ -NN belongs to non-parametric methods for density estimation, see section 2.5 from [1]. (Figure from [1])

You may try it yourself, <https://scikit-learn.org/stable/modules/density.html#kernel-density>

# Precision and Recall, and ...

Consider digit **detection** (is there a digit?) or SPAM/HAM, Male/Female classification

**Recall** :

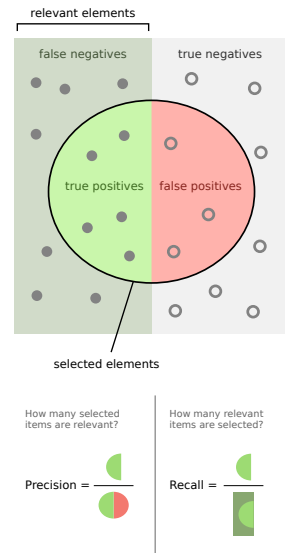
- ▶ How many relevant items are selected?
- ▶ Are we missing some items?
- ▶ Also called: **True positive rate** (TPR), sensitivity, hit rate ...

**Precision**

- ▶ How many selected items are relevant?
- ▶ Also called: Positive predictive value

**False positive rate** (FPR)

- ▶ Probability of false alarm



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## Notes

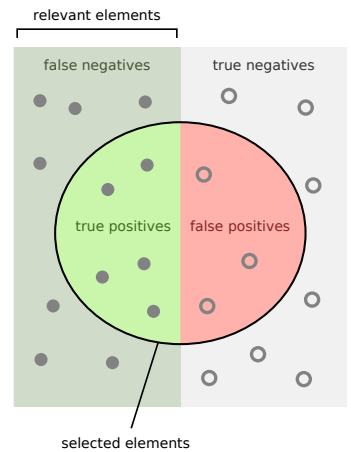
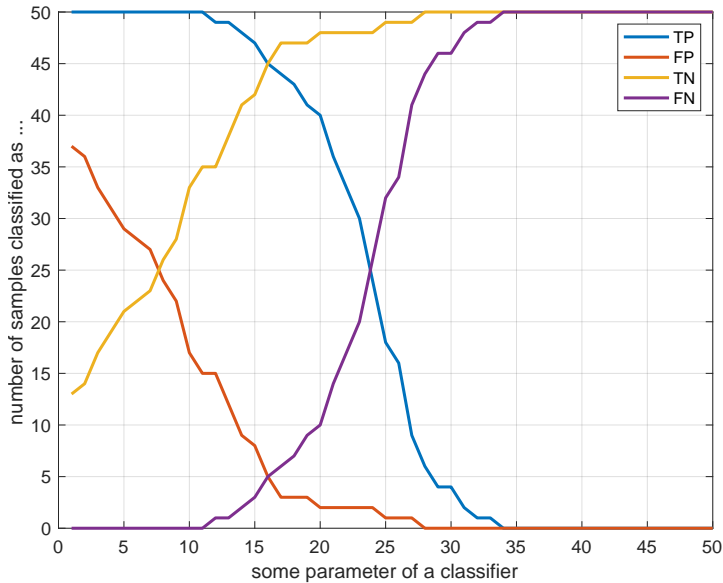
$$\text{TPR} = \frac{\text{TP}}{P} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

$$\text{FPR} = \frac{\text{FP}}{N} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

Think about TPR vs FPR graph, what is the best classifier?

# Studying a classifier ...



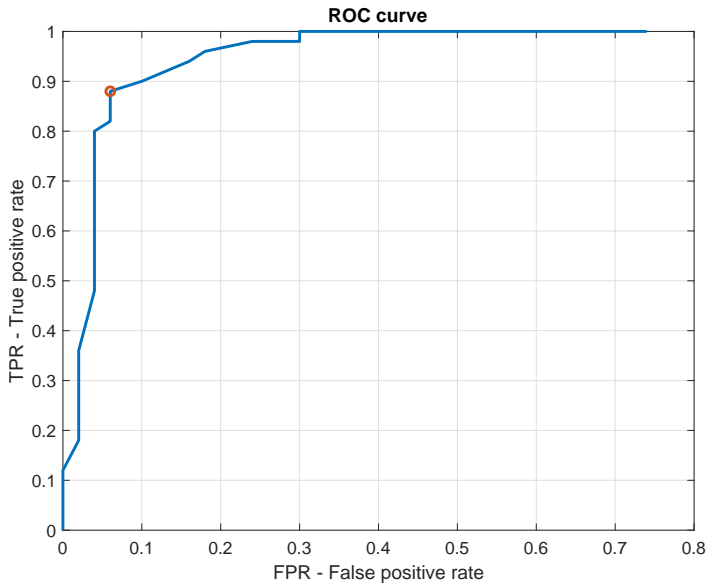
How many data samples  $x_i$ ?

- A 50
- B 100
- C 150
- D 200

## Notes

How many data samples in the testing (evaluation) set?

# ROC – Receiver operating characteristics curve

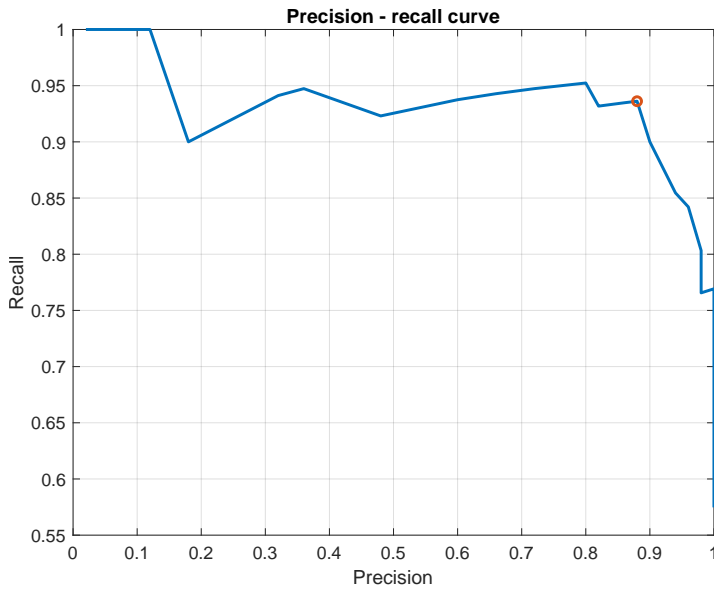


$$\text{TPR} = \frac{\text{TP}}{P} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$
$$\text{FPR} = \frac{\text{FP}}{N} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

## Notes

- How do you slide along the curve?
- What is the meaning of the diagonal?
- What would be the shape of the curve for the ideal/worst classifier?
- How would you compare various curve and select the best classifier?
- Think/read about other ways to evaluate/visualise classification results.

# Precision – recall curve



$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

## Notes

Think about a different classifier (curve), how would you compare?

# How to evaluate a multi-class classifier? Confusion table

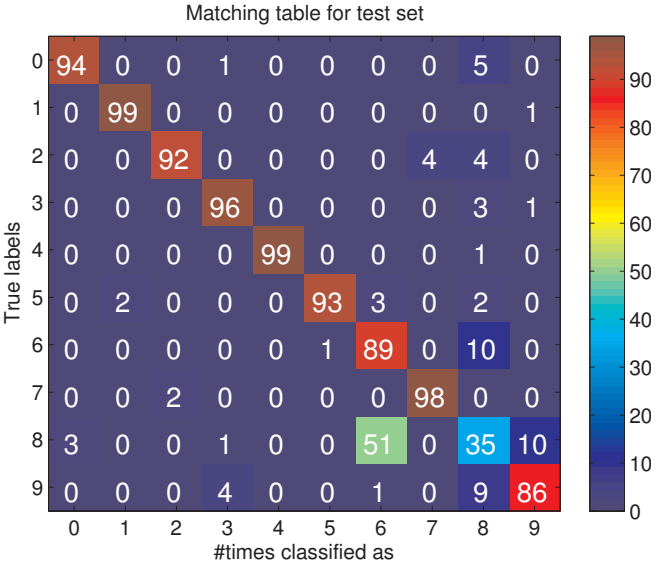


Figure from [6]

## Notes

A result for a one particular classifier and its setting (parameters), one particular testing set.



# Product of many small numbers ...

$$P(s|\vec{x}) = \frac{P(\vec{x}|s)P(s)}{P(\vec{x})} = \frac{P(s)}{P(\vec{x})} P(x[1]|s) \cdot P(x[2]|s) \cdot \dots$$

$P(\vec{x})$  not needed, .....

$$\log(P(x[1]|s)P(x[2]|s)\dots) = \log(P(x[1]|s)) + \log(P(x[2]|s)) + \dots$$

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## Notes

just try

- `prod(rand(1,100))` and `prod(rand(1,10000))` in Matlab.
- `prod(rand(1,100)) == 0` and `prod(rand(1,10000)) == 0` in Matlab.

or in python console:

- ```
>>> import numpy as np
```
- ```
>>> np.prod(np.random.rand(100))==0
```
- ```
>>> np.prod(np.random.rand(1000))==0
```
- ```
>>> a = np.random.rand(1000)
>>> b = np.random.rand(1000)
>>> np.prod(a)>np.prod(b)
False
>>> np.prod(a)<np.prod(b)
False
>>> np.sum(np.log(a))>np.sum(np.log(b))
True
```

Hitting the limit of number representation.

What is the way out?

$P(\vec{x})$  not needed – does not depend on the class.

Laws of logarithms...

# References I

Further reading: Chapter 13 and 14 of [5]. Books [1] and [3] are classical textbooks in the field of pattern recognition and machine learning. This lecture has been also inspired by the 21st lecture of CS 188 at <http://ai.berkeley.edu> (e.g., Laplace smoothing). Many Matlab figures created with the help of [4].

[1] Christopher M. Bishop.

*Pattern Recognition and Machine Learning.*

Springer Science+Business Media, New York, NY, 2006.

<https://www.microsoft.com/en-us/research/uploads/prod/2006/01/Bishop-Pattern-Recognition-and-Machine-Learning-2006.pdf>.

[2] Yen-Chi Chen.

Lecture 7: Density estimation: k-nearest neighbor and basis approach.

Lecture within STAT 425: Introduction to Nonparametric Statistics, 2018.

[http://faculty.washington.edu/yenchic/18W\\_425/Lec7\\_knn\\_basis.pdf](http://faculty.washington.edu/yenchic/18W_425/Lec7_knn_basis.pdf).

# References II

- [3] Richard O. Duda, Peter E. Hart, and David G. Stork.  
*Pattern Classification*.  
John Wiley & Sons, 2nd edition, 2001.
- [4] Vojtěch Franc and Václav Hlaváč.  
Statistical pattern recognition toolbox.  
<http://cmp.felk.cvut.cz/cmp/software/stprtool/index.html>.
- [5] Stuart Russell and Peter Norvig.  
*Artificial Intelligence: A Modern Approach*.  
Prentice Hall, 3rd edition, 2010.  
<http://aima.cs.berkeley.edu/>.

## References III

[6] Tomáš Svoboda, Jan Kybic, and Hlaváč Václav.

*Image Processing, Analysis and Machine Vision — A MATLAB Companion.*

Thomson, Toronto, Canada, 1<sup>st</sup> edition, September 2007.

<http://visionbook.felk.cvut.cz/>.