Classifiers: Naïve Bayes, k-NN, evaluation

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thanks to Daniel Novák and Filip Železný, Ondřej Drbohlav

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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 probababilities

$$r(\delta) = \sum_x \sum_s \ell(s, \delta(x)) P(x, s) = \sum_s \sum_x \ell(s, \delta(x)) P(s|x) P(x)$$

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

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, ...
- **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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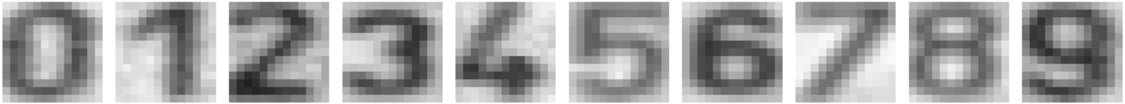
Example: Digit recognition/classification



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

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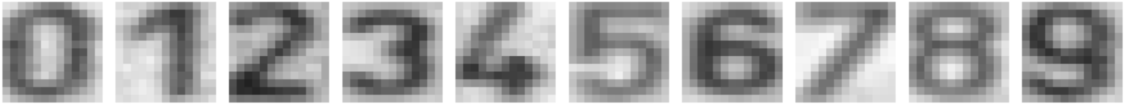

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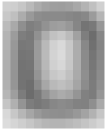
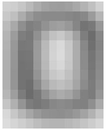
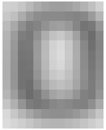
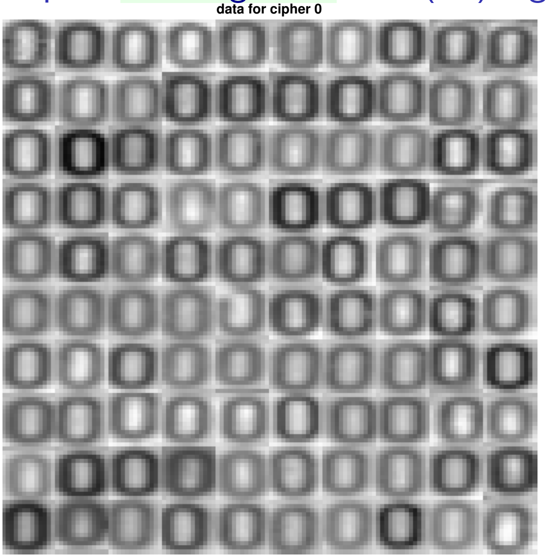
Decision/classification problem : What cipher is in the (query) image? 

Optimal (Bayes) Classification

$\delta^*($  $) = \arg\max_d P(d \mid$  $)$

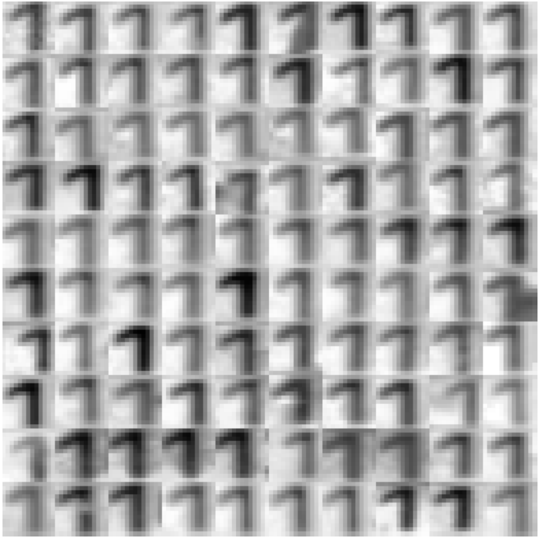
Machine Learnine: Prepare training data , let (an) algorithm learn itself



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

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

data for cipher 1



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

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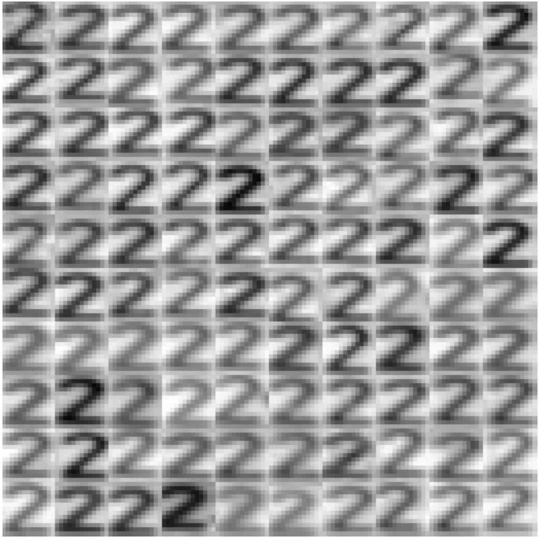


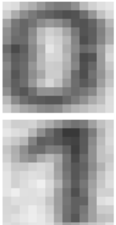
Training samples: $(\vec{x}_i, s = 2)$

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



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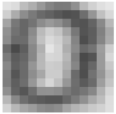
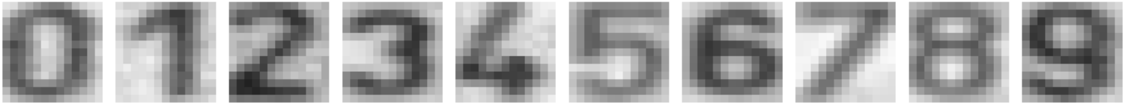


How many images?



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

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

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

- 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

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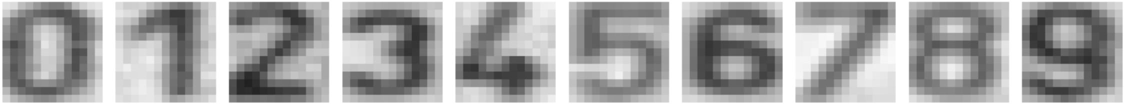

- Input: 8-bit image 13×13, pixel intensities $0 - 255$. (0 means black, 255 means white)
- Output: Digit $0 - 9$. Decision about the class, classification.
- Features: Pixel intensities . . .

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 $s^* = \text{argmax}_s P(s|\vec{x})$.

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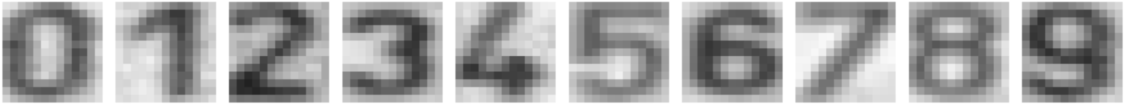

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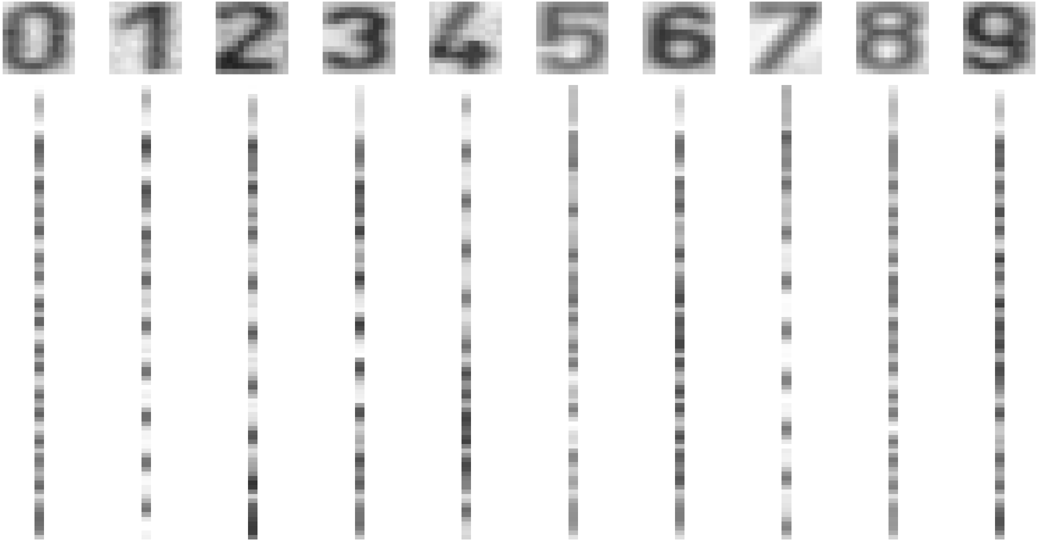
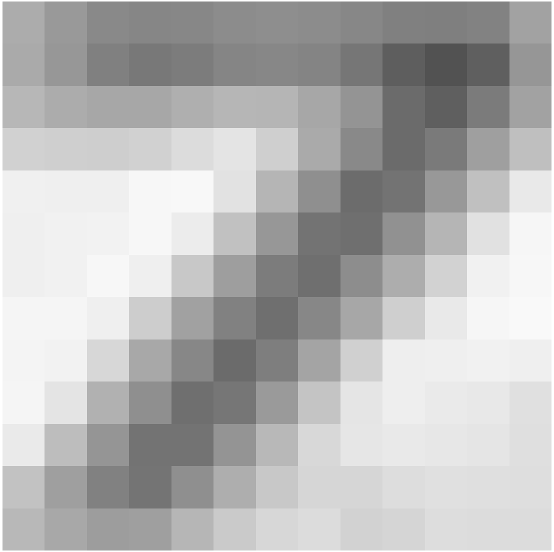
From images to $\vec{x}$



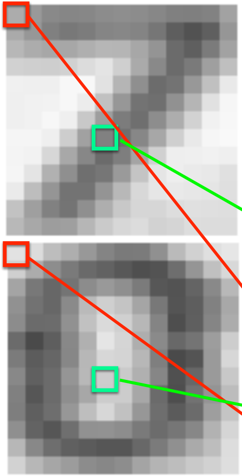
Conditional probabilities, likelihoods



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

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

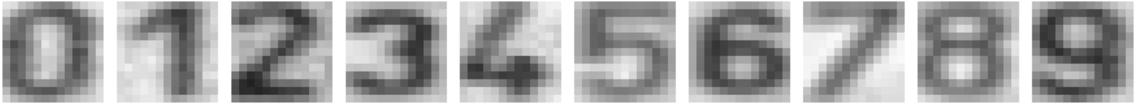


$P(x_{0,0} = 25|s_k)$ $P(x_{7,5} = 25|s_k)$

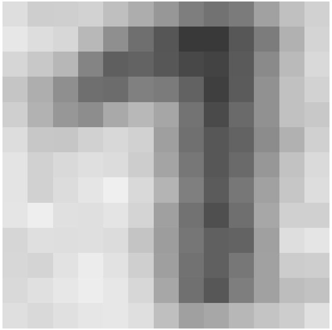
s_k	$P(x_{0,0} = 25\|s_k)$
1	0.0009
2	0.05
3	0.00006
4	0.0005
5	0.07
6	0.0007
7	0.1
8	0.0006
9	0
0	0

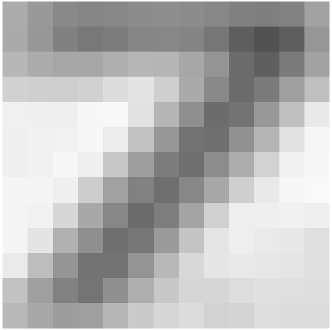
s_k	$P(x_{7,5} = 25\|s_k)$
1	0.0009
2	0.05
3	0.00006
4	0.0005
5	0.004
6	0.07
7	0.1
8	0.006
9	0.08
0	0.005

Unseen events



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





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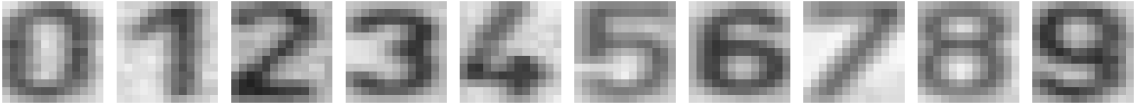
\end{aligned}
$$

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

Unseen events



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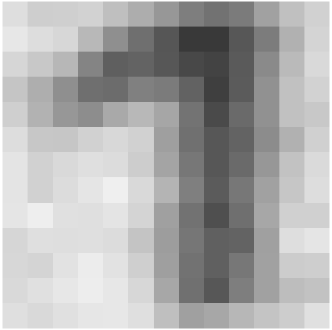

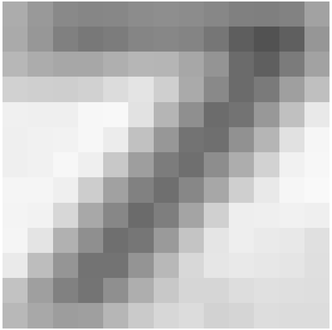

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Unseen event, how to decide?

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

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

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).

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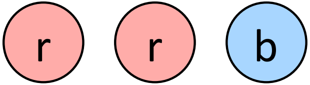
$$P_{\text{LAP}}(x) = \frac{c(x)+1}{\sum_x [c(x)+1]} = \frac{c(x)+1}{N+|X|} = ?$$

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.

Laplace smoothing - as a hyperparameter k

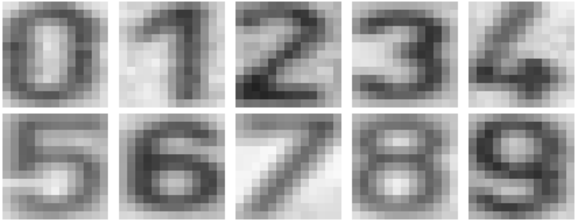
Pretend you see every sample k extra times:

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

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

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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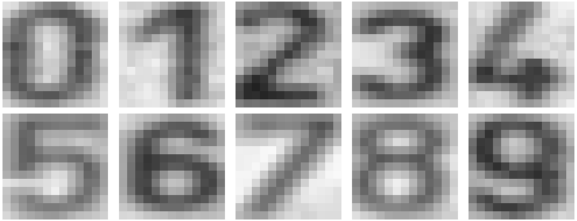

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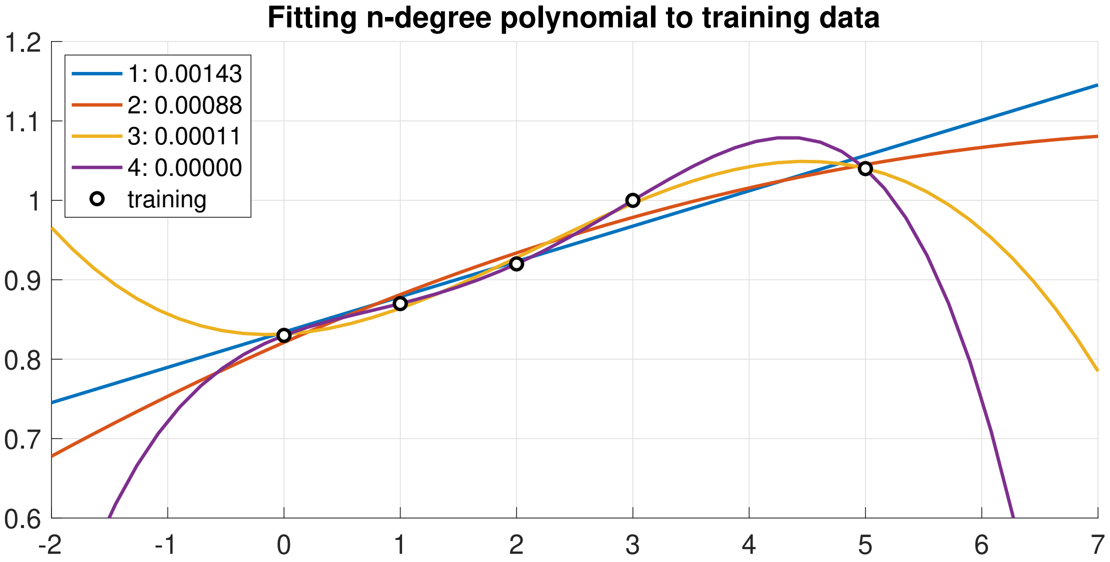

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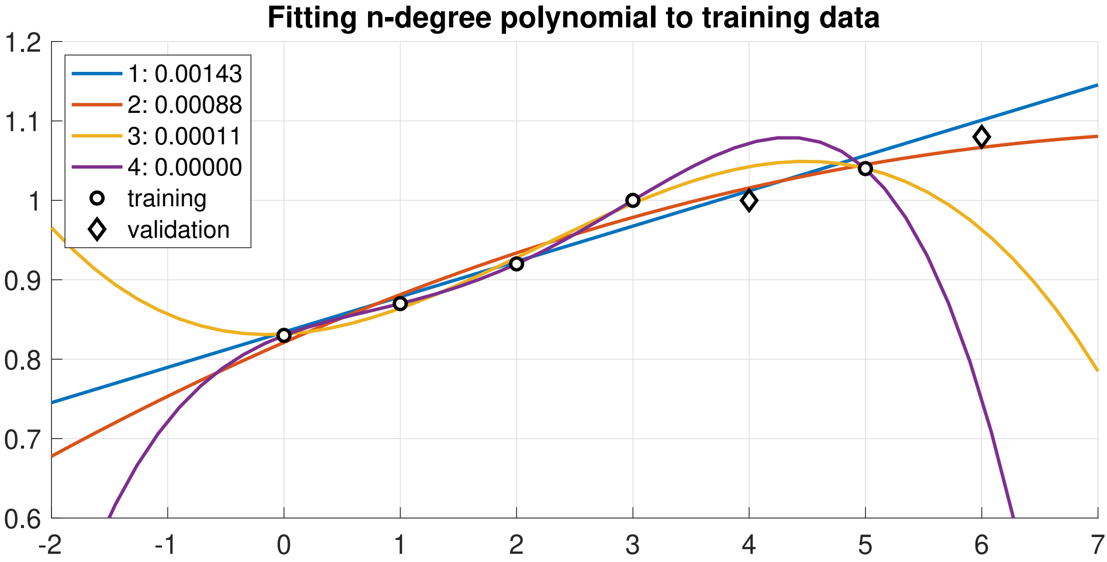
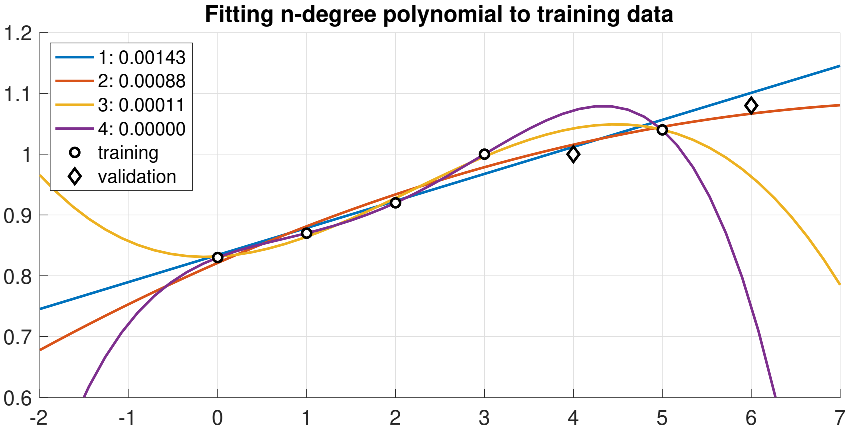


Generalization and overfitting

- 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.

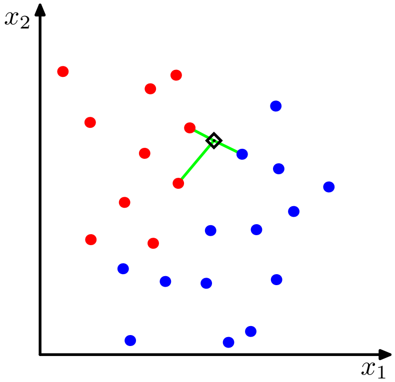
$K-$ Nearest Neighbor and Bayes $j^* = \text{argmax}_j P(s_j|\vec{x})$

Assume data:

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

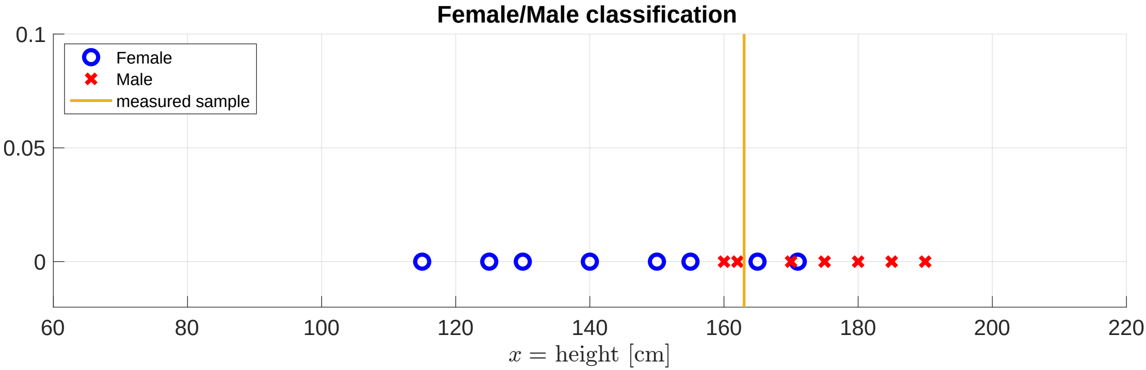
We want classify to $\vec{x}$. We draw a circle (hypher-sphere) centered at $\vec{x}$ containing K points irrespective of class. V is the volume of this sphere. $P(s_j|\vec{x}) = ?$

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



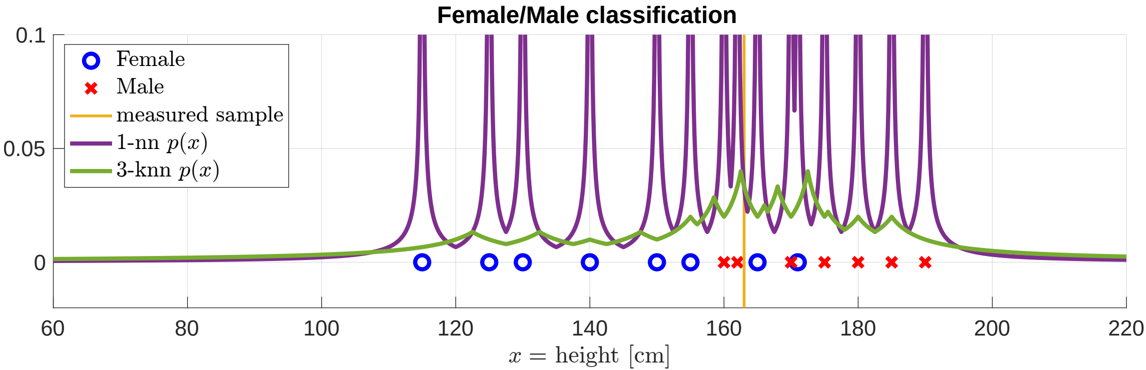
(a)

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?

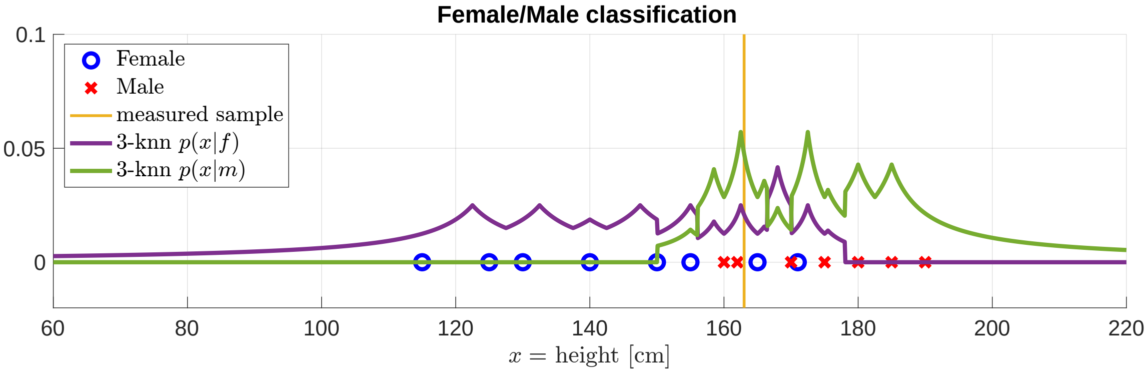
$K-$NN $p(x)$ estimate



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

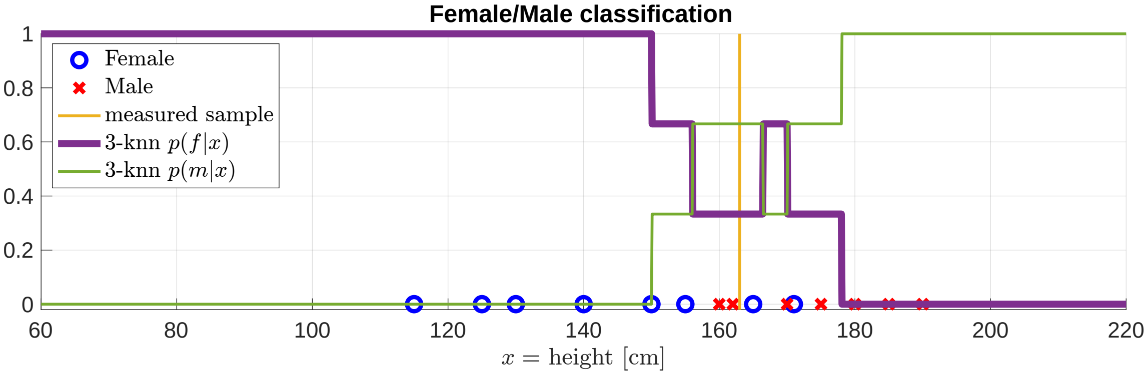
$V = 2r_k(x)$, where $r_k(x)$ is the distance of $k-$th nearest data point to x

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



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

K−NN $p(s_j|x)$ posteriors



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

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

Precision and Recall, and . . .

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

Recall :

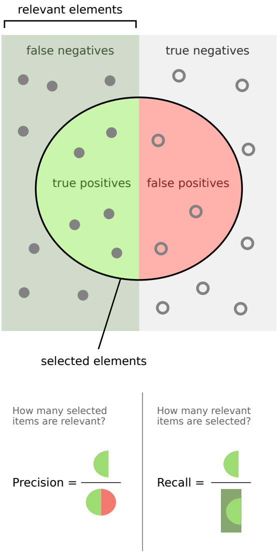
- How many relevant items are selected?
- Are we missing some items?
- Also called: True positive rate (TPR), sensitivity, hit rate . . .

Precision

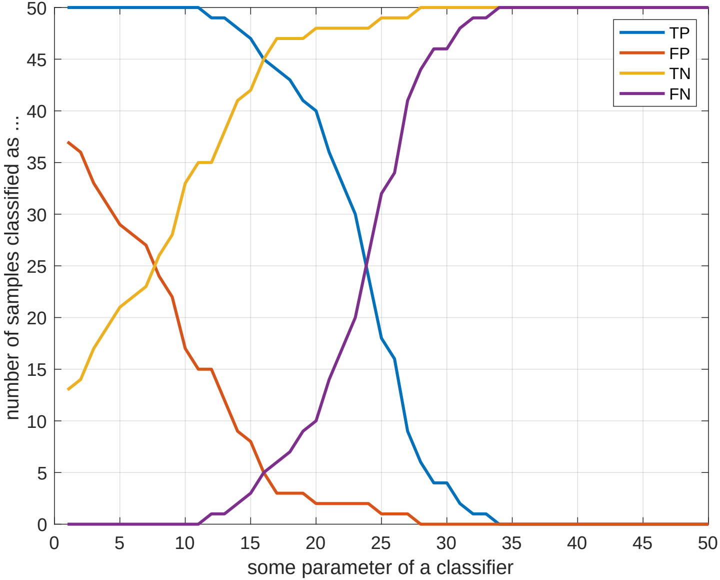
- How many selected items are relevant?
- Also called: Positive predictive value

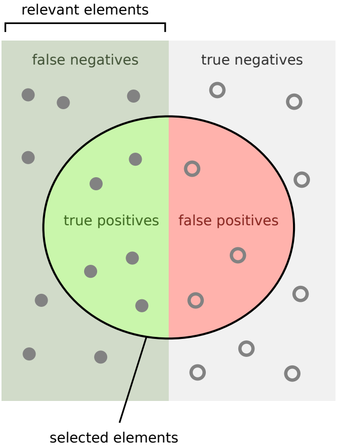
False positive rate (FPR)

- Probability of false alarm



Studying a classifier . . .





How many data samples x_i?

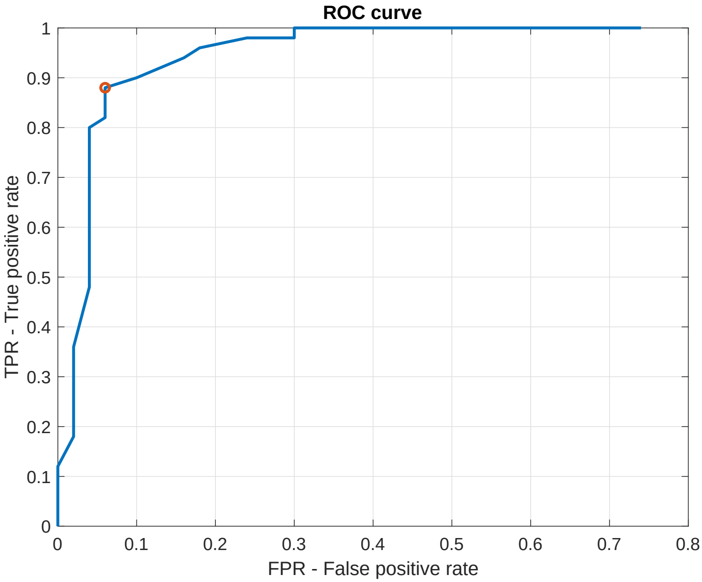
A 50

B 100

C 150

D 200

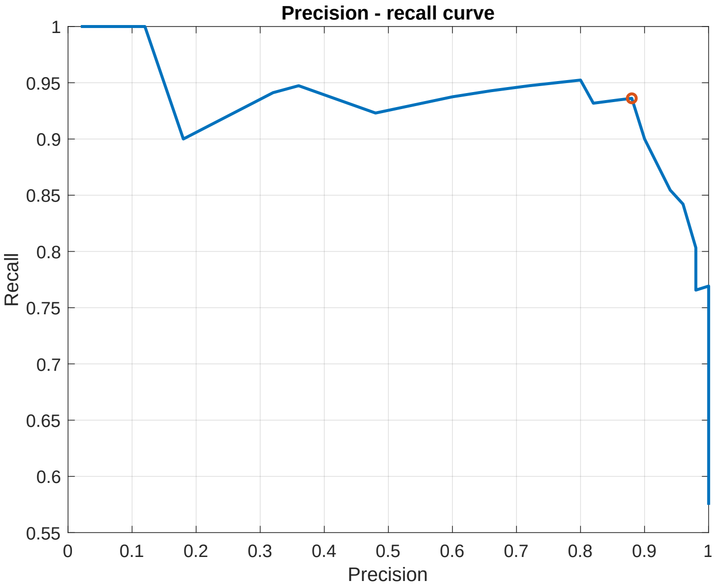
ROC – Receiver operating characteristics curve



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

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

Precision – recall curve



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

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

How to evaluate a multi-class classifier? Confusion table

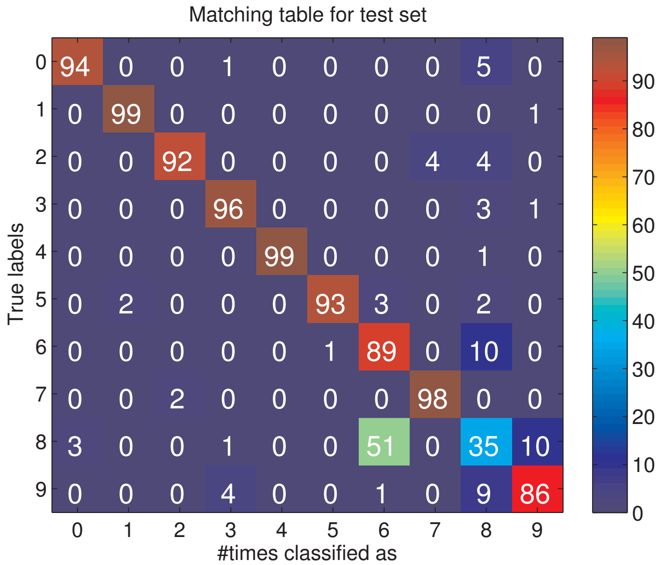


Figure from [6]

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, ...

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

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, ...

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

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].

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