Classifiers, intro, evaluation

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thanks to Daniel Novák and Filip Železný, Ondřej Drbohlav

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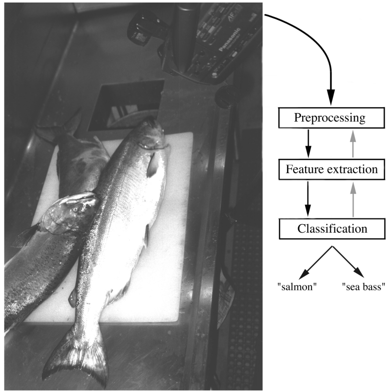
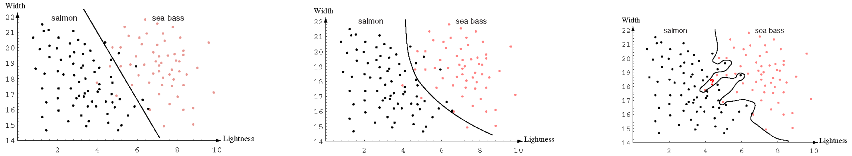
May 22, 2018

Classification example: What's the fish?



- Factory for fish processing
- 2 classes $s_{1,2}$:
  - salmon
  - sea bass
- Features $\vec{x}$: length, width, lightness etc. from a camera

Fish classification in feature space



- Linear, quadratic, k-nearest neighbor classifier

- Feature frequency per class shown using histograms
- Classification errors due to histogram overlap

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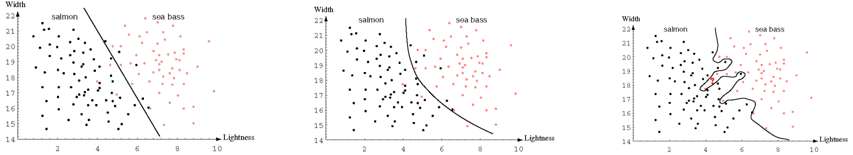

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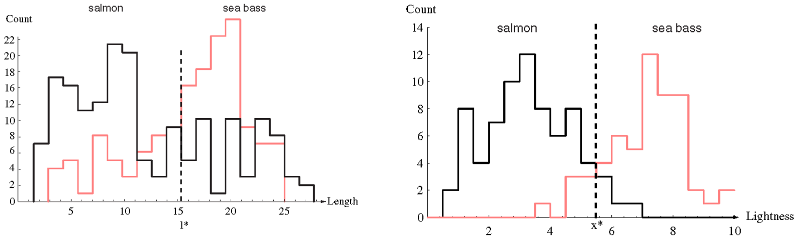

- Feature frequency per class shown using histograms
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Fish – classification using probability

$$posterior = \frac{likelihood \times prior}{evidence}$$

- Notation for classification problem
  - Classes $s_j \in S$ (e.g., salmon, sea bass)
  - Features $x_i \in X$ or feature vectors ($\vec{x}_i$) (also called attributes)
- Optimal classification of $\vec{x}$:

$$\delta^*(\vec{x}) = \arg\max_j P(s_j|\vec{x})$$

- We thus choose the most probable class for a given feature vector.
- Both likelihood and prior are taken into account – recall Bayes rule:

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

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

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

- 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

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

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Naïve Bayes classification

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

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

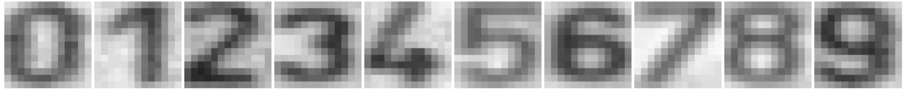
- Use simple Bayes law and maximize:

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

- 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

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



- Input: 8-bit image 13×13, intensities $0 - 255$.
- 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 $s^* = \operatorname{argmax}_s P(s|\vec{x})$.

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

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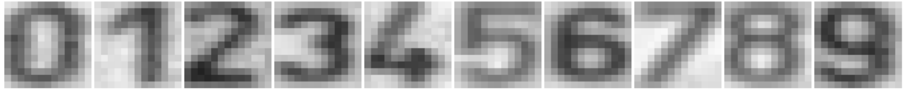

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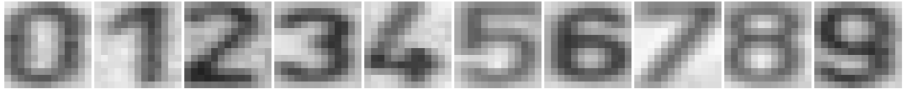

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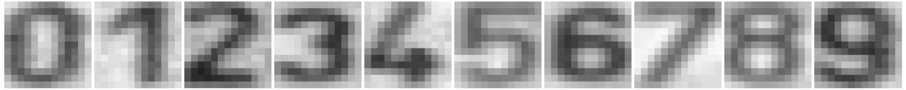

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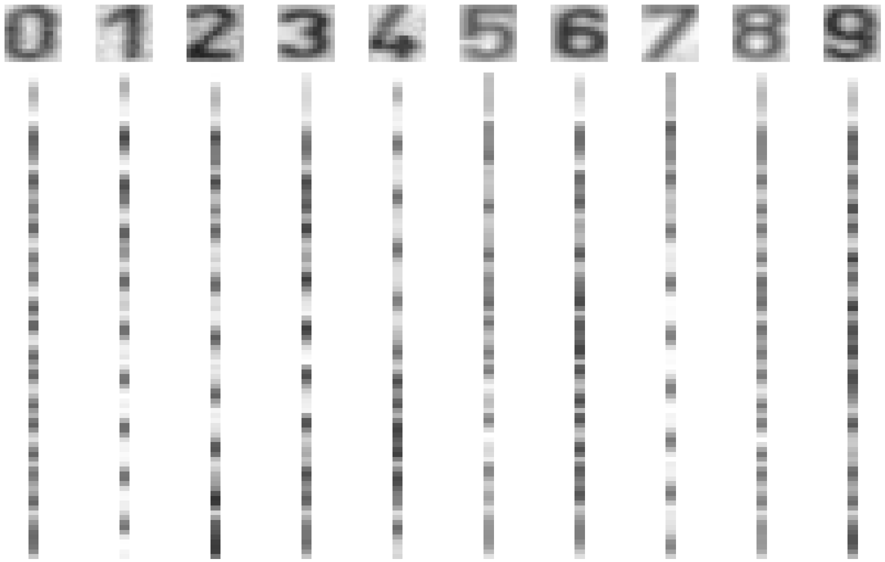
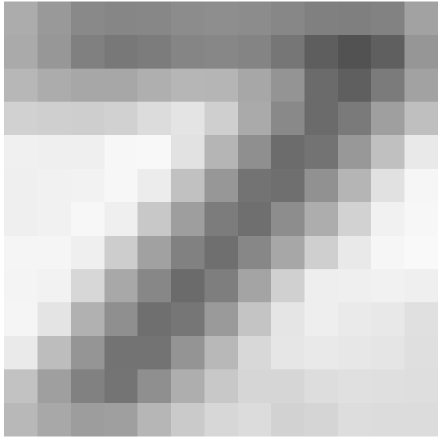
From images to $\vec{x}$

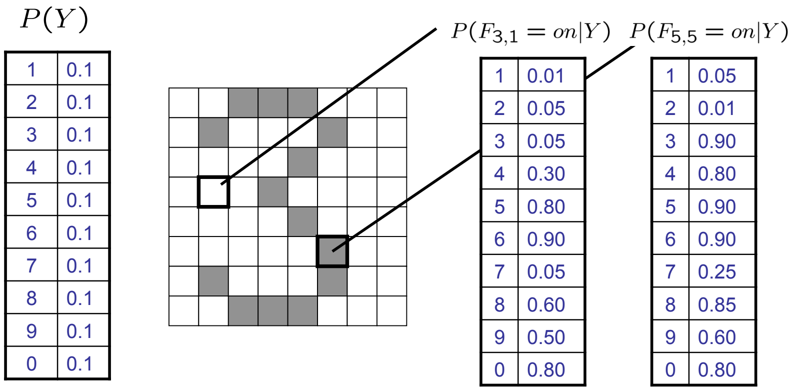


Conditional probabilities



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

We can rearrange pixels into vector - then using a linear index $P(x_j = I_i | s_k)$.



Y	$P(Y)$	$P(F_{3,1} = on\|Y)$	$P(F_{5,5} = on\|Y)$
1	0.1	0.01	0.05
2	0.1	0.05	0.01
3	0.1	0.05	0.90
4	0.1	0.30	0.80
5	0.1	0.80	0.90
6	0.1	0.90	0.90
7	0.1	0.05	0.25
8	0.1	0.60	0.85
9	0.1	0.50	0.60
0	0.1	0.80	0.80

image by courtesy of P. Abeel, http://ai.berkeley.edu

Training and testing

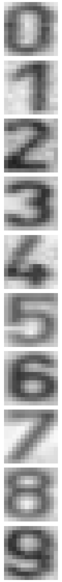
Data labeled instances.

- 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.



We will be talking about hyperparameters in a minute

Generalization and overfiting

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

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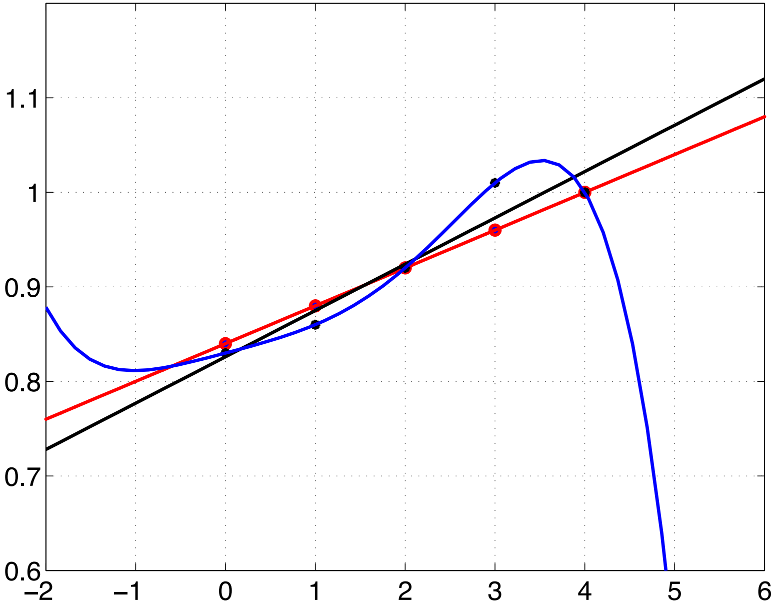
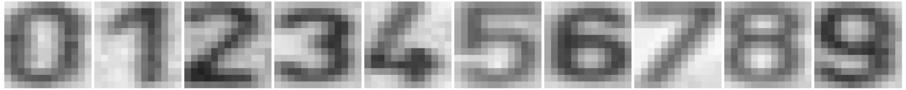
Overfiting

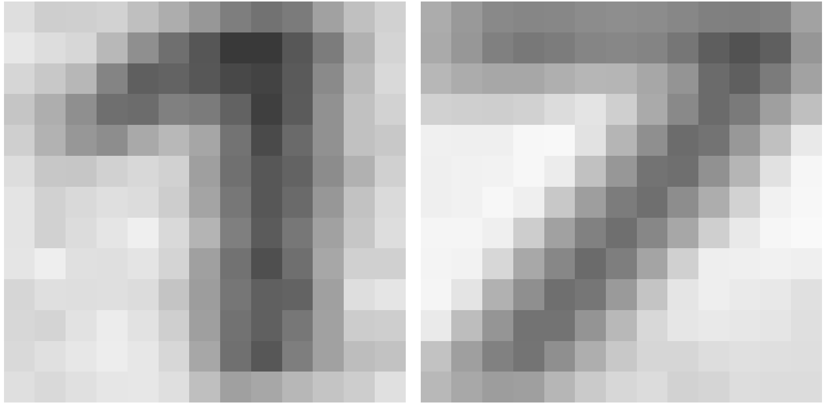


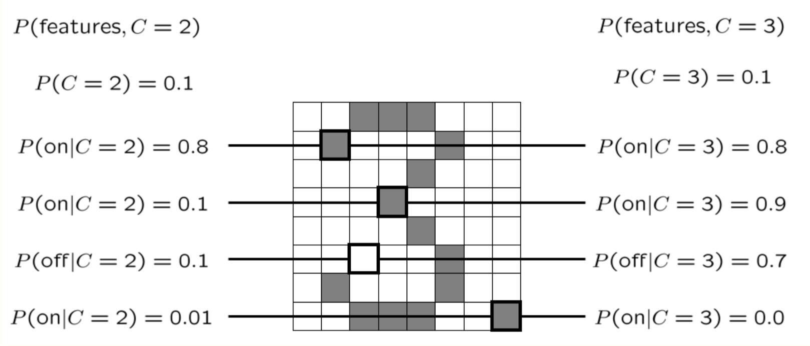
see the `overfit.m` demo

Unseen events



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





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Laplace smoothing

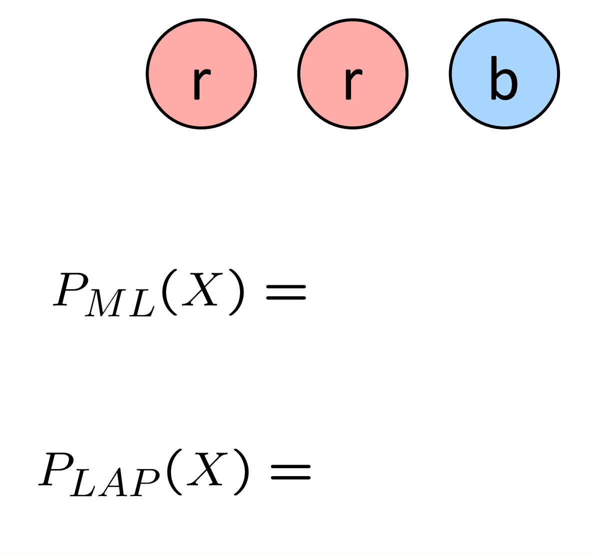
$$P(x) = \frac{\text{count}(x)}{\text{total samples}}$$

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

Pretend you see the sample one more time.

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

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



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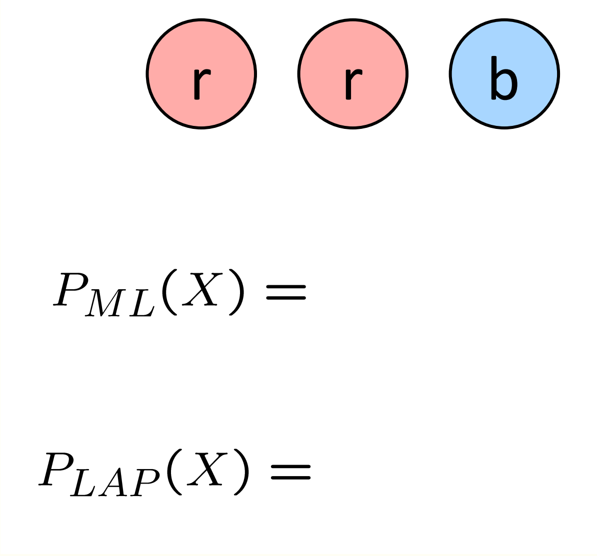

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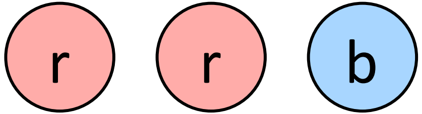

$$P_{ML}(X) =$$

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

image by courtesy of P. Abeel, http://ai.berkeley.edu

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

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

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, ...

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

just try `prod(rand(1,100))` and `prod(rand(1,10000))` in Matlab.
What is the way out?

Product of many small numbers ...

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Inference and decision

Inference stage - learning models/function/parameters from data.
Decision stage - decide about a query $\vec{x}$.

- Generative model : Learn (infer) $P(\vec{x}, s)$. Decide by computing $P(s|\vec{x})$.
- Discriminative model : Learn $P(s|\vec{x})$
- Discriminant function : Learn $f(\vec{x})$ which maps $\vec{x}$ directly into class labels.

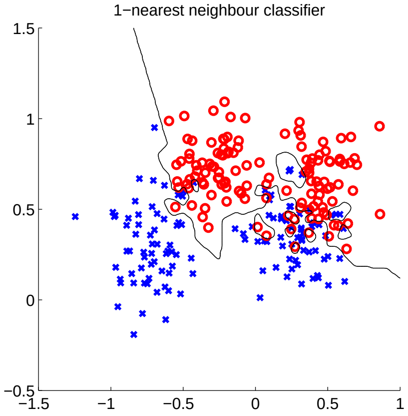
Generative models because by sampling from them it is possible to generate synthetic data points $\vec{x}$.
For the discriminative model one can consider, e.g. logistic function:

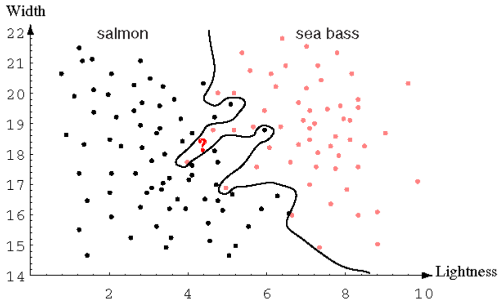
$$f(x) = \frac{1}{1 + e^{-k(x-x_0)}}$$

K-Nearest neighbors classification

For a query $\vec{x}$:

- Find K nearest $\vec{x}$ from the tranining (labeled) data.
- Classify to the class with the most exemplars in the set above.





$K-$ Nearest Neighbor and Bayes

Assume data:

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

We want classify $\vec{x}$. We draw a sphere centered at $\vec{x}$ containing K points irrespective of class. V is the volume of this sphere.

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

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

$$P(s_j) = \frac{N_j}{N}$$

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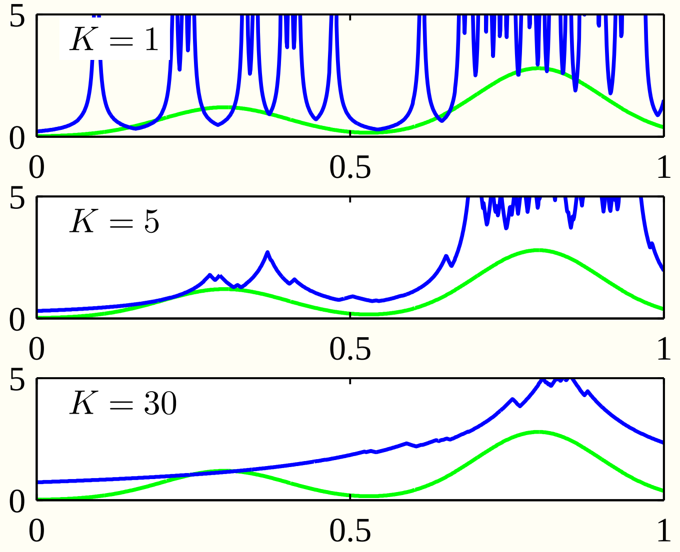

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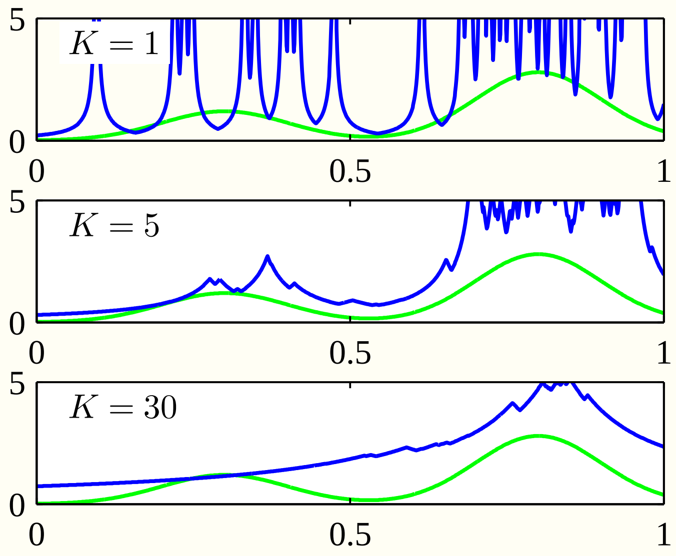
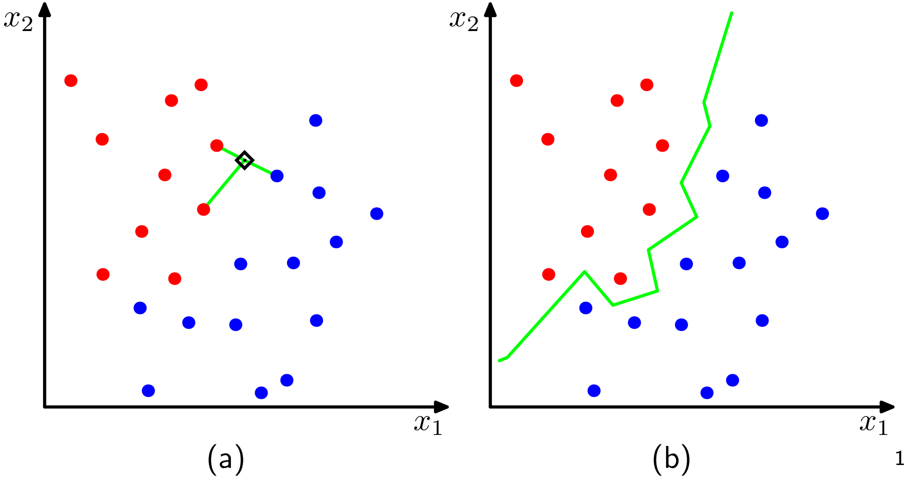


NN classification example



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1 Figs from [1]

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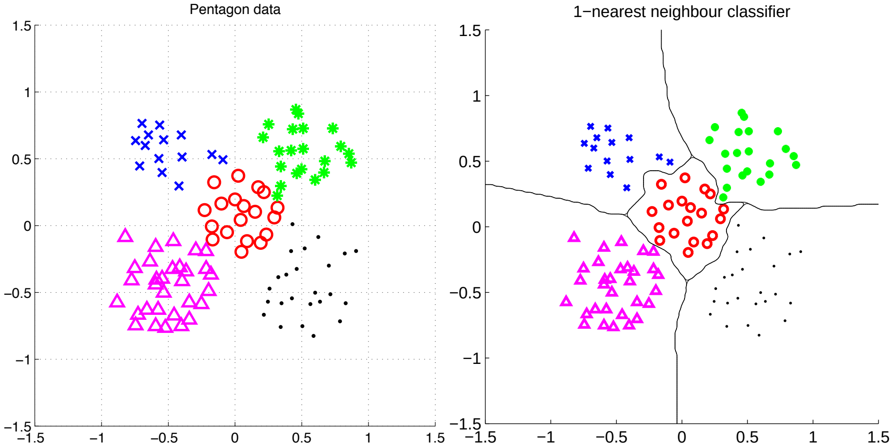
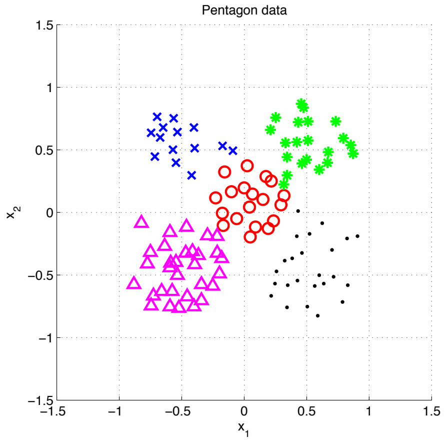
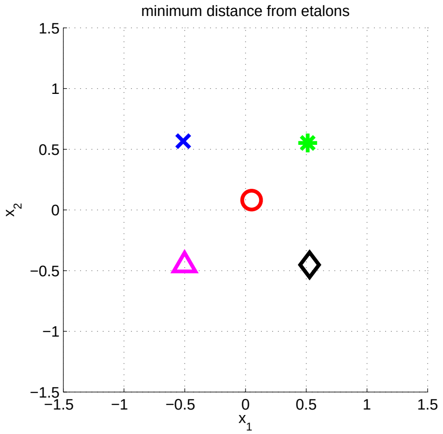


Etalon based classification

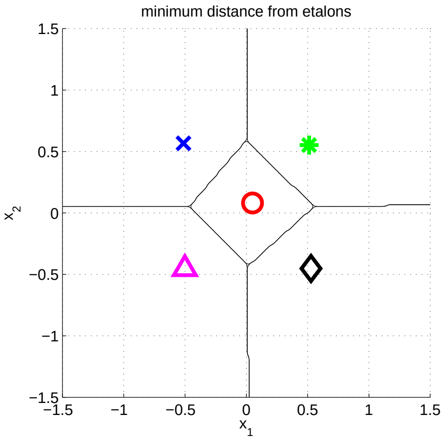




Represent $\vec{x}$ by etalon , $\vec{e}_s$ per each class $s \in S$

Separate etalons

$$f(\vec{x}) = \arg\min_{s \in S}(||\vec{x} - \vec{e}_s||^2 + o_s)$$

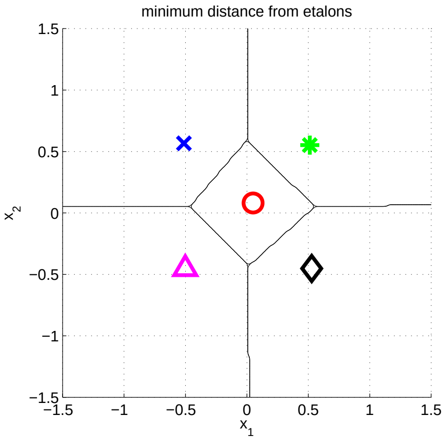


What etalons?

If $\mathcal{N}(\vec{x}|\vec{\mu},\Sigma)$; all classes same covariance matrices, then

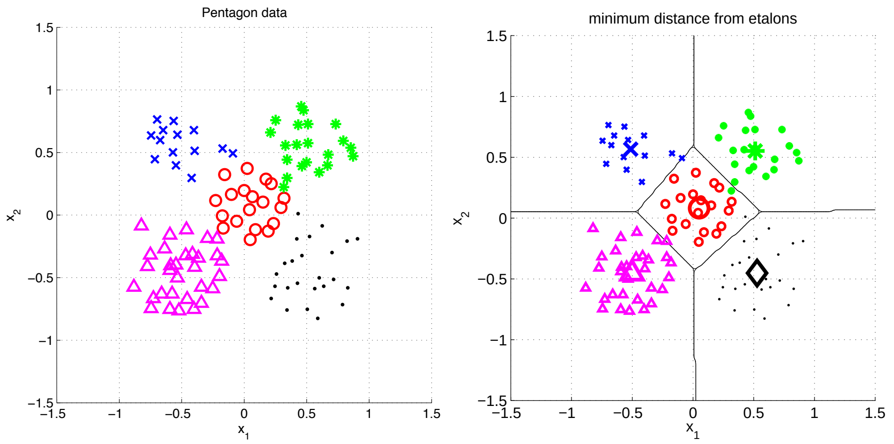
$$\vec{e}_s \stackrel{\text{def}}{=} \vec{\mu}_s = \frac{1}{|\mathcal{X}^s|}\sum_{i\in\mathcal{X}^s}\vec{x}_i^s$$

and separating hyperplanes halve distances between pairs.



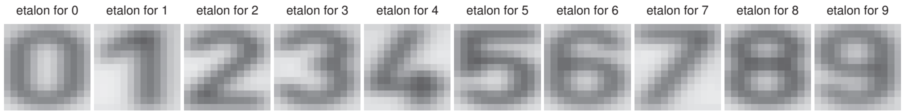
$$\mathcal{N}(\vec{x}|\vec{\mu},\Sigma) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\Sigma|^{1/2}}\exp\{-\frac{1}{2}(\vec{x}-\vec{\mu})^\top\Sigma^{-1}(\vec{x}-\vec{\mu})\}$$

Etalon based classification, $\vec{e}_s = \vec{\mu}_s$



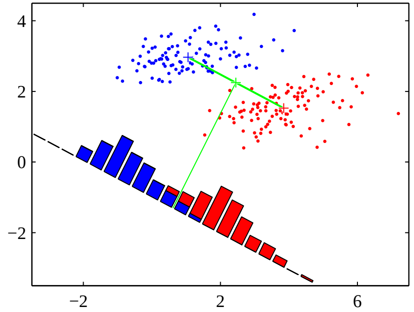
Some wrongly classified samples. We like the simple idea. Are there better etalons? How to find them?

Digit recognition - etalons $\vec{e}_s = \vec{\mu}_s$



Figures from [5]

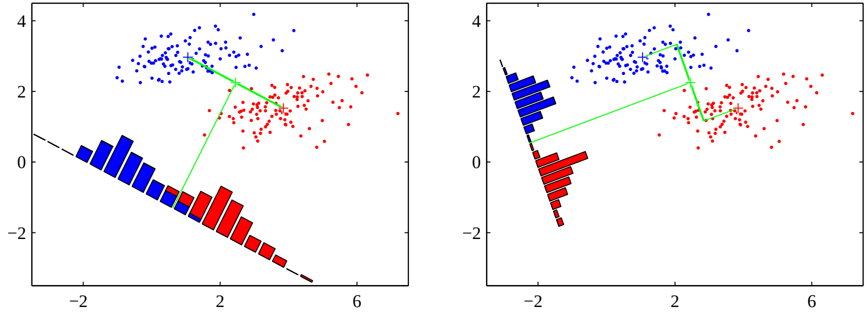
Better etalons – Fischer linear discriminant



- Dimensionality reduction
- Maximize distance between means, ...
- ...and minimize within class variance. (minimize overlap)

Figures from [1]

Better etalons – Fischer linear discriminant



- Dimensionality reduction
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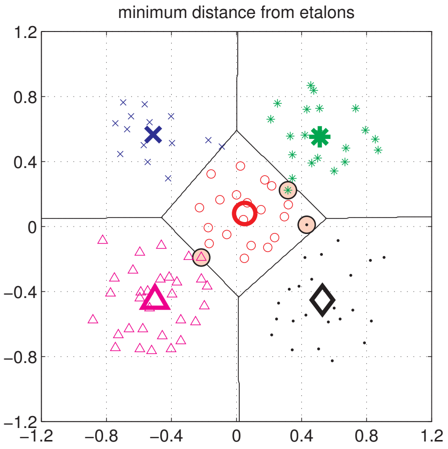
- ...and minimize within class variance. (minimize overlap)

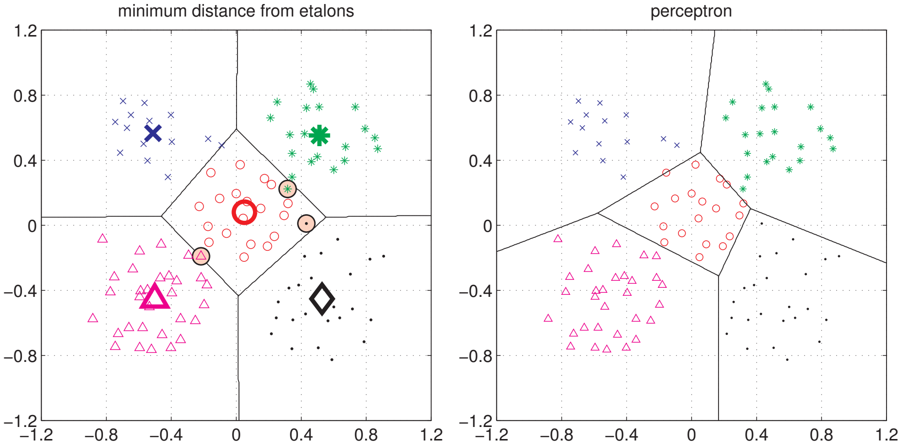
Figures from [1]

Better etalons - Perceptron



Figures from [5]

Better etalons - Perceptron



Figures from [5]

Etalon classifier – Linear classifier

$$f(\vec{x}) = \arg\min_{s \in S} \left(\|\vec{x} - \vec{e}_s\|^2 + o_s \right) = \arg\min_{s \in S} (\vec{x}^\top \vec{x} - 2\,\vec{e}_s^\top \vec{x} + \vec{e}_s^\top \vec{e}_s + o_s) =$$

$$= \arg\min_{s \in S} \left(\vec{x}^\top \vec{x} - 2\left(\vec{e}_s^\top \vec{x} - \frac{1}{2}(\vec{e}_s^\top \vec{e}_s + o_s)\right) \right) =$$

$$= \arg\min_{s \in S} (\vec{x}^\top \vec{x} - 2\,(\vec{e}_s^\top \vec{x} + b_s)) =$$

$$= \boxed{\arg\max_{s \in S} (\vec{e}_s^\top \vec{x} + b_s)} = \arg\max_{s \in S} f_s(\vec{x}). \qquad b_s = -\frac{1}{2}(\vec{e}_s^\top \vec{e}_s + o_s)$$

Linear function (plus offset)

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$$

Etalon classifier – Linear classifier

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\begin{aligned}
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$$

Linear function (plus offset)

$$f(\mathbf{x}) = \mathbf{w}^\top\mathbf{x} + w_0$$

Perceptron learning - problem set up

We seek $\mathcal{K} = \left\{(\mathbf{w}_s, w_{0s}) \mid s \in S\right\}$

$$f(\mathbf{x}) = \arg\max_{s \in S} \left(\mathbf{w}_s^\top \mathbf{x} + w_{0s}\right)$$

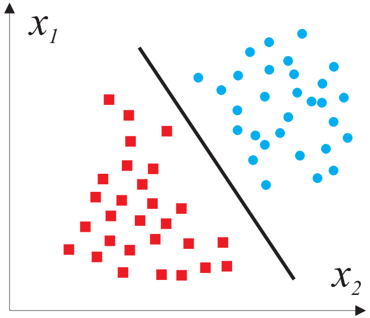
achieves no error on training set $\mathcal{T} = \left\{(\mathbf{x}^i,\, s^i),\ i = 0, 1, \ldots, m\right\}$

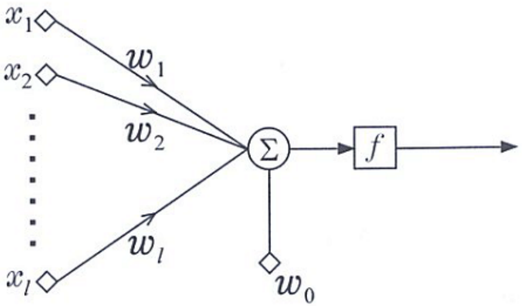
$$\epsilon_{tr} = \frac{1}{m} \sum_{j=1}^{m} \mathbf{1}\left(s^j \neq f(\mathbf{x}^j)\right), \qquad \mathbf{1}(s) = \begin{cases} 1 & s \text{ True} \\ 0 & s \text{ False} \end{cases}$$

Perceptron, two classes linearly separable

$|S| = 2$, i.e. two states (typically also classes)

$$f(\mathbf{x}) = \begin{cases} s = 1\,, & \text{if} \quad \mathbf{w}^\top \mathbf{x} + w_0 > 0\,, \\ s = -1\,, & \text{if} \quad \mathbf{w}^\top \mathbf{x} + w_0 < 0\,. \end{cases}$$





Linear seaparability - hyperplane separates/divides space into two half-spaces

Perceptron learning – Algorithm

$\mathbf{x}'_j = s_j \begin{bmatrix} 1 \\ \mathbf{x}_j \end{bmatrix}$, $\mathbf{w}' = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$ drop the dashes to avoid notation clutter.

Goal: Find a weight vector $\mathbf{w} \in \Re^{D+1}$ (original feature space dimensionality is D) such that:

$$\mathbf{w}^\top \mathbf{x}_j > 0 \qquad (\forall j \in \{1, 2, ..., m\})$$

Perceptron algorithm (Rosenblat 1962):

1. $t \leftarrow 0$, $\mathbf{w}^{(t)} \leftarrow 0$.
2. Find a wrongly classified observation $\mathbf{x}_j$:

$$\mathbf{w}^{(t)\top} \mathbf{x}_j \leq 0, \qquad (j \in \{1, 2, ..., m\}.)$$

3. If there is no misclassified observation then terminate. Otherwise,

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + \mathbf{x}_j \,.$$

4. Goto 2.

Perceptron learning – Algorithm

$\mathbf{x}'_j = s_j \begin{bmatrix} 1 \\ \mathbf{x}_j \end{bmatrix}$, $\mathbf{w}' = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$ drop the dashes to avoid notation clutter.

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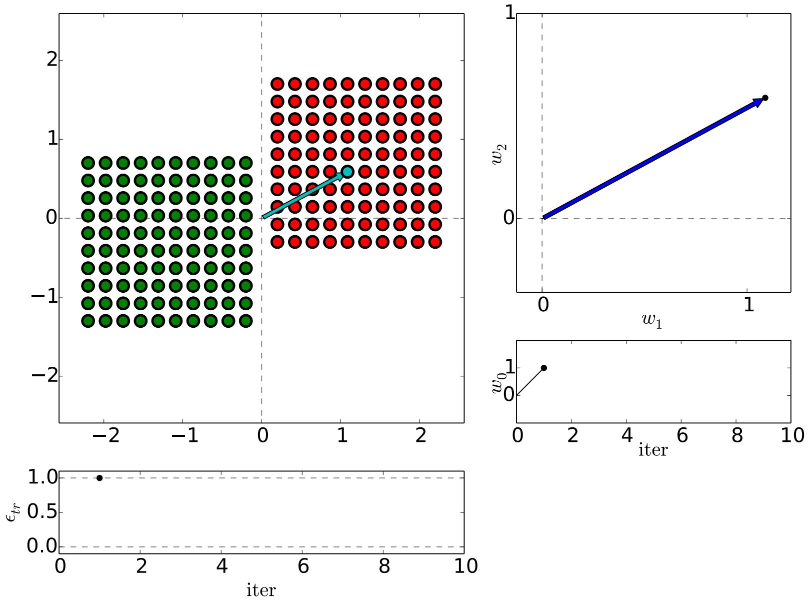
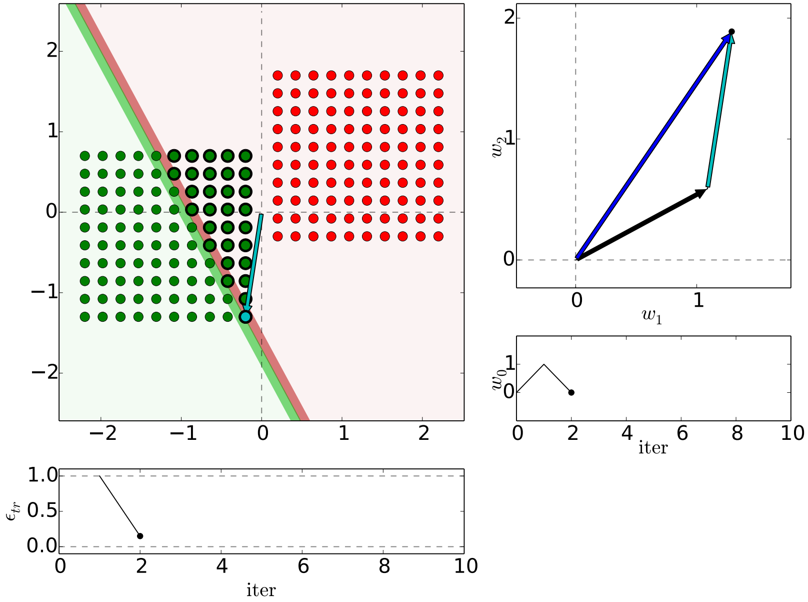
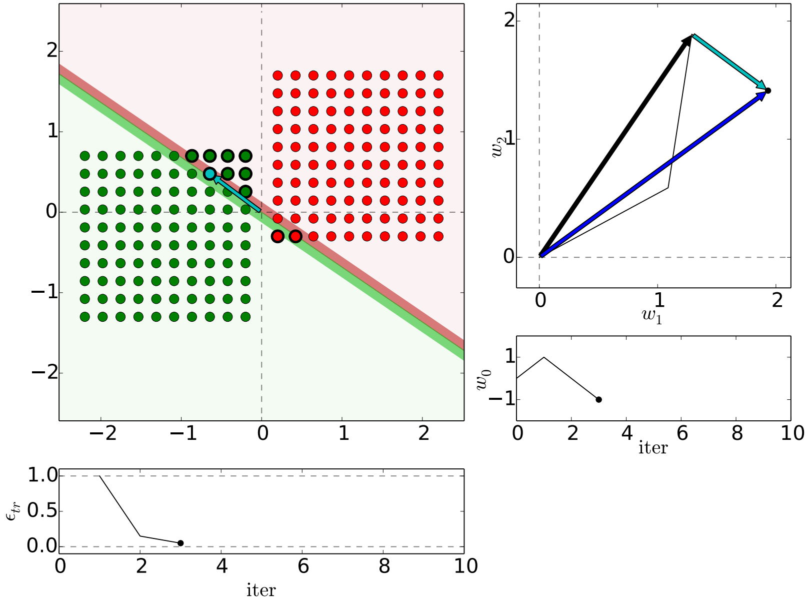
Perceptron iterations



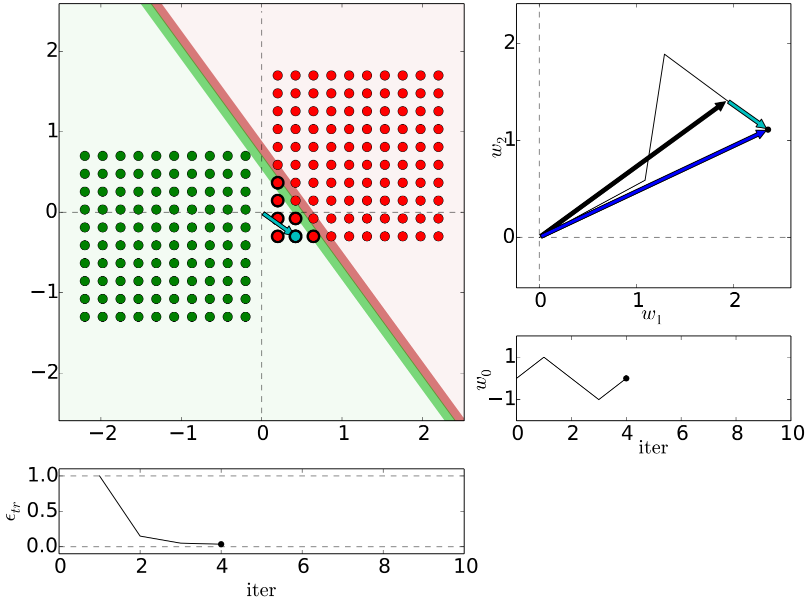
Perceptron iterations



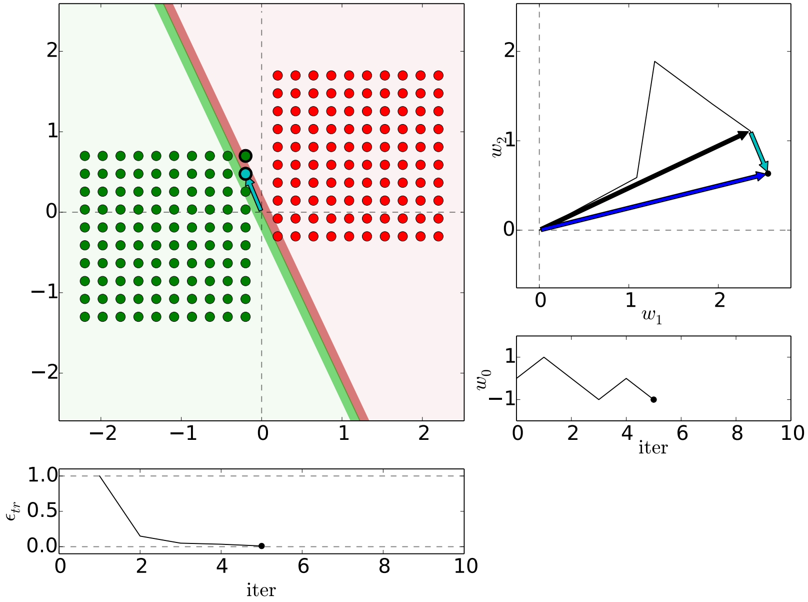
Perceptron iterations



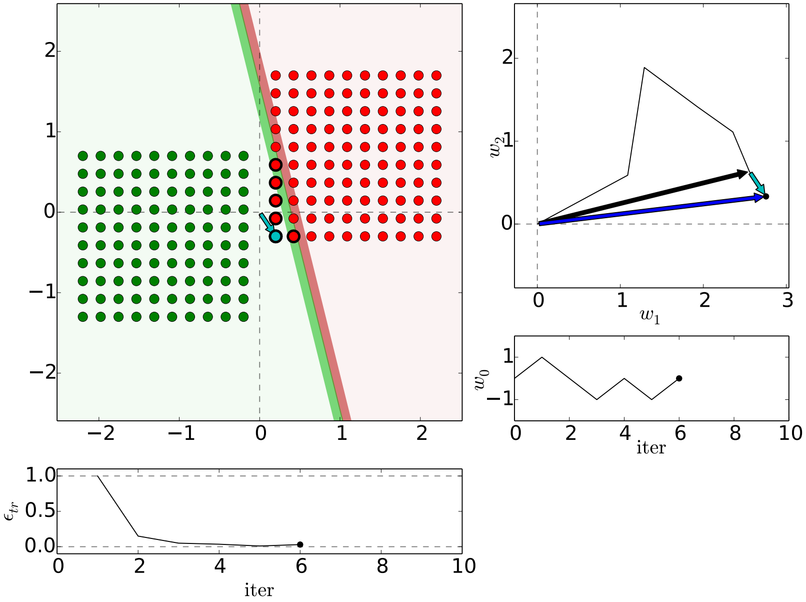
Perceptron iterations



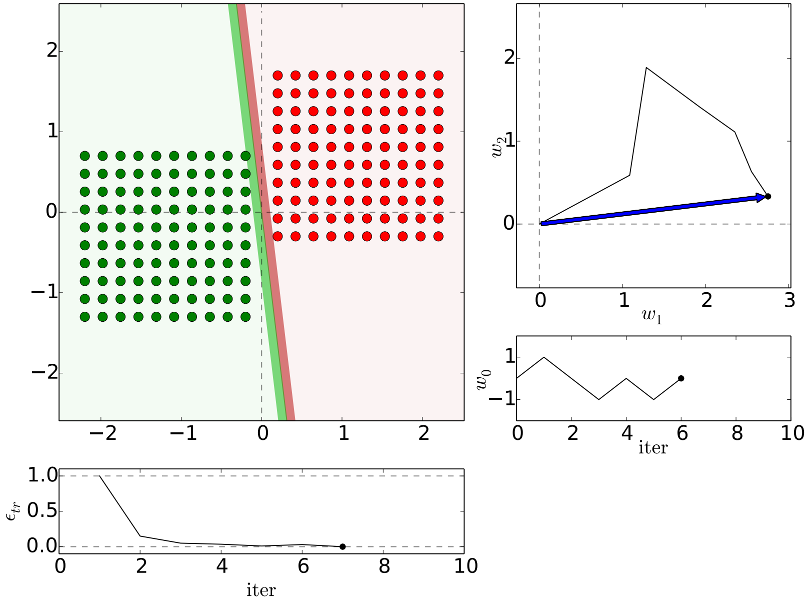
Perceptron iterations



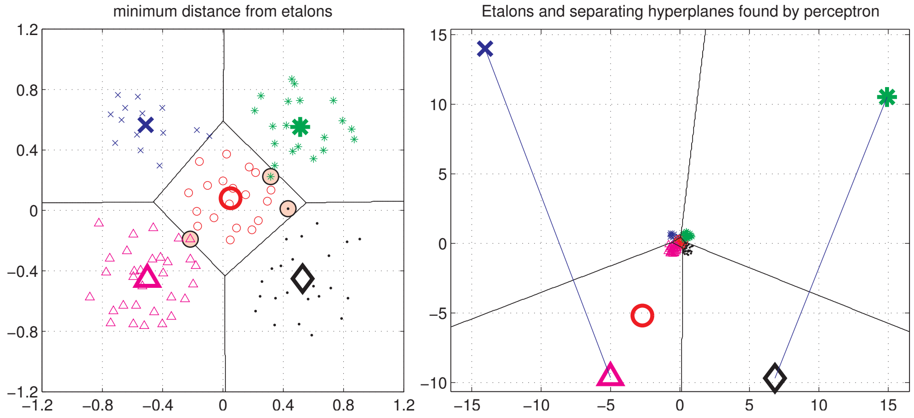
Perceptron iterations



Perceptron iterations

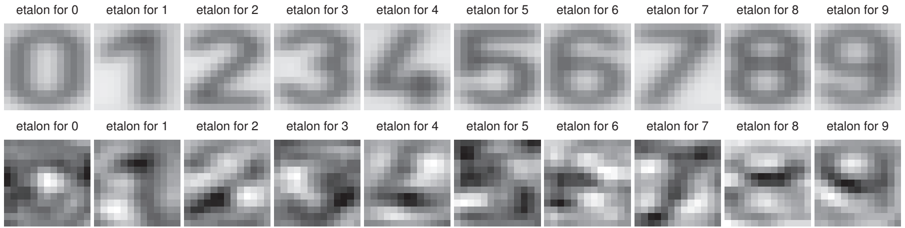


Etalons: means vs found be perceptron



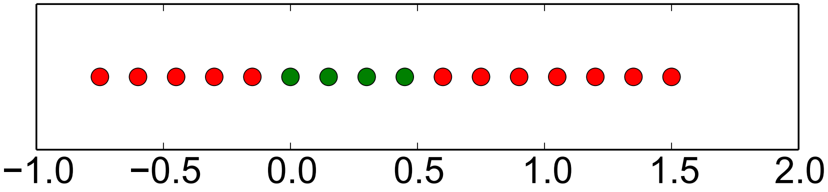
Figures from [5]

Digit recognition - etalons means vs. perceptron



Figures from [5]

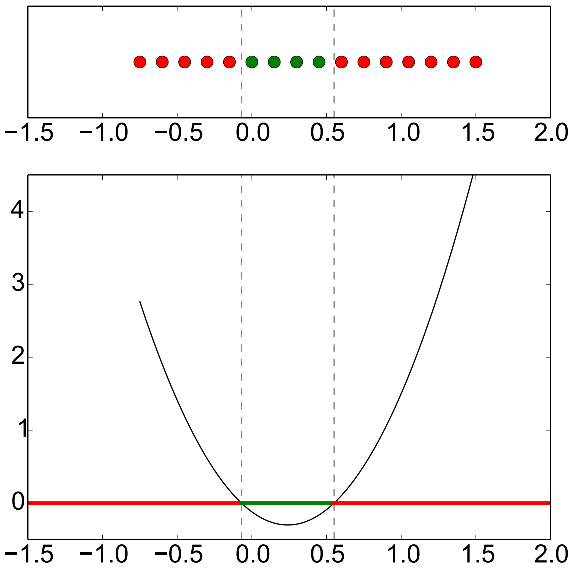
What if not lin separable?



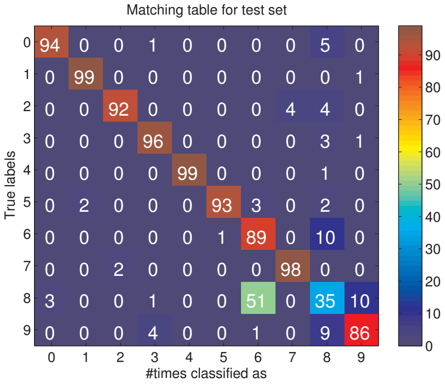
Dimension lifting

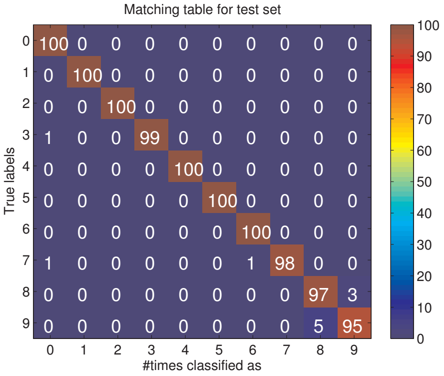
$$\mathbf{x} = [x, x^2]^\top$$

Dimension lifting, $\mathbf{x} = [x, x^2]^\top$



Performance comparison, parameters fixed





Why there some errors in perceptron results? we said zero error on training set.

Precision and Recall, Confusion matrix

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

Confusion matrix :

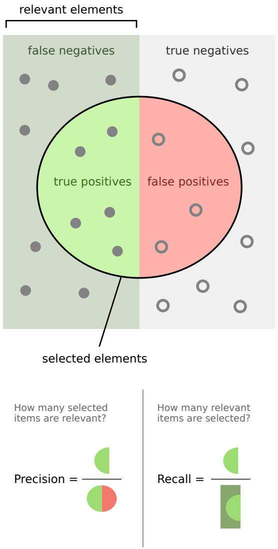
- Classification (prediction) vs Truth state

Recall :

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

Precision

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



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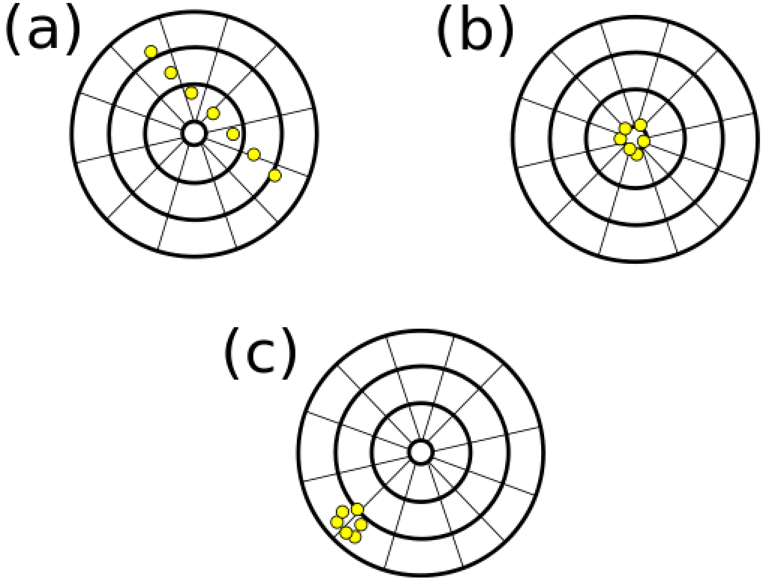
https://commons.wikimedia.org/w/index.php?curid=36926283

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

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

Think about precision vs recall graph, what is the best classifier?

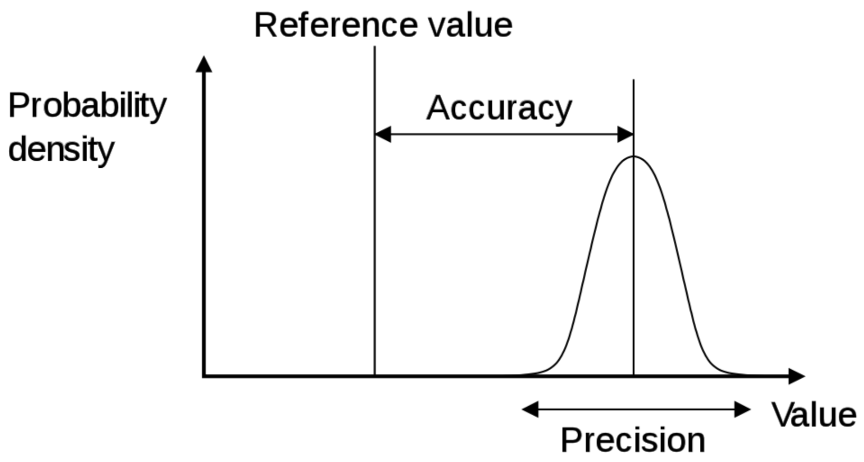
Accuracy vs precision



https://commons.wikimedia.org/wiki/File:Precision_versus_accuracy.svg

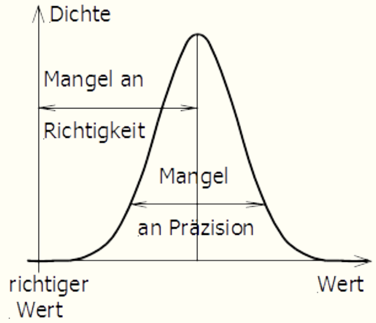
Accuracy: how close (is your model) to the true. Precision: how consistent/stable

Accuracy vs precision



https://en.wikipedia.org/wiki/Accuracy_and_precision

Accuracy: how close (is your model) to the true. Precision: how consistent/stable.
Think about terms *bias* and *error*. In Czech perhaps accuracy≈správnost, precision≈přesnost.



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. Many Matlab figures created with the help of [3]

[1] Christopher M. Bishop.
Pattern Recognition and Machine Learning.
Springer Science+Bussiness Media, New York, NY, 2006.

[2] Richard O. Duda, Peter E. Hart, and David G. Stork.
Pattern Classification.
John Wiley & Sons, 2nd edition, 2001.

[3] Votjěch Franc and Václav Hlaváč.
Statistical pattern recognition toolbox.
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References II

[4] Stuart Russell and Peter Norvig.
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http://aima.cs.berkeley.edu/.

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