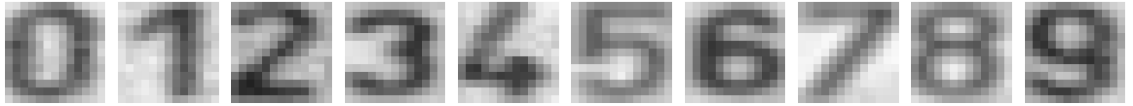# Classifiers: Naïve Bayes, evaluation

Tomáš Svoboda and Matěj Hoffmann
thanks to Daniel Novák and Filip Železný, Ondřej Drbohlav

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April 27, 2022

Notes

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.
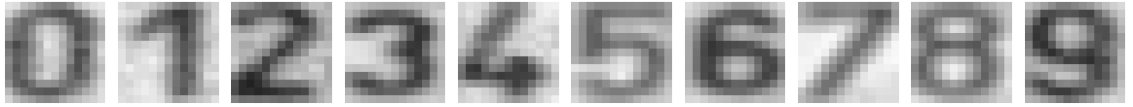- ▶ Features: Pixel intensities ...

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

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───────────────── **Notes** ─────────────────

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Classification as a special case of statistical decision theory

- ▶ Attribute vector $\vec{x} = [x_1, x_2, \ldots]^{\top}$: pixels 1, 2, ...
- ▶ **State set $\mathcal{S} = $ decision set $\mathcal{D} = \{0, 1, \ldots 9\}$.**
- ▶ State = actual class, Decision = recognized class
- ▶ Loss function: $l(s, d) = \begin{cases} 0, & d = s \\ 1, & d \neq s \end{cases}$
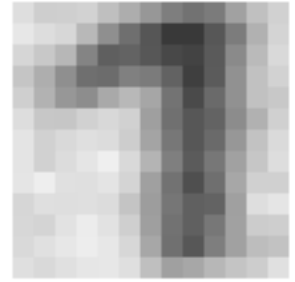
Optimal decision strategy:

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

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:

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

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?

Optimal (Bayes) Classification

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

Notes

Machine Learnine: Prepare training data , let (an) algorithm learn itself
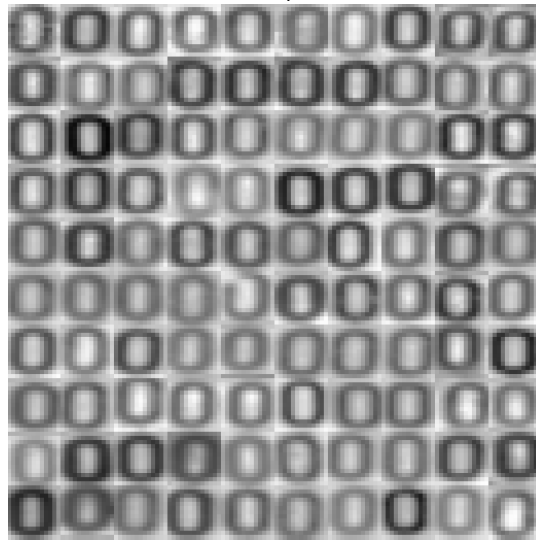
data for cipher 0

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

Notes

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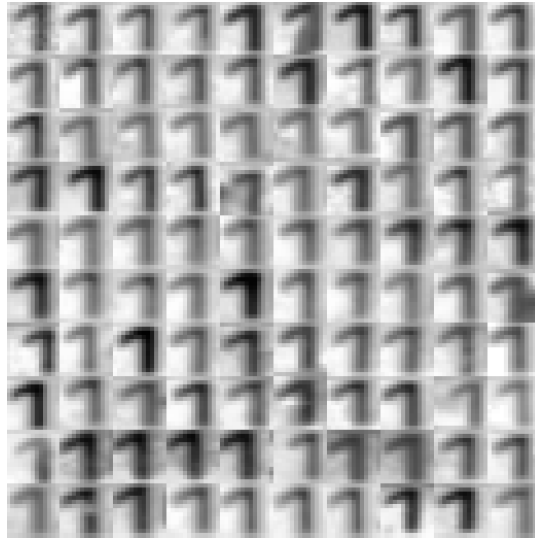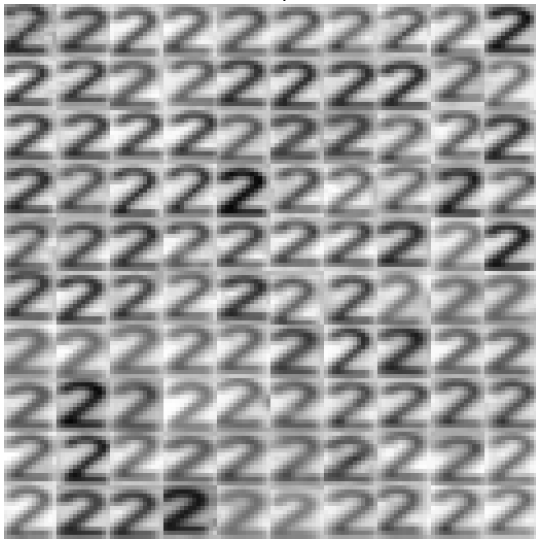

data for cipher 1

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

Notes

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

data for cipher 2

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

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 $(\vec{x}_1, s_1), (\vec{x}_2, s_2), \ldots (\vec{x}_l, s_l)$
  ▶ 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:

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

▶ 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

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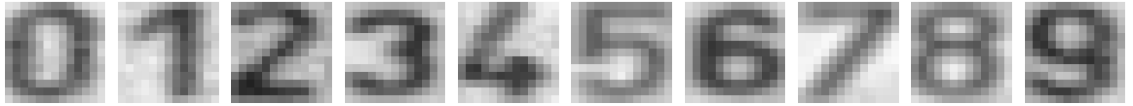
Why hard? Way too many various $\vec{x}$.

What is the difference between set and multiset?

Reminder about math notation. In literature, vectors are mostly denoted by bold lower case **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).

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
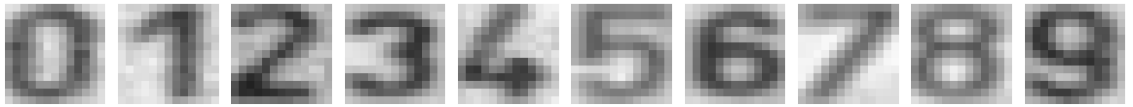
―――――――――――――――――――― **Notes** ――――――――――――――――――――

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

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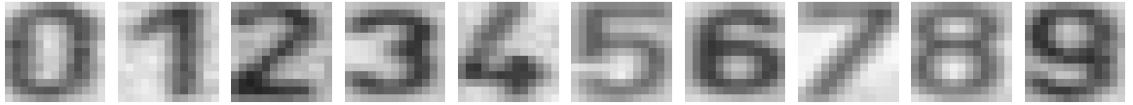- ▶ Classify $s^* = \text{argmax}_s P(s|\vec{x})$.

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)

Example: Digit recognition/classification

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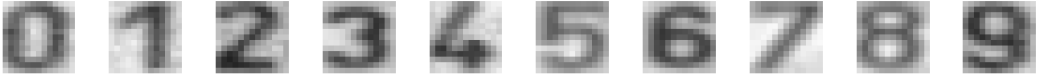- ▶ Classify $s^* = \text{argmax}_s P(s|\vec{x})$.

--- **Notes** ---

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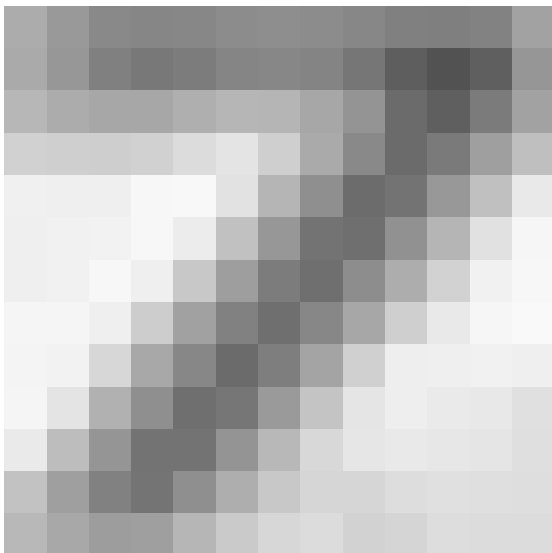Dimension of $\vec{x}$ is $13 \times 13 = 169$. There are 256^{169} possible images. (we already know)

From images to $\vec{x}$

Notes

Conditional probabilities, likelihoods

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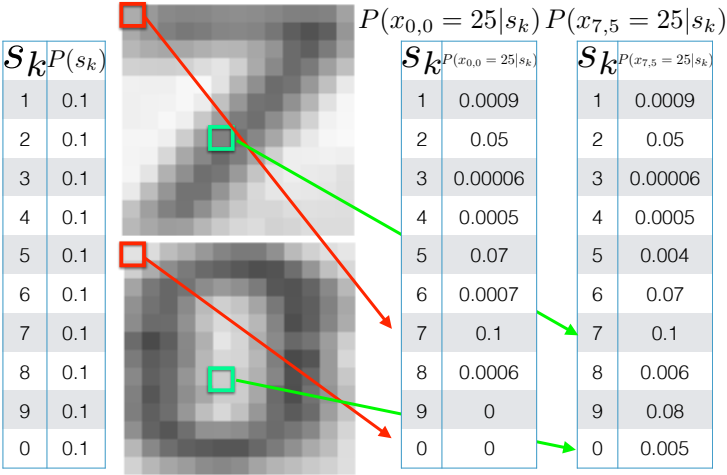- ▶ Likelihoods for pixels. $P(x_{r,c} = I_i | s_k)$

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).
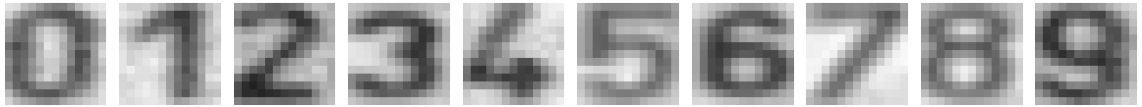
Conditional likelihoods

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

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

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

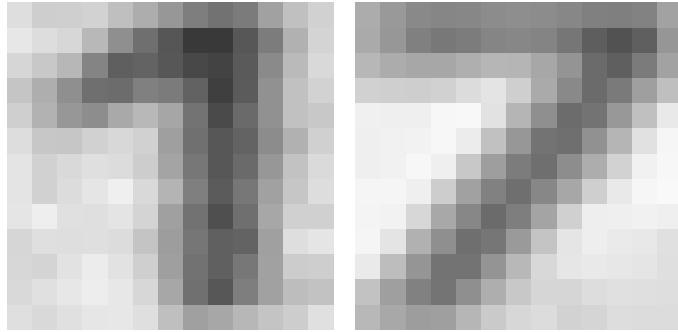| S_k	$P(x_{7,5} = 25|s_k)$
1	0.0009
2	0.05
3	0.00006
4	0.0005
5	0.004
6	0.07
7	0.1
8	0.006
9	0.08
0	0.005

Notes

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

Unseen events

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

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

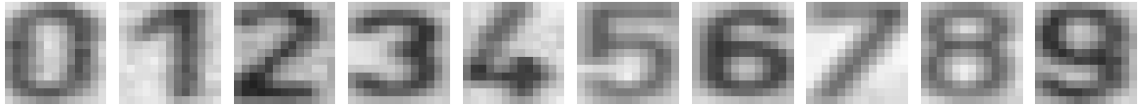A new (not in training) query image with $x_{0,0} = 101$. How would you classify?

Notes

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

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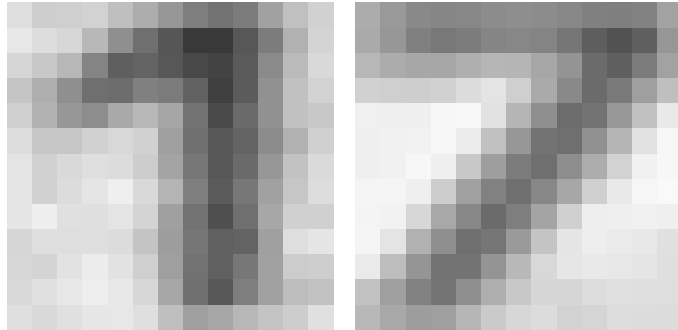Think about the problem of classifying numerals. Some $P(x_{r,c} = I \mid s) = 0$. What about an example:

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$$\vdots = \vdots$$

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

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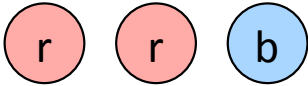Pretend you see the (any) sample one more time.

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Notes

$P_{\text{LAP}}(x) = ?$

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:

- $P(red) = 2/3$
- $P(blue) = 1/3$

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

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

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

Laplace smoothing - as a hyperparameter k
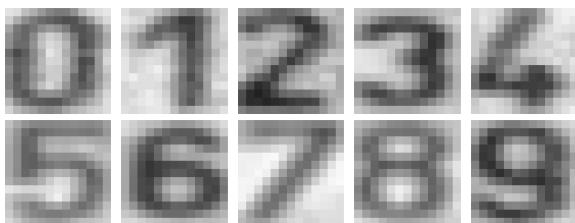
Pretend you see every sample k extra times:

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

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

For conditional, smooth each condition independently

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

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.
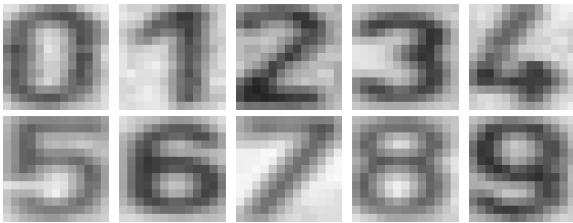
Laplace smoothing - as a hyperparameter k

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For conditional, smooth each condition independently

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

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:

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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

Legend:
- 1: 0.00143
- 2: 0.00088
- 3: 0.00011
- 4: 0.00000
- ○ training
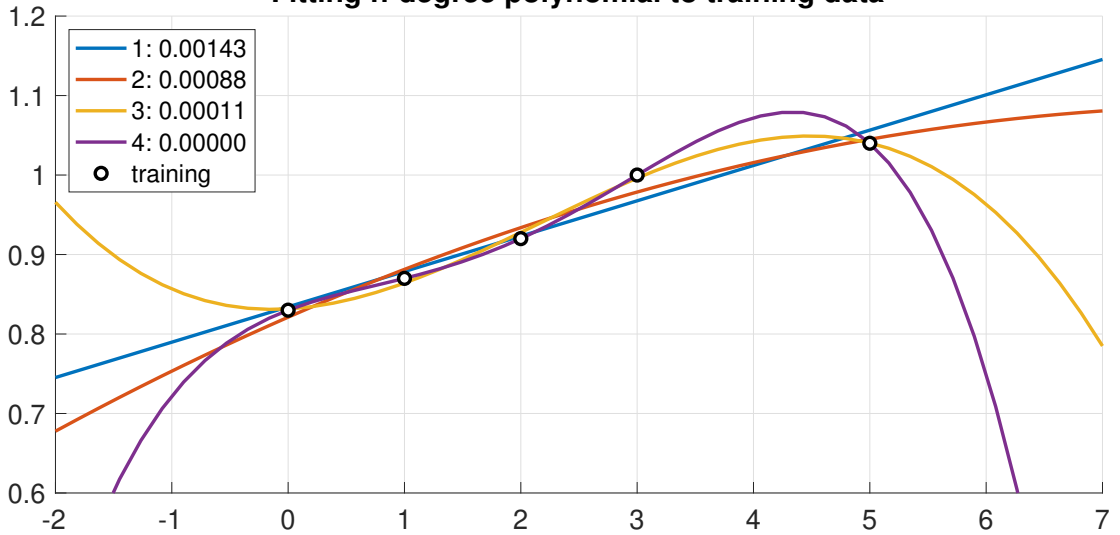
Notes

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

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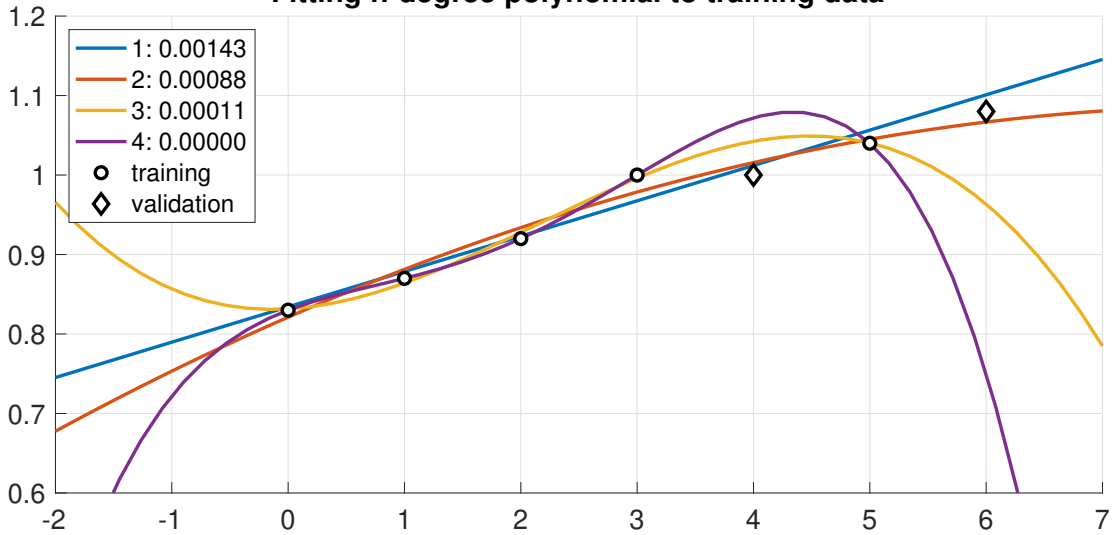
Notes

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

Generalization and overfitting

▶ Data: training, validating, testing . Wanted classifier performs well on what data?

▶ Overfitting: too close to training, poor on testing.

Fitting n-degree polynomial to training data

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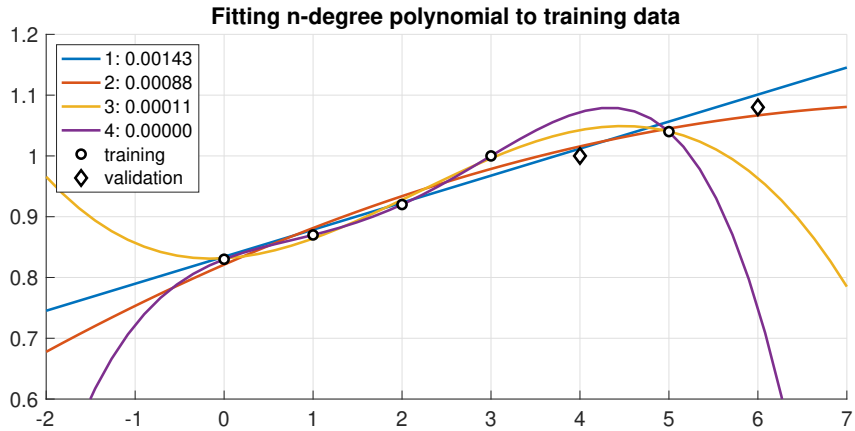
Training and testing
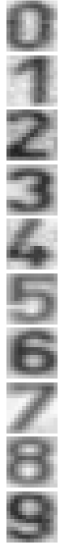
Data labeled instances.

- ▶ 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.
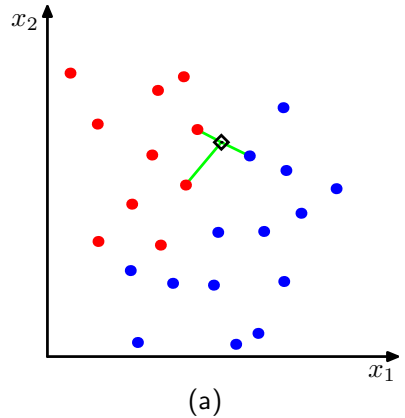
Notes

Training set - biggest part.

$K-$ 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 ---

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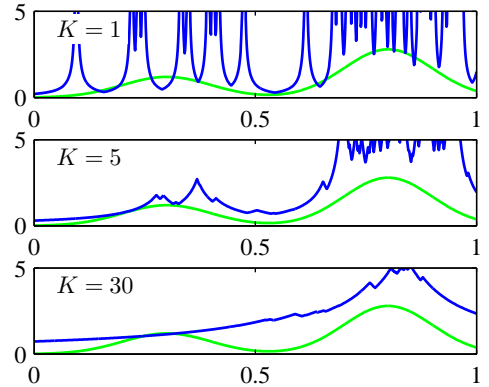$$

$k - NN$ for non-parametric density estimation

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

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

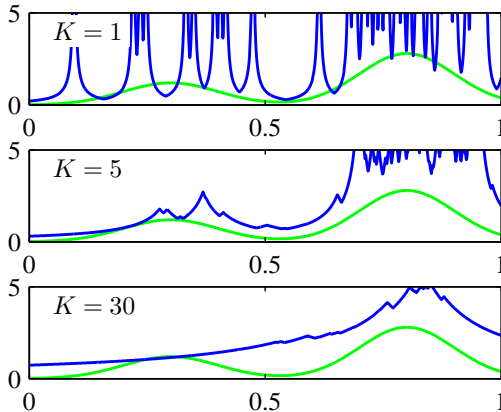$R_k(\vec{x})$ - distance from $\vec{x}$ to its $k-$th nearest neighbour point (radius)

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

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])
Try yourself, https://scikit-learn.org/stable/modules/density.html#kernel-density

How to evaluate a classifier? Confusion table
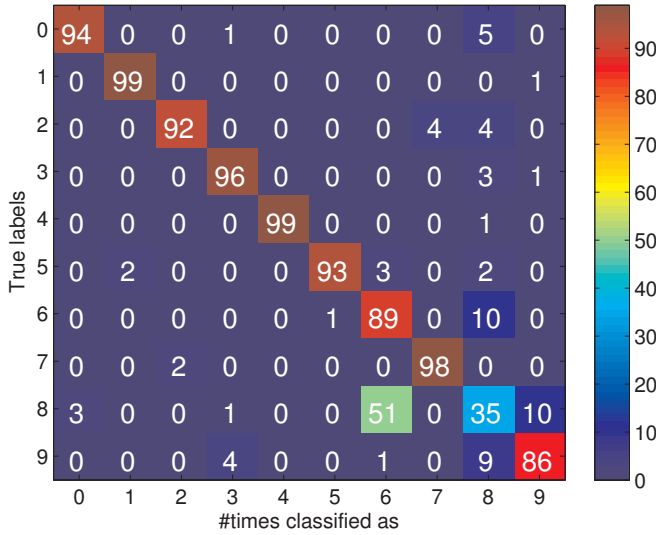

Figure from [6]

___

Notes

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

Precision and Recall, and . . .

Consider digit detection (is there a digit?) or SPAM/HAM 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

relevant elements

false negatives   true negatives

true positives   false positives

selected elements

How many selected items are relevant?

How many relevant items are selected?

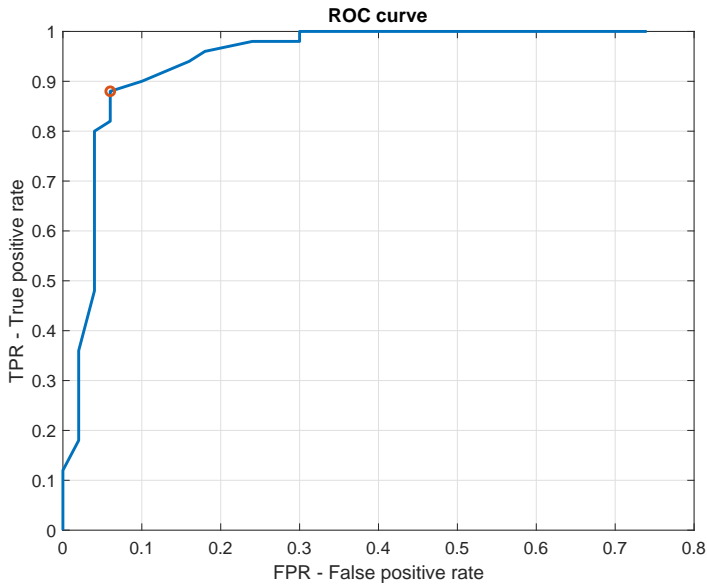$\text{Precision} = \dfrac{}{}$ $\text{Recall} = \dfrac{}{}$
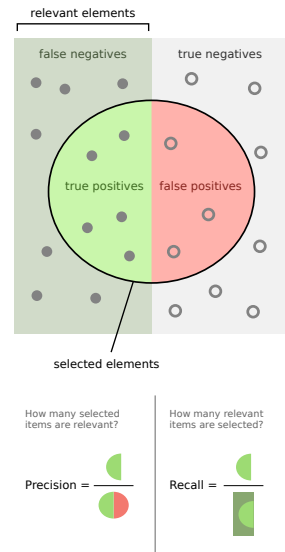
Notes

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

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

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

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

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.

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...

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, ...

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—————————————— **Notes** ——————————————

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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].

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

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Notes

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Notes

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Notes