Classifiers, Learning

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thanks to Daniel Novák and Filip Železný, Ondřej Drbohlav

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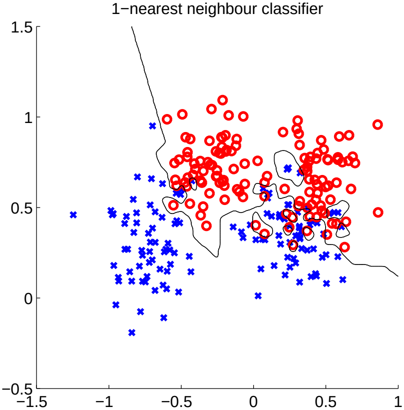
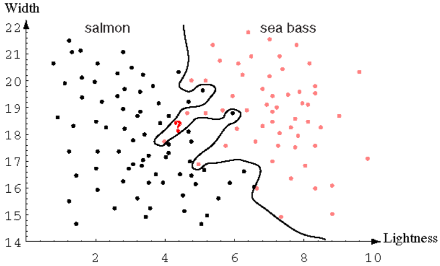
K-Nearest neighbors classification

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

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

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

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

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

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

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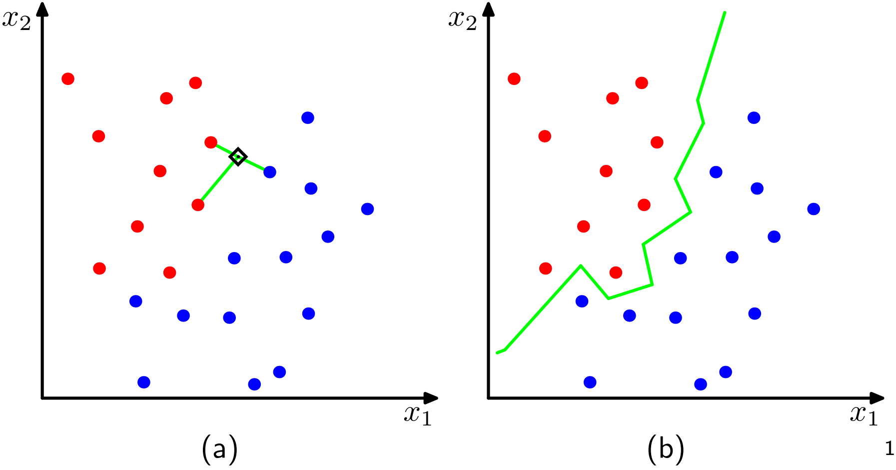
NN classification example



[1]

[1]Figs from [1]

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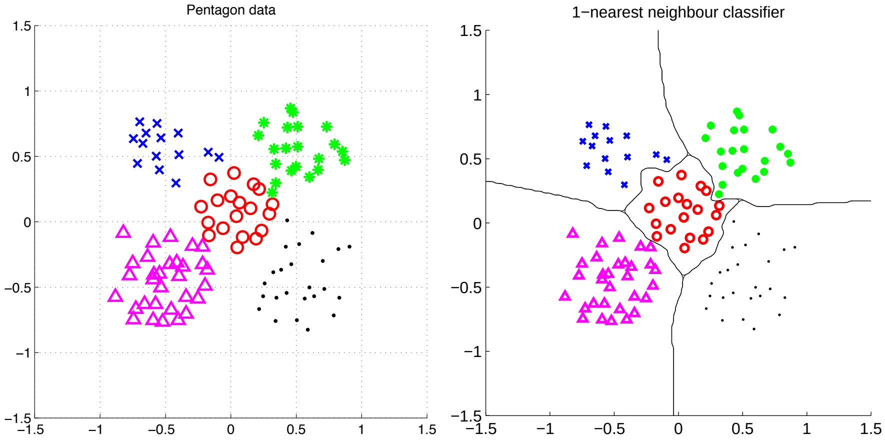
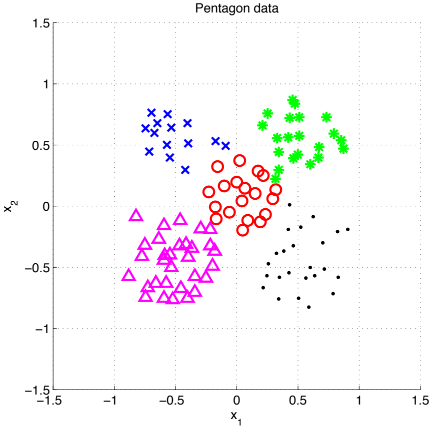
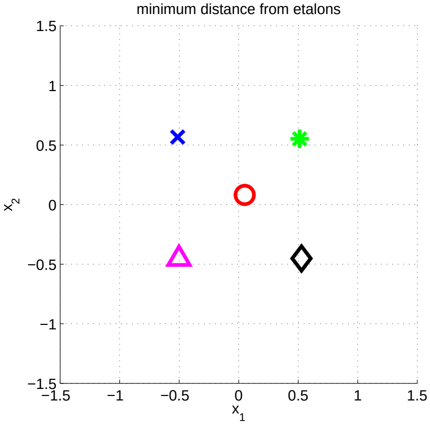


Metrics for NN classification

Etalon based classification

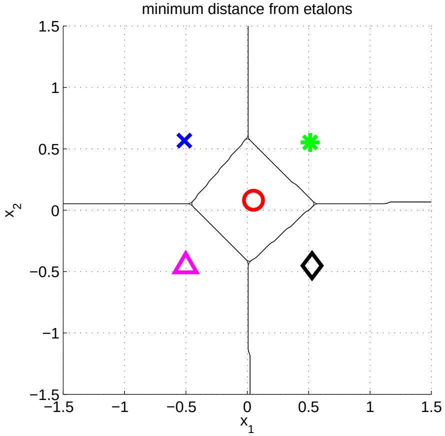




Represent $\vec{x}$ by etalon , $\vec{e}_s$ per each class $s \in S$

Separate etalons

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

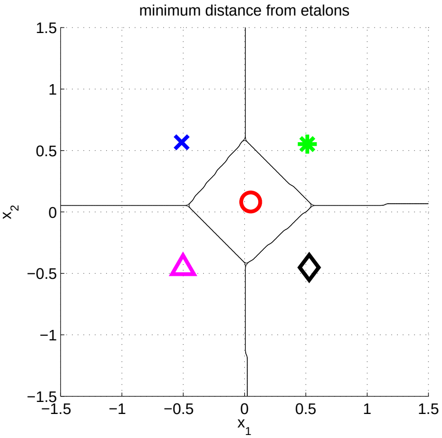


What etalons?

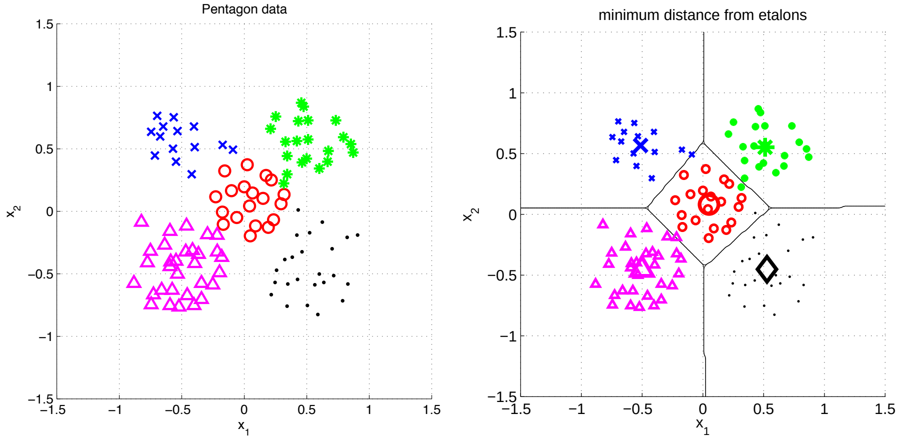
If $\mathcal{N}(\vec{x}|\vec{\mu},\Sigma)$; all classes same covariance matrices, then

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

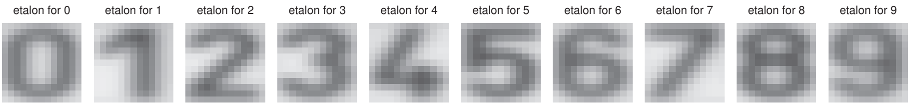
and separating hyperplanes halve distances between pairs.



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

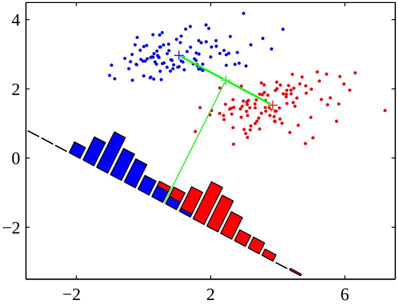


Digit recognition - etalons $\vec{e}_s = \vec{\mu}_s$



Figures from [5]

Better etalons – Fischer linear discriminant



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

Figures from [1]

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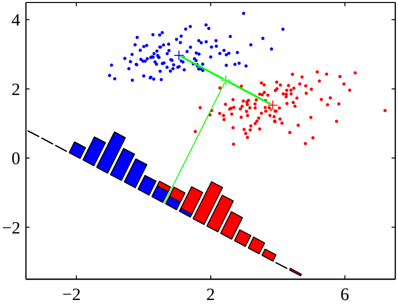

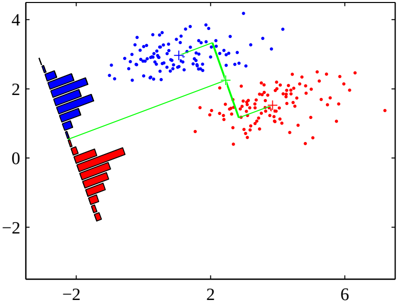

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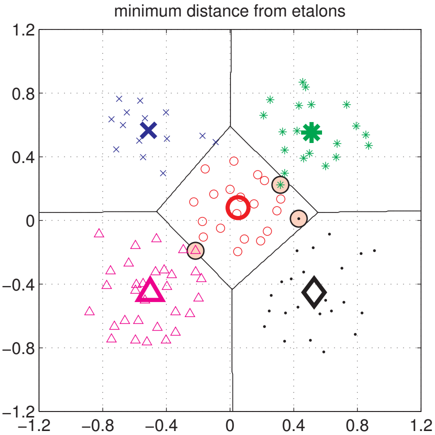

Figures from [5]

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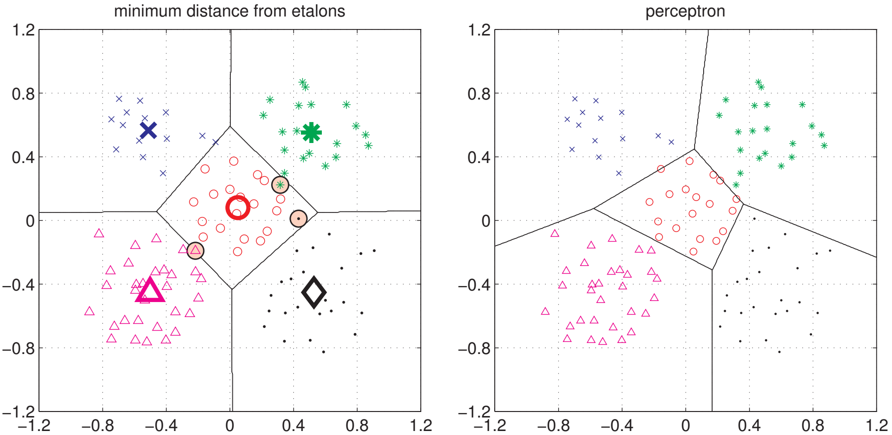

Figures from [5]

Etalon classifier – Linear classifier

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

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

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

Linear function (plus offset)

$$g_s(\mathbf{x}) = \mathbf{w}_s^\top \mathbf{x} + w_{s0}$$

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Learning and decision

Learning stage - learning models/function/parameters from data.

Decision stage - decide about a query $\vec{x}$.

What to learn?

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

Linear discriminant function - two class case

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

Decide s_1 if $g(\mathbf{x}) > 0$ and s_2 if $g(\mathbf{x}) < 0$

Figure from [2]

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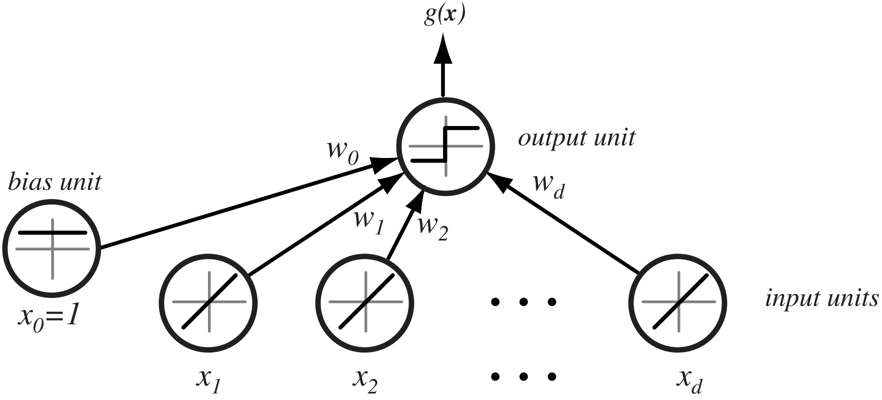

Figure from [2]

Separating hyperplane

$$\mathbf{w}^\top \mathbf{x}_1 + w_0 = \mathbf{w}^\top \mathbf{x}_2 + w_0$$
$$\mathbf{w}^\top (\mathbf{x}_1 - \mathbf{x}_2) = 0$$

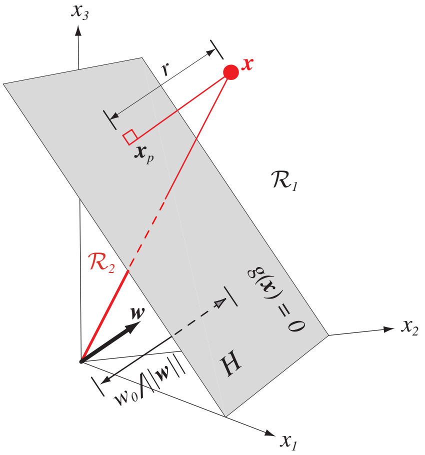

Figure from [2]

Multiclass case

Two classes set-up

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

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

$\mathbf{x}'_j = s_j \begin{bmatrix} 1 \\ \mathbf{x}_j \end{bmatrix}$, $\mathbf{w}' = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$

for all $\mathbf{x}'$

$$\mathbf{w}'^\top \mathbf{x}' > 0$$

drop the dashes to avoid notation clutter.

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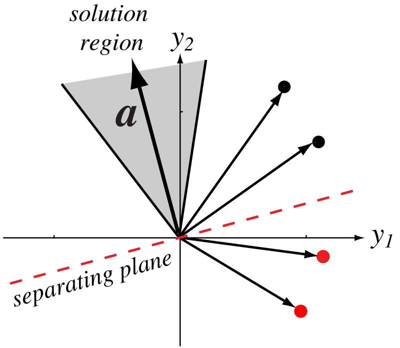
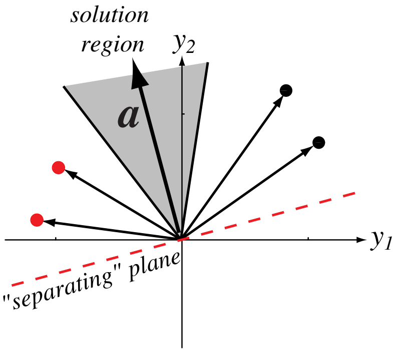
Solution (graphically)





Substitute $\mathbf{a} \leftarrow \mathbf{w}$ and $y_1, y_2 \leftarrow x_1, x_2$

Figure from [2]

Learning $\mathbf{w}$, gradient descent

A criterion to be minimized $J(\mathbf{w})$

Initialize $\mathbf{w}$, threshold θ, learning rate α

$k \leftarrow 0$

repeat

  $k \leftarrow k + 1$

  $\mathbf{w} \leftarrow \mathbf{w} - \alpha(k)\nabla J(\mathbf{w})$

until $|\alpha(k)\nabla J(\mathbf{w})| < \theta$

return $\mathbf{w}$

Learning **w** - Perceptron criterion

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) Criterion to be minimized:

$$J(\mathbf{w}) = \sum_{\mathbf{x} \in \mathcal{X}} -\mathbf{w}^\top \mathbf{x}$$

where $\mathcal{X}$ is a set of missclassified $\mathbf{x}$.

$$\nabla J(\mathbf{w}) = \sum_{\mathbf{x} \in \mathcal{X}} -\mathbf{x}$$

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(Batch) Perceptron algorithm

Initialize **w**, threshold θ, learning rate α
$k \leftarrow 0$
repeat
  $k \leftarrow k + 1$
  $\mathbf{w} \leftarrow \mathbf{w} + \alpha(k) \sum_{\mathbf{x} \in \mathcal{X}(k)} \mathbf{x}$
until $|\alpha(k) \sum_{\mathbf{x} \in \mathcal{X}(k)} \mathbf{x}| < \theta$
return **w**

Fixed-increment single-sample Perceptron

n patterns/samples, we are looping over all patterns repeatedly

Initialize $\mathbf{w}$

$k \leftarrow 0$

repeat

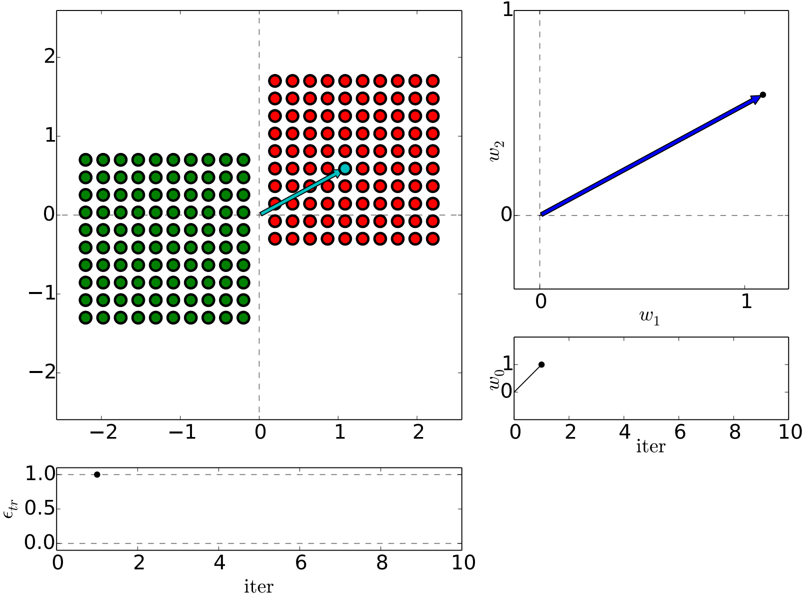
$k \leftarrow (k+1) \bmod n$

if $\mathbf{x}^k$ missclassified, **then** $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{x}^k$

until all $\mathbf{x}$ correctly classified

return $\mathbf{w}$

Perceptron iterations/loops



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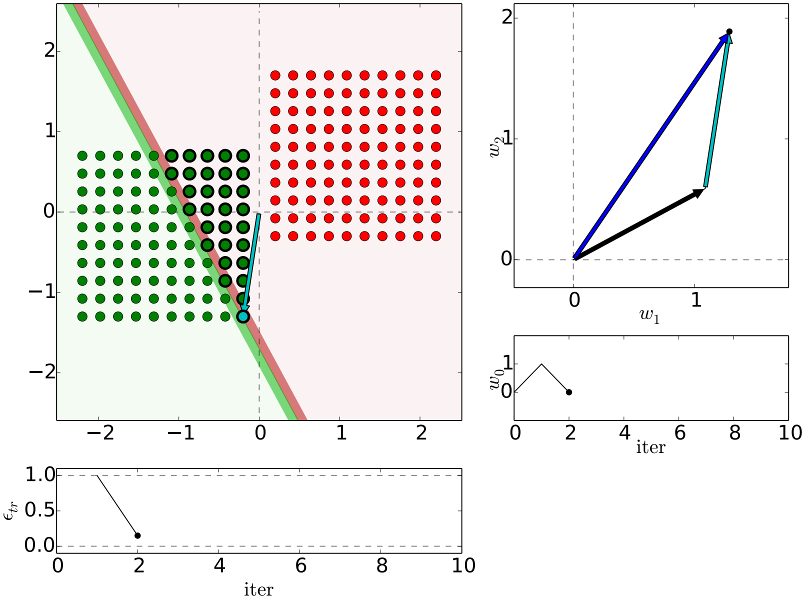

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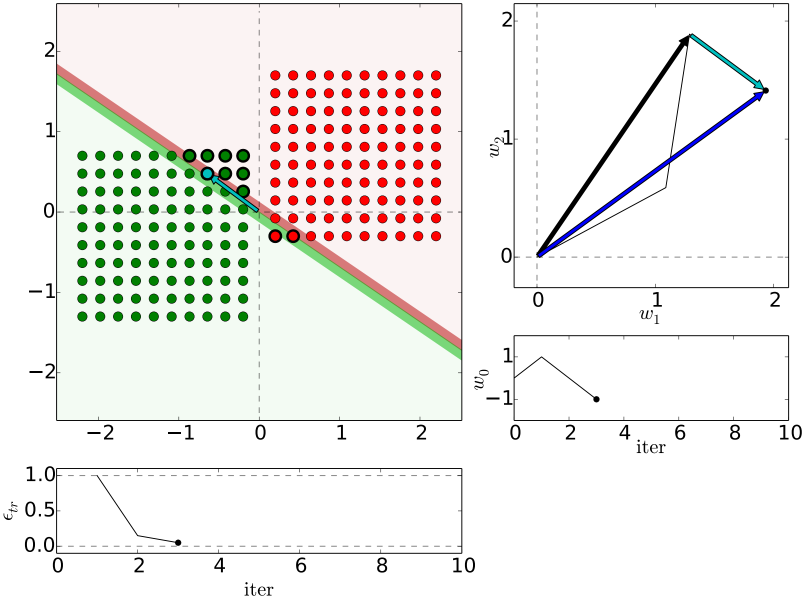

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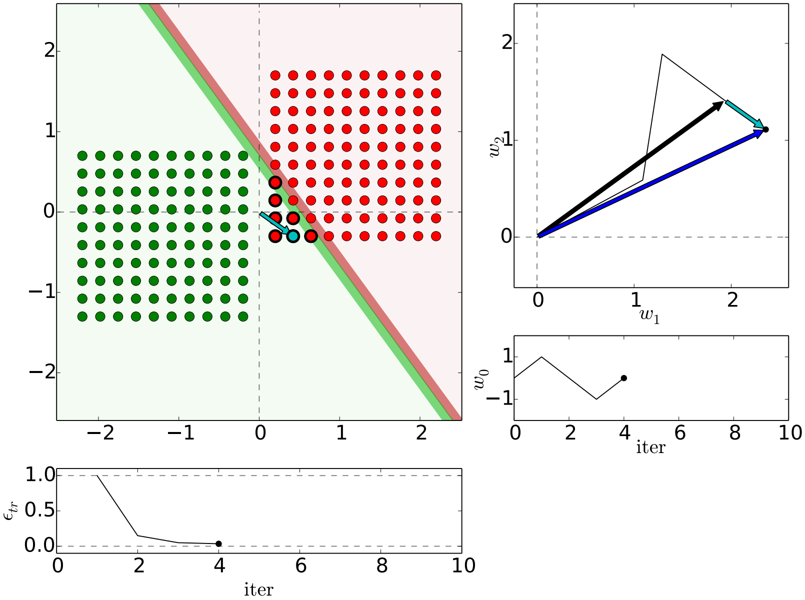
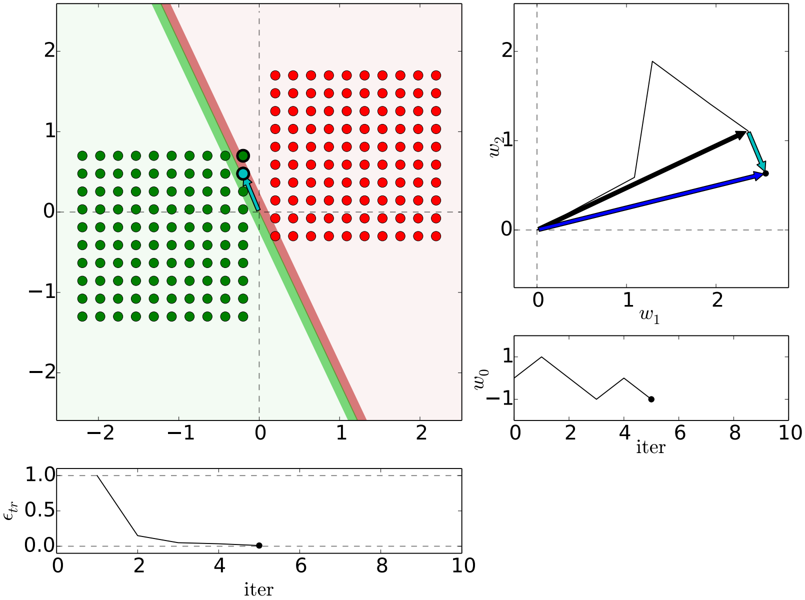
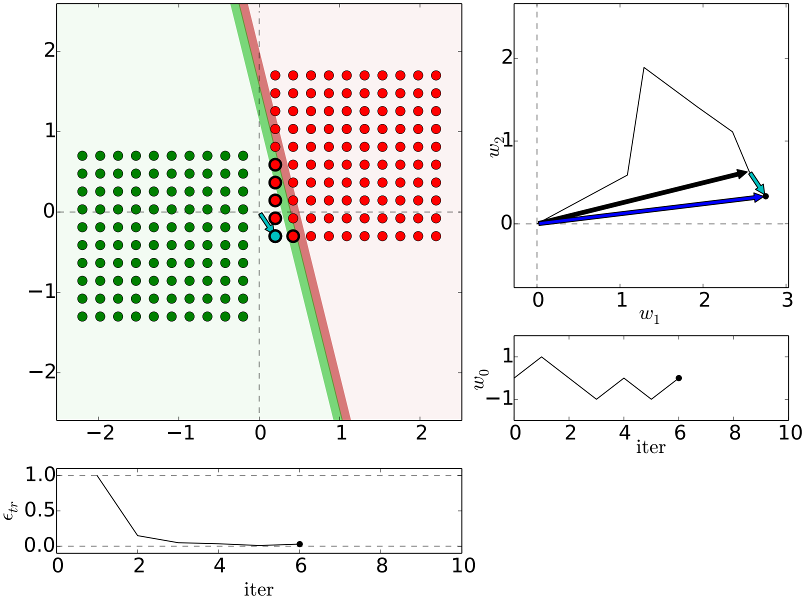


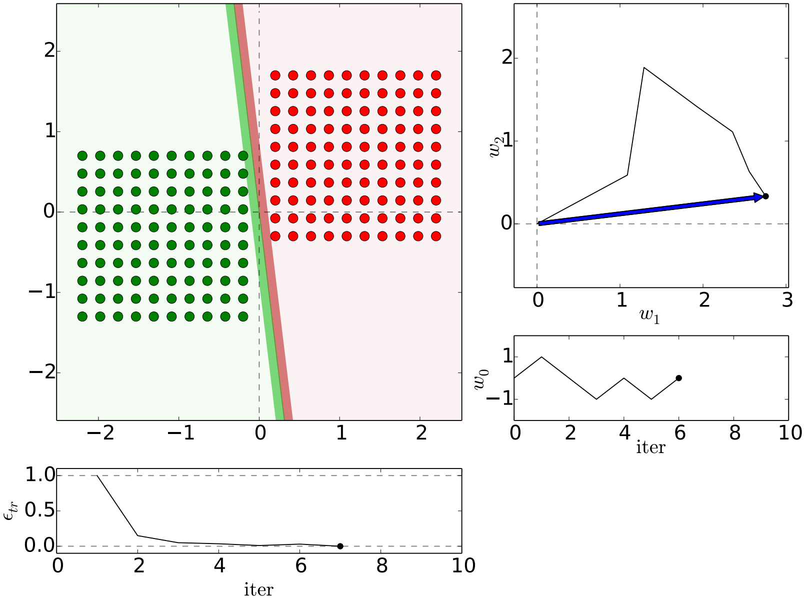
Perceptron iterations/loops



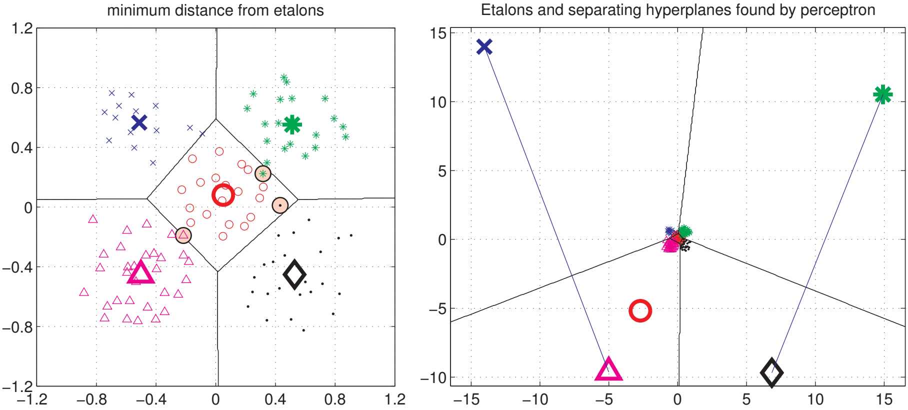
Perceptron iterations/loops



Perceptron iterations/loops

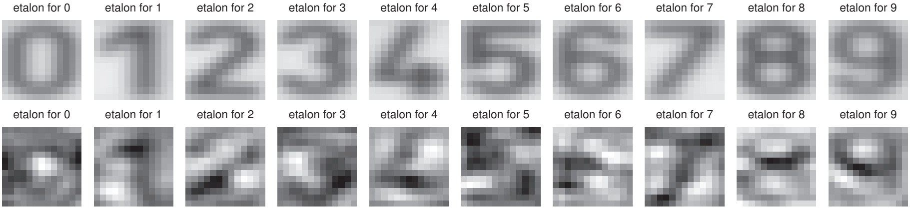


Etalons: means vs found be perceptron



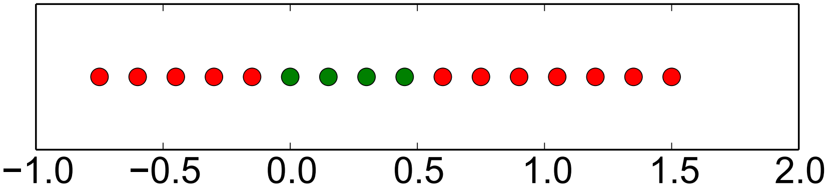
Figures from [5]

Digit recognition - etalons means vs. perceptron



Figures from [5]

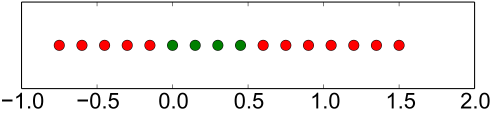
What if not lin separable?

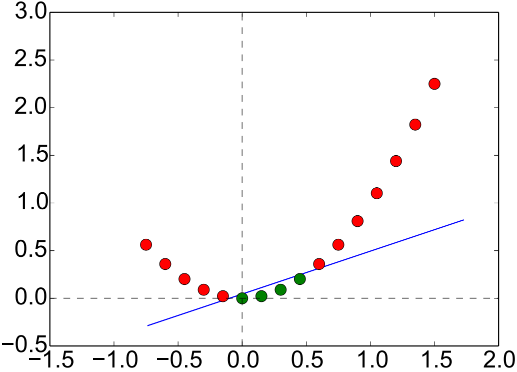


Dimension lifting

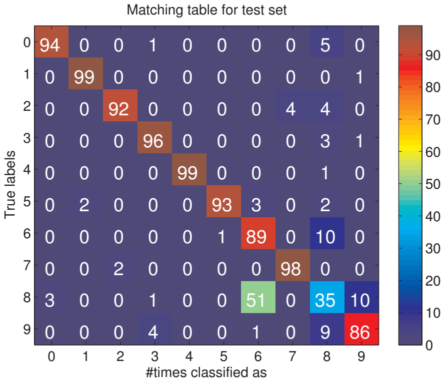
$$\mathbf{x} = [x, x^2]^\top$$

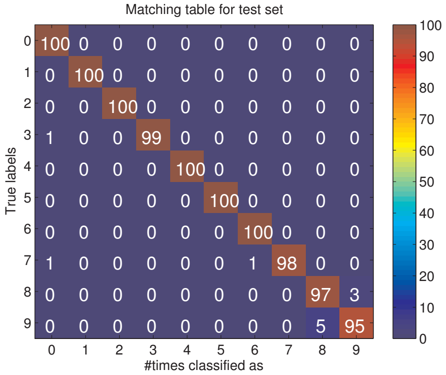
Dimension lifting, $\mathbf{x} = [x, x^2]^\top$





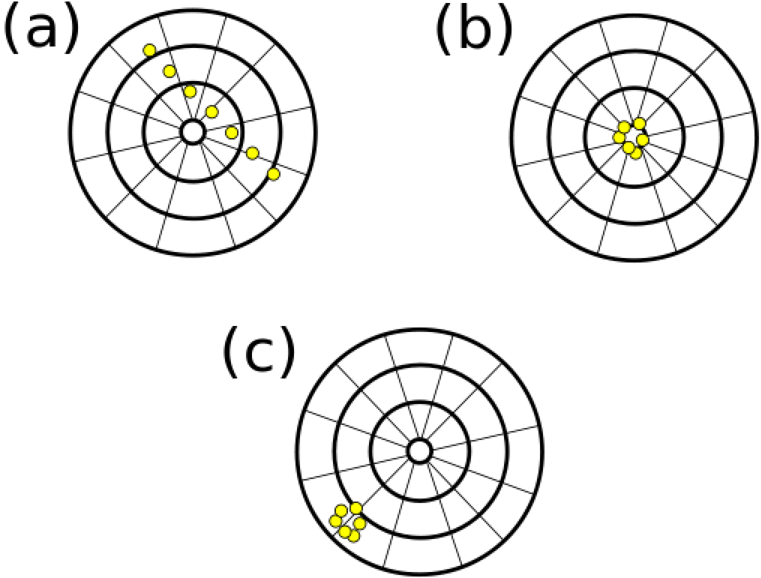
Performance comparison, parameters fixed





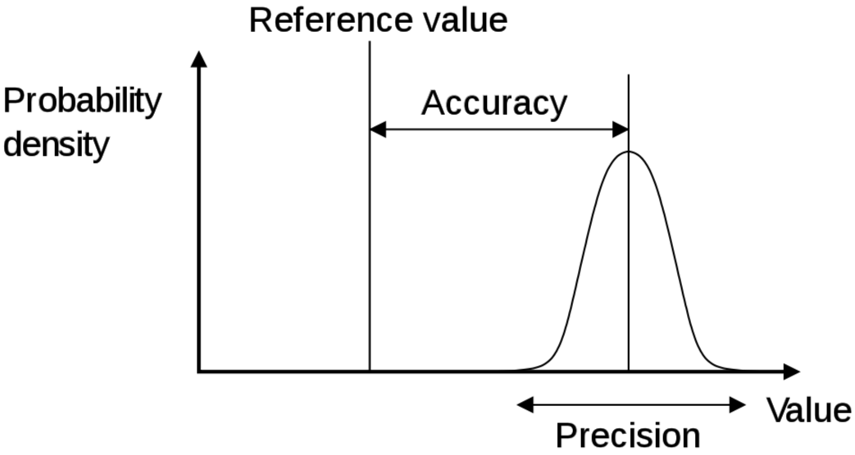
LSQ approach to linear classification

Accuracy vs precision



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

Accuracy vs precision



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

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.
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[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.
http://cmp.felk.cvut.cz/cmp/software/stprtool/index.html.

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[4] Stuart Russell and Peter Norvig.
Artificial Intelligence: A Modern Approach.
Prentice Hall, 3rd edition, 2010.
http://aima.cs.berkeley.edu/.

[5] Tomáš Svoboda, Jan Kybic, and Hlaváč Václav.
Image Processing, Analysis and Machine Vision — A MATLAB Companion.
Thomson, Toronto, Canada, 1^{st} edition, September 2007.
http://visionbook.felk.cvut.cz/.