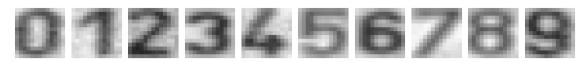
### Classifiers: Naïve Bayes, evaluation

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

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Department of Cybernetics
Faculty of Electrical Engineering, Czech Technical University in Prague

May 13, 2020

### Example: Digit recognition/classification



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

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

# Classification as a special case of statistical decision theory

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

$$I(s,d) = \left\{ egin{array}{ll} 0, & d=s \ 1, & d 
eq s \end{array} 
ight.$$

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

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?

## Bayes classification in practice

- ▶ 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  $(\vec{x}_1, s_1), (\vec{x}_2, s_2), \dots (\vec{x}_l, s_l)$ 
  - so-called i.i.d (independent, identically distributed) multiset
  - every  $(\vec{x_i}, s)$  is drawn independently from  $P(\vec{x}, s)$
- ▶ 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  $\vec{x}$ . 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?

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.

## 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:

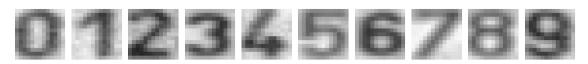
$$P(s|\vec{x}) = \frac{P(\vec{x}|s)P(s)}{P(\vec{x})} = \frac{P(s)}{P(\vec{x})}P(x[1]|s) \cdot P(x[2]|s) \cdot \ldots =$$

- 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?)
- $\triangleright$  P(s) may be provided apriori.
- naïve = when used despite statistical dependence

#### Notes -

Why naïve at all? Consider N- dimensional space, 8-bit values. Instead of problem  $8^N$  we have  $8\times N$  problem. 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)
- ightharpoonup Output: Digit 0 9. Decision about the class, classification.
- ► Features: Pixel intensities ...

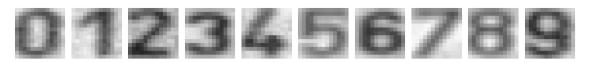
Collect data , . .

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

#### 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  $255^{169}$  possible images.

## Example: Digit recognition/classification



- ▶ Input: 8-bit image  $13 \times 13$ , pixel intensities 0 255. (0 means black, 255 means white)
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### Collect data , ...

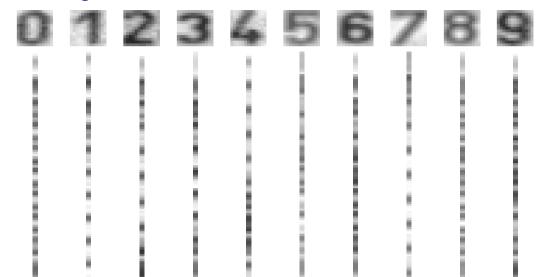
- $\triangleright$   $P(\vec{x})$ . What is the dimension of  $\vec{x}$ ? How many possible images?
- Learn  $P(\vec{x}|s)$  per each class (digit).
- ► Classify  $s^* = \operatorname{argmax}_s P(s|\vec{x})$ .

#### Notes -

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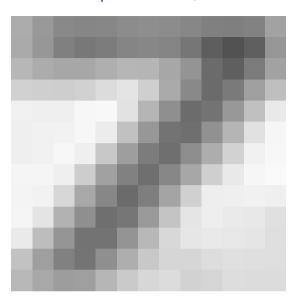
Dimension of  $\vec{x}$  is  $13 \times 13 = 169$ . There are  $255^{169}$  possible images.

From images to  $\vec{x}$ 



Notes -

## Conditional probabilities, likelihoods



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

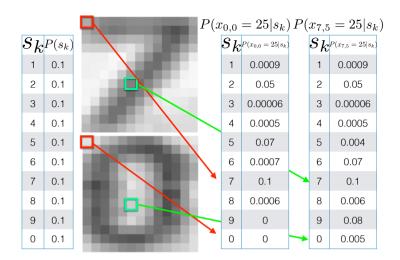
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#### Notes -

A lexical, 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 zup 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).

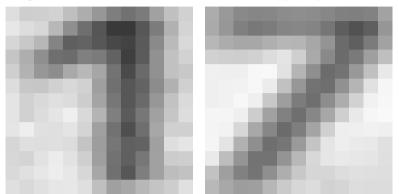
## Conditional likelihoods



### Unseen events



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



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### Notes -

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

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

$$P(x_{0,0} = 101 \mid s = 7) = 0$$

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

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

# Laplace smoothing ("additive smoothing")

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

Problem: count(x) = 0

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

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

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

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

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Observation:







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

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

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

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

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

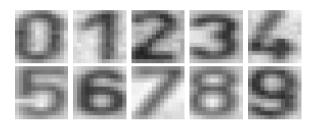
Pretend you see every sample k extra times:

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

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

For conditional, smooth each condition independently

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



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:

• 
$$P_{LAP}(red) = (2 + 100)/(3 + 100 * 2) = 102/203$$

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

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

Pretend you see every sample *k* extra times:

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

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

For conditional, smooth each condition independently

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



What is |X| equal to?

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C: 256

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#### Notes -

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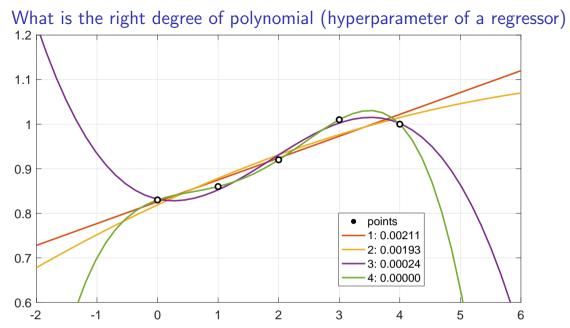
• 
$$P_{LAP}(red) = (2 + 100)/(3 + 100 * 2) = 102/203$$

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Conditional: relevant for the Naïve Bayes case.



Notes -

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see the overfit.m demo

# Generalization and overfiting

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

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# Generalization and overfiting

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

### How to evaluate a classifier? Confusion table



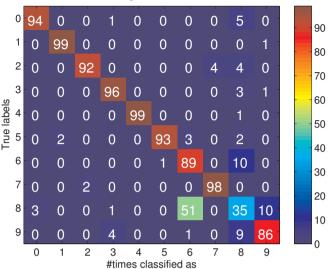


Figure from [5]

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:

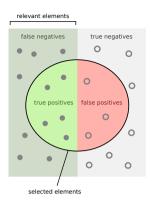
- ► How many relevant items are selected?
- ► Are we missing some items?
- Also called: True positive rate (TPR), sensitivity, hit rate . . .

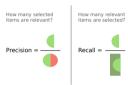
### Precision

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

### False positive rate (FPR)

Probability of false alarm





By Walber - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=36926283

#### Notes -

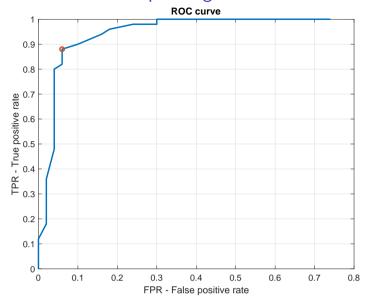
$$\mathsf{TPR} = \frac{\mathsf{TP}}{P} = \frac{\mathsf{TP}}{\mathsf{TP} + \mathsf{FN}}$$

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

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

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

## ROC - Receiver operating characteristics curve



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

#### 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.

## Discriminant functions $f(\vec{x}, s)$

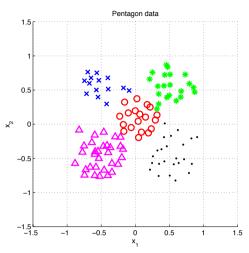
$$s^* = \operatorname*{argmax} f(\vec{x}, s)$$

Conditional likelihoods:  $\mathcal{N}(\vec{x}|\vec{\mu}_s, \Sigma_s)$ 

$$\frac{1}{2\pi |\Sigma_s|^{1/2}} \exp\{-\frac{1}{2} (\vec{x} - \vec{\mu}_s)^\top \Sigma_s^{-1} (\vec{x} - \vec{\mu}_s)\}$$

Bayes:

$$s^* = \operatorname*{argmax}_{s \in \mathcal{S}} P(s|\vec{x}) = \frac{P(\vec{x} \mid s)P(s)}{P(\vec{x})}$$



$$f(\vec{x}, s) = P(s) \frac{1}{2\pi |\Sigma_s|^{1/2}} \exp\{-\frac{1}{2}(\vec{x} - \vec{\mu}_s)^{\top} \Sigma_s^{-1}(\vec{x} - \vec{\mu}_s)\}$$

#### Notes

Normal distribution for general dimensionality D:

$$\mathcal{N}(\vec{x}|\vec{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\{-\frac{1}{2} (\vec{x} - \vec{\mu})^{\top} \Sigma^{-1} (\vec{x} - \vec{\mu})\}$$

How about learning  $f(\vec{x}, s)$  directly without explicit modeling of underlying probabilities? What about  $f(\vec{x}, s) = \vec{w}_s^{\top} \vec{x} + w_{s0}$ 

Towards linear classifier, geometrical thoughts . . .

$$f(\vec{x},s) = P(s) \frac{1}{2\pi |\Sigma_s|^{1/2}} \exp\{-\frac{1}{2} (\vec{x} - \vec{\mu}_s)^{\top} \Sigma_s^{-1} (\vec{x} - \vec{\mu}_s)\}$$

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, ......

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

#### **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)</pre>

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...

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

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

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#### **Notes**

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 $P(\bar{x})$  not needed – does not depend on the class. Laws of logarithms...

### References I

Further reading: Chapter 13 and 14 of [4]. Books [1] and [2] 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 [3].

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