Classifiers: Naïve Bayes, k-NN, evaluation

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Notes

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 probababilities

$$r(\delta) = \sum_x \sum_s \ell(s,\delta(x))P(x,s) = \sum_s \sum_x \ell(s,\delta(x))P(s|x)P(x)$$
$$= \sum_x P(x) \underbrace{\sum_s \ell(s,\delta(x))P(s|x)}_{\text{Conditional risk}} = \sum_x P(x) r\left(\delta(x),x\right)$$

  where conditional risk $r(d,x) = \sum_s \ell(s,d)P(s|x)$.
- Risk of a strategy is a weighted sum of conditional risks (conditioned on x)
- The optimal strategy is obtained by minimizing the conditional risk *separately* for each x:

$$\delta^*(x) = \operatorname*{argmin}_d r(d,x) = \arg\min_d \sum_s \ell(s,d)P(s|x)$$

Notes

A special case - Bayesian *classification*

- Attribute vector $\vec{x} = (x_1, x_2, \dots)$: pixels 1, 2, ...
- **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:

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

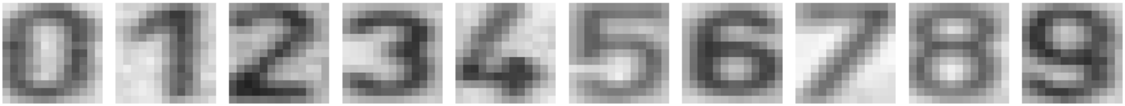
Inserting into above:

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

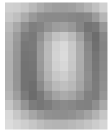
Notes

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 classificaions – equally painful, contrary to decision problem – remember "What to cook for dinner" problem?

Example: Digit recognition/classification



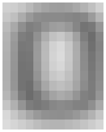
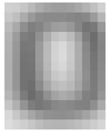
- Input: 8-bit image 13×13, pixel intensities $0 - 255$. (0 means black, 255 means white)
- Output: Digit $0 - 9$. Decision about the class, classification.
- Features: Pixel intensities ...

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

Notes

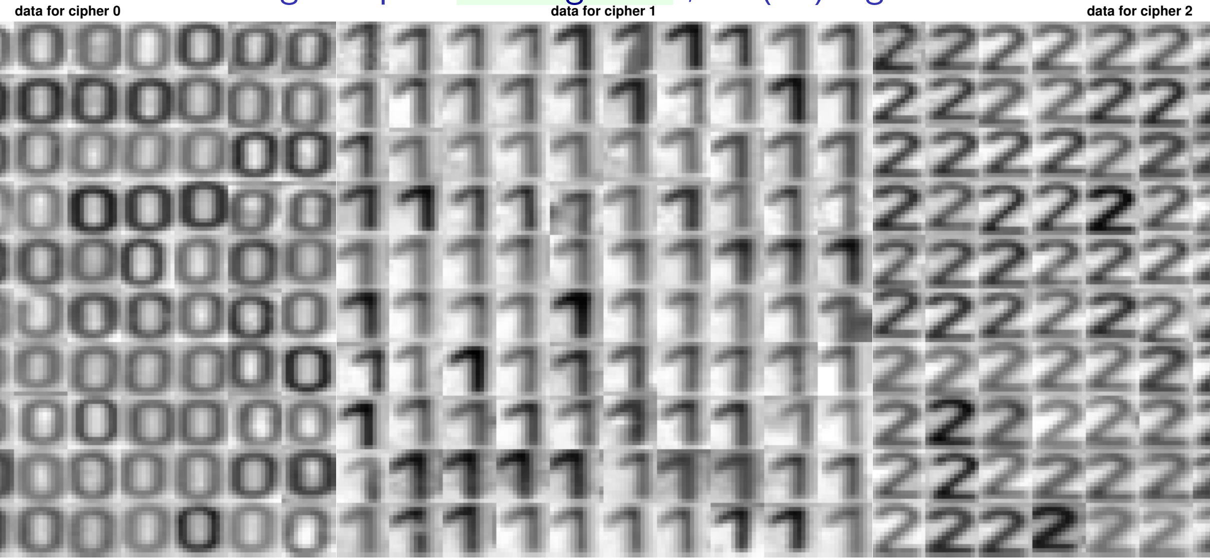
Digit recognition is a very classical example of classification problem. It has been used for decades, and it is used till today, see e.g. MNIST demo at PyTorch

Optimal (Bayes) Classification

$\delta^*($  $) = \arg\max_{d} P(d|$  $)$

Notes

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



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

Notes

What we need to learn:

- Known: the decision rule (function)
- To be learned: parameters of the function

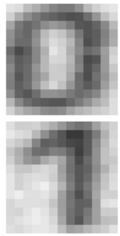
A simplest example: male/female classification beased on height. A simple thresholding function, but what i the threshold?

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 $(\vec{x}_1, s_1), (\vec{x}_2, s_2), \ldots (\vec{x}_l, s_l)$
  - every $(\vec{x}_i, s)$ is drawn independently from $P(\vec{x}, s)$, i.e. sample i does not depend on $1, \cdots, i-1$
  - so-called i.i.d (independent, identically distributed) multiset
- Without knowing anything about the distribution, a non-parametric estimate:

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

- 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

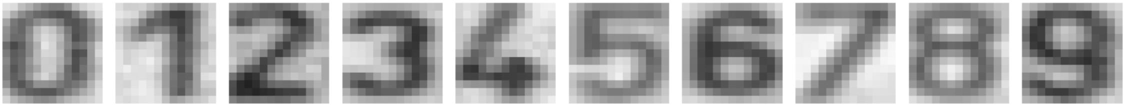


Notes

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 13×13, pixel intensities $0 - 255$. (0 means black, 255 means white)

- A: 169^{256}
- B: 256^{169}
- C: 13^{13}
- D: 169×256
- E: different quantity

Notes

Think about simple binary 10×10 image - $\vec{x}$ contains $0, 1$, position matters. What is the total number of unique images? Think binary, 1×8 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).

Naive Bayes

Notes

Naïve Bayes classification

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

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

- Use simple Bayes law and maximize:

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

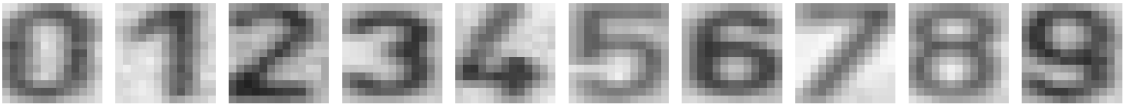
- No combinatorial curse in estimating $P(s)$ and $P(x[i]|s)$ separately for each i and s.
- No need to estimate $P(\vec{x})$. (Why?)
- $P(s)$ may be provided apriori.
- naïve $=$ when used despite statistical dependence

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 13×13, pixel intensities $0 - 255$. (0 means black, 255 means white)
- Output: Digit $0 - 9$. Decision about the class, classification.
- Features: Pixel intensities ...

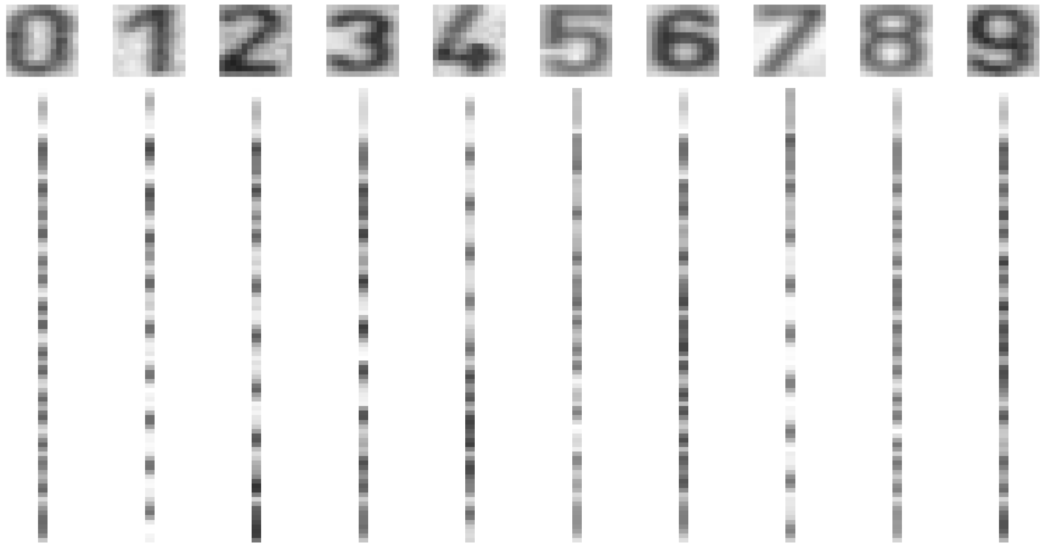
Collect data , ...

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

Notes

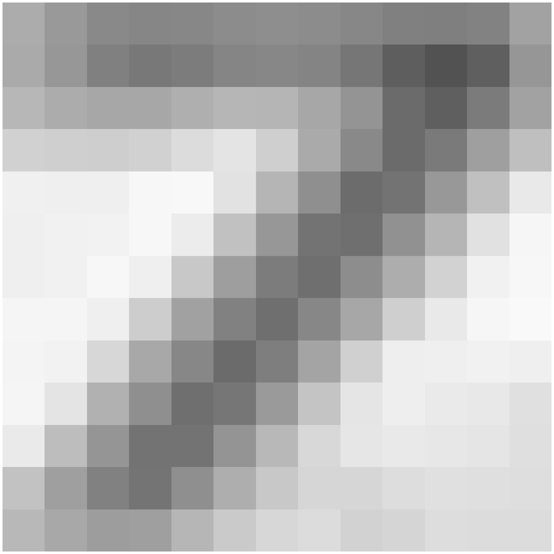
We can create many more features than just pixel intensities. But first things first.
We are assuming all errors are equally important - minimizing the number of wrong decisions.
Dimension of $\vec{x}$ is $13 \times 13 = 169$. There are 256^{169} possible images. (we already know)

From images to $\vec{x}$



Notes

Conditional probabilities, likelihoods



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

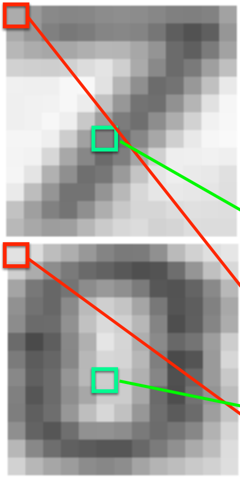
Notes

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 obervation of a dark pixel in the top right corner was generate by an image of 7. Jak věrohodné to je?

Conditional likelihoods

s_k	$P(s_k)$
1	0.1
2	0.1
3	0.1
4	0.1
5	0.1
6	0.1
7	0.1
8	0.1
9	0.1
0	0.1



$P(x_{0,0} = 25|s_k)$ $P(x_{7,5} = 25|s_k)$

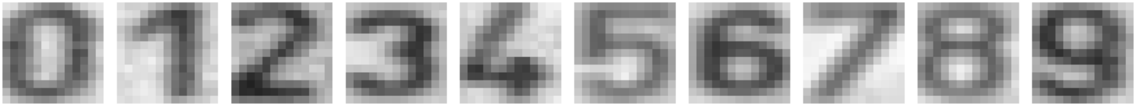
s_k	$P(x_{0,0} = 25\|s_k)$
1	0.0009
2	0.05
3	0.00006
4	0.0005
5	0.07
6	0.0007
7	0.1
8	0.0006
9	0
0	0

s_k	$P(x_{7,5} = 25\|s_k)$
1	0.0009
2	0.05
3	0.00006
4	0.0005
5	0.004
6	0.07
7	0.1
8	0.006
9	0.08
0	0.005

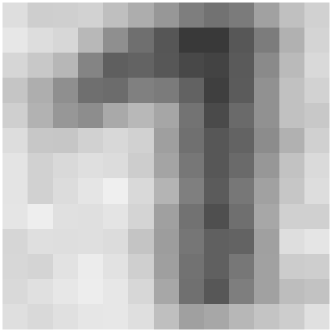
Notes

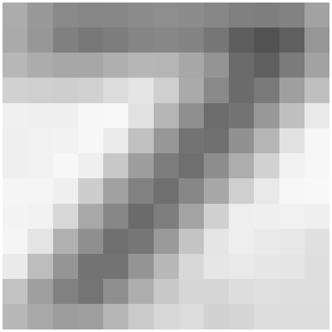
For each pixel (position) and possible instensity (image/pixel value) we create such a table.

Unseen events (sparsity of training data)



Images 13×13, intensities $0 - 255$, 100 exemplars per each class.





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

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

Notes

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

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

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?

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

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.

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

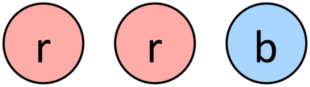
$$P_{\text{LAP}}(x) = \frac{c(x) + 1}{N + |X|}$$

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

Notes

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

Observation:



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

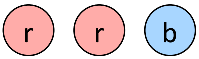
A: $P_{\text{LAP}}(X = \text{red}) = 7/10$, $P_{\text{LAP}}(X = \text{blue}) = 3/10$

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

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

D: None of the above.

Notes



$P_{ML}(X) =$

$P_{LAP}(X) =$

originally:

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

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

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

this slide: courtesy of P. Abeel, http://ai.berkeley.edu. 21st lecture of CS 188.

Laplace smoothing - as a hyperparameter k

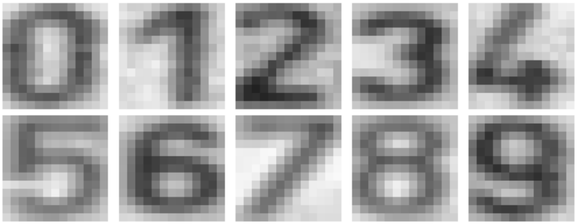
Pretend you see every sample k extra times:

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

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

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

Notes

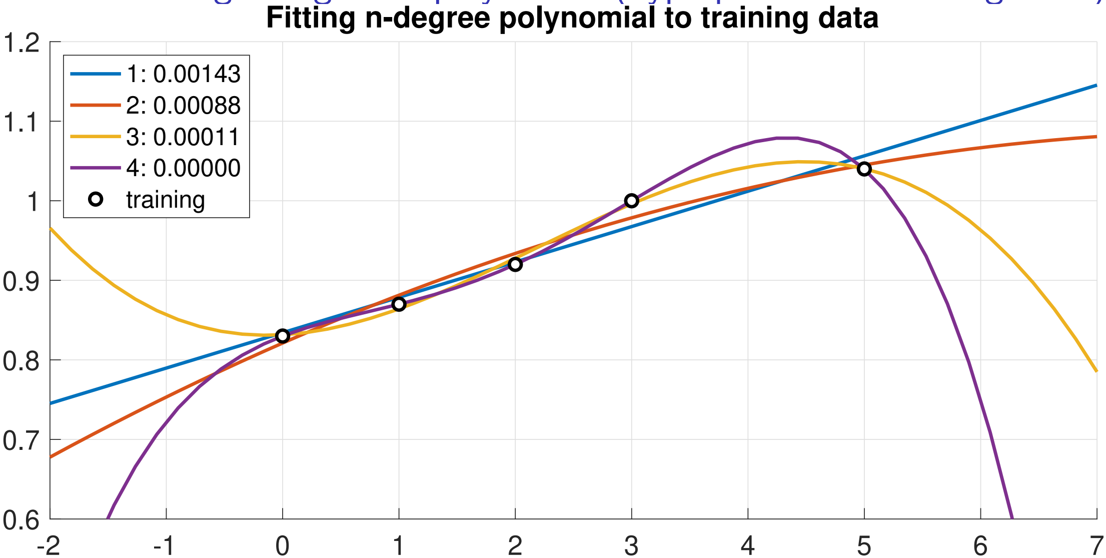
Hyperparameter would be tuned along with your classifier
For $k = 100$ and blue and red, you would get:

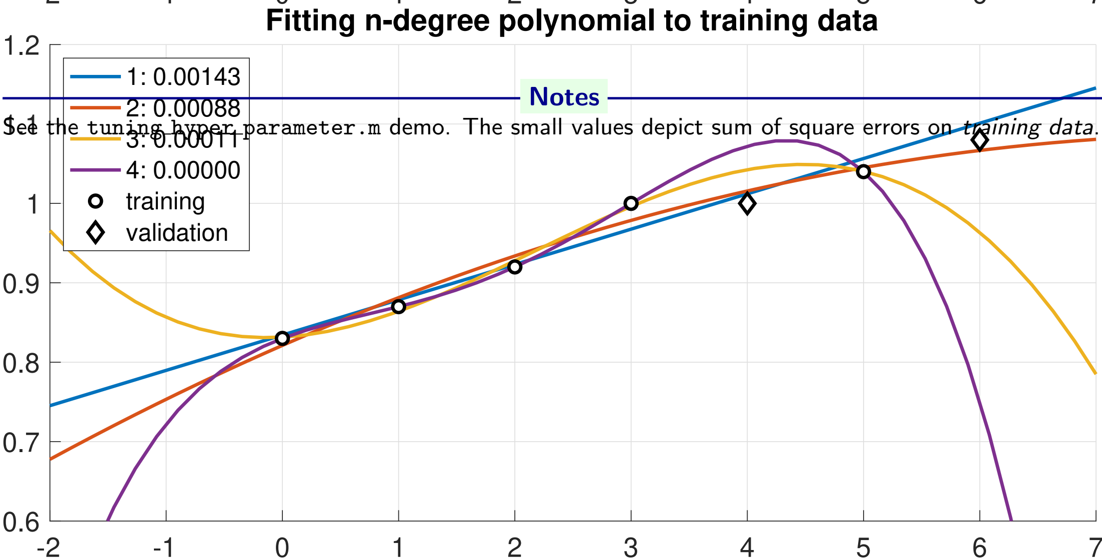
- $P_{LAP}(red) = (2 + 100)/(3 + 100 * 2) = 102/203$
- $P_{LAP}(blue) = (1 + 100)/(3 + 100 * 2) = 101/203$

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)



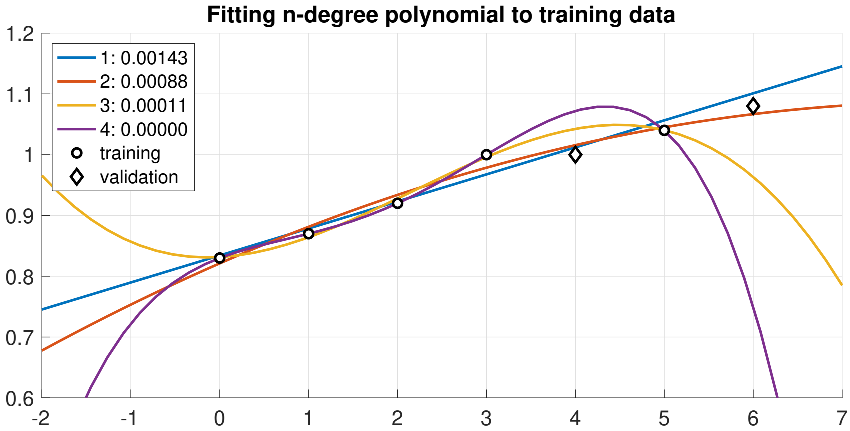


Notes

See the `tuning_hyper_parameter.m` demo. The small values depict sum of square errors on *training data*.

Generalization and overfiting

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



Notes

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.

Notes

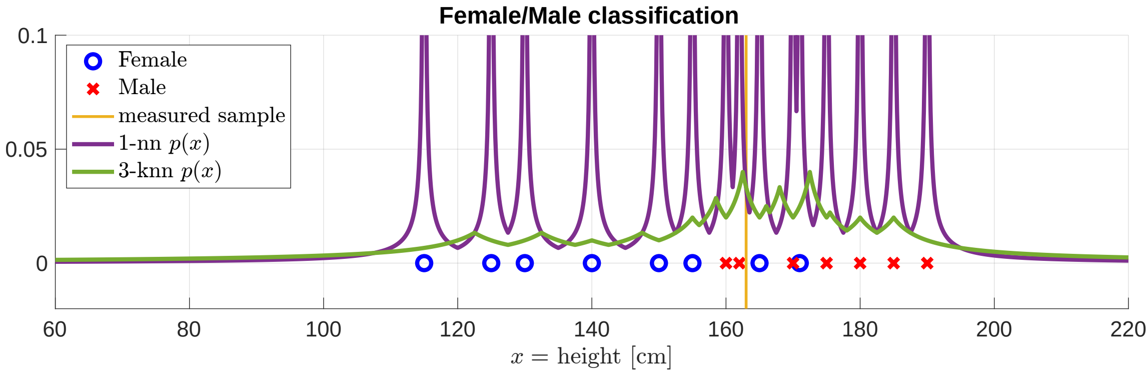
Training set - biggest part.

Nearest Neighbour classifier

1. Query x
2. Select N nearest neighbours of x from the training set. N is odd.
3. Pick up the class the majority of neighbours belongs to.

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

Notes

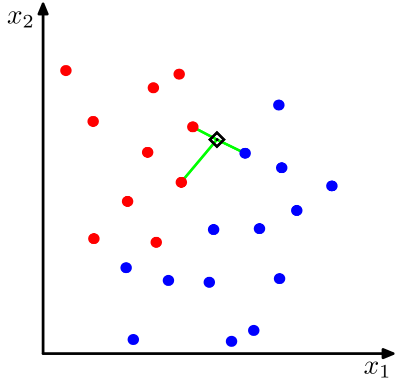
$K-$ Nearest Neighbor and Bayes $j^* = \text{argmax}_j\, P(s_j|\vec{x})$

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 (hypher-sphere) centered at $\vec{x}$ containing K points irrespective of class. V is the volume of this sphere. $P(s_j|\vec{x}) = ?$

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

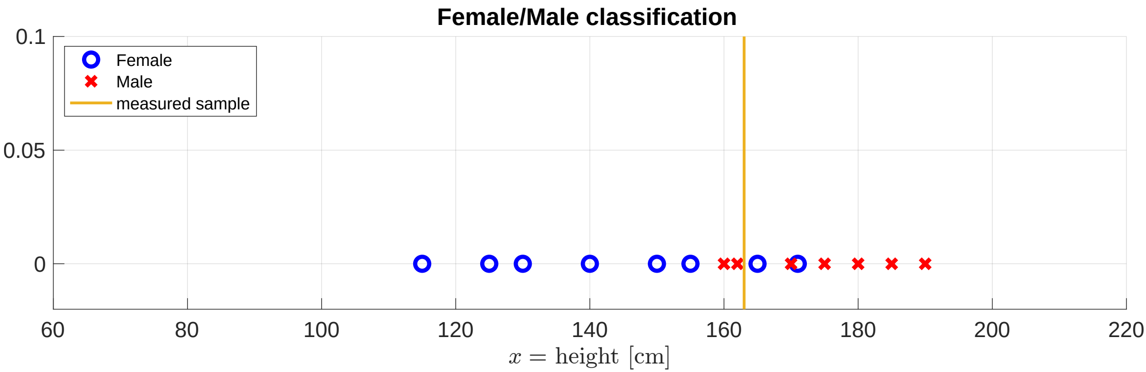


(a)

Notes

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

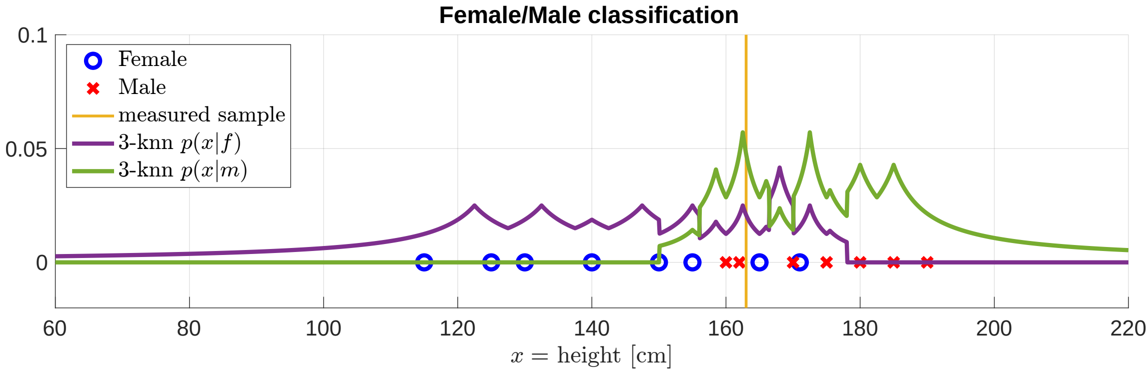
Female/male classification based on height. N data points available.



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

Notes

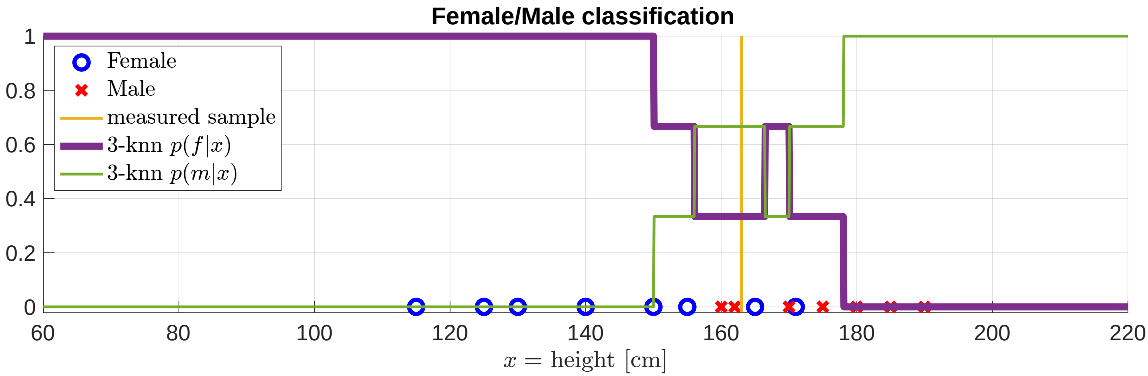
K−NN $p(x|s_j)$ estimates



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

Notes

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.

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

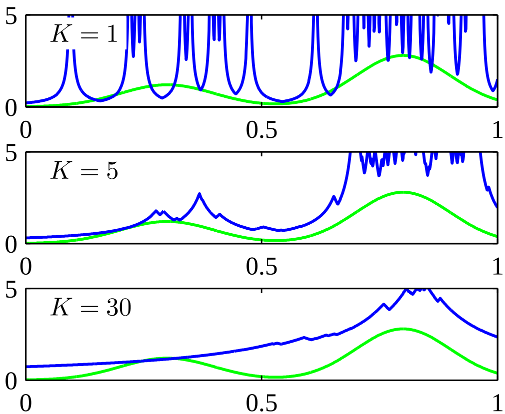
$$V = V_d R_k^d(\vec{x})$$

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

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

volume od unit $d-$dimensional sphere,
Γ denotes gamma function.
$V_1 = 2, V_2 = \pi, V_3 = \frac{4}{3}\pi$

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

Evaluation (comparisons) of classifiers

Notes

Precision and Recall, and ...

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

Recall :

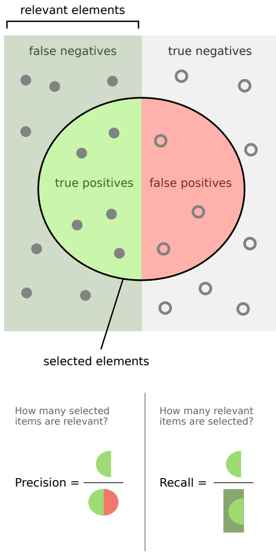
- How many relevant items are selected?
- Are we missing some items?
- Also called: True positive rate (TPR), sensitivity, hit rate ...

Precision

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

False positive rate (FPR)

- Probability of false alarm



Notes

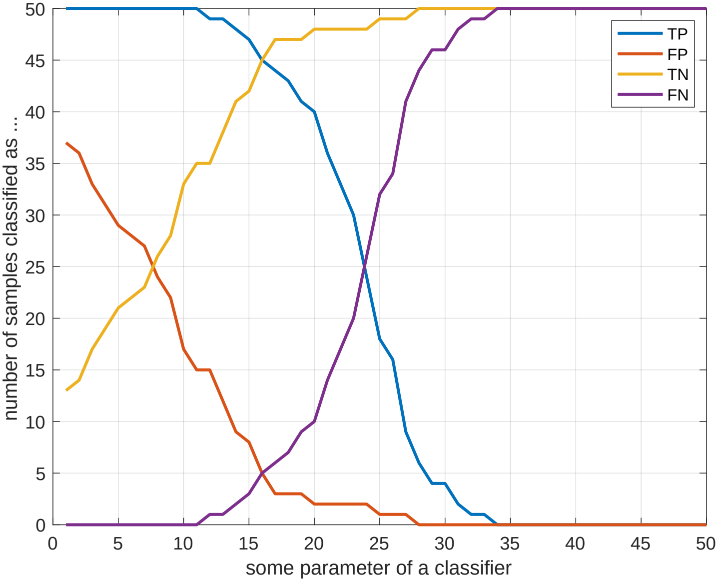
$$\mathrm{TPR} = \frac{\mathrm{TP}}{P} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}$$

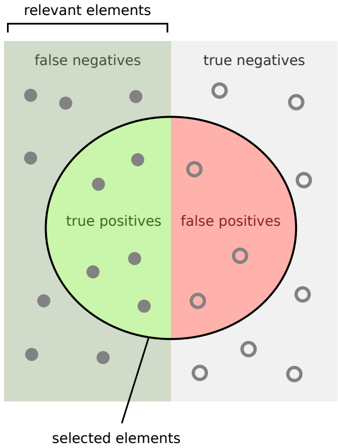
$$\mathrm{Precision} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FP}}$$

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

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

Studying a classifier . . .





How many data samples x_i?

A 50

B 100

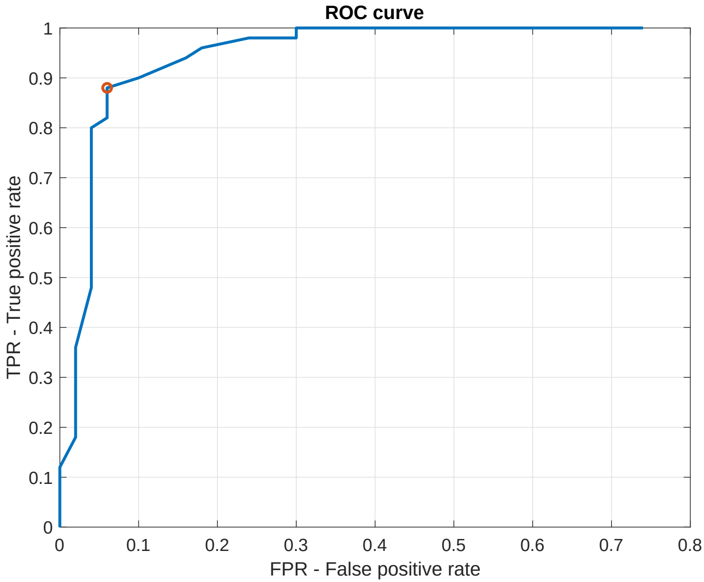
C 150

D 200

Notes

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

ROC – Receiver operating characteristics curve



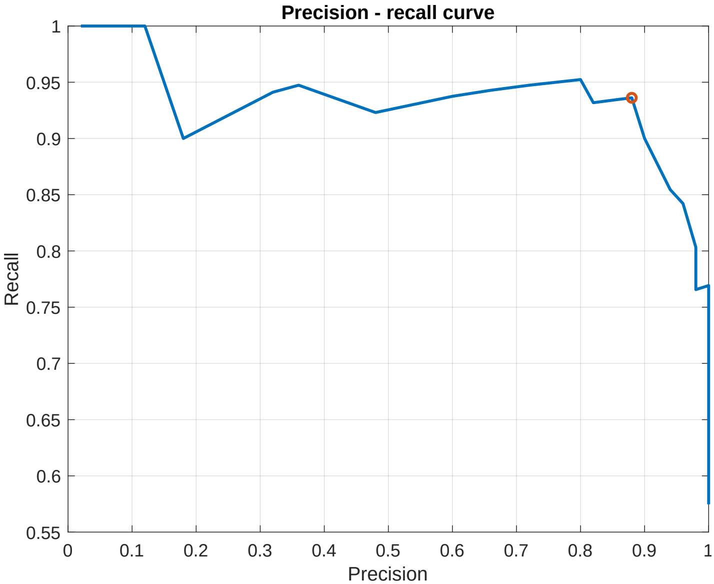
$$\mathrm{TPR} = \frac{\mathrm{TP}}{P} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

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

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



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

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

Notes

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

Try to explain meaning of Precision and Recall from the user's (buyer's) perspective.

How to evaluate a multi-class classifier? Confusion table

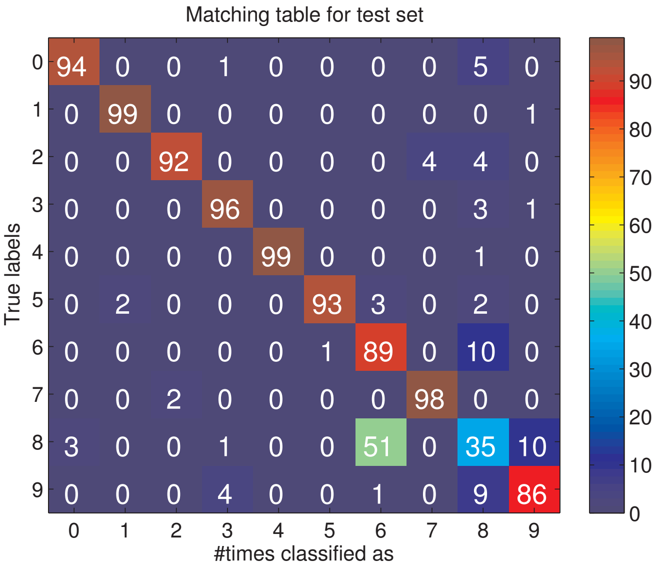


Figure from [6]

Notes

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

Product of many small numbers ...

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

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

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

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.
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[2] Yen-Chi Chen.
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Notes

References II

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[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.
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Notes

References III

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