

Classifiers, Learning

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

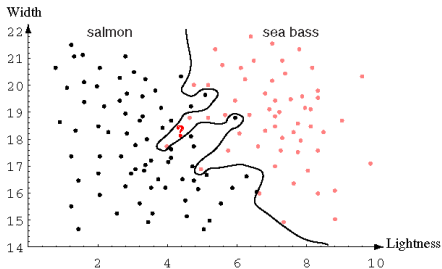
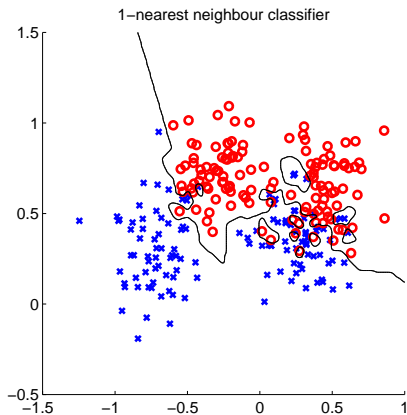
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May 20, 2019

K-Nearest neighbors classification

For a query \vec{x} :

- ▶ Find K nearest \vec{x} from the training (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. $P(s_j|\vec{x}) = ?$

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

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

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

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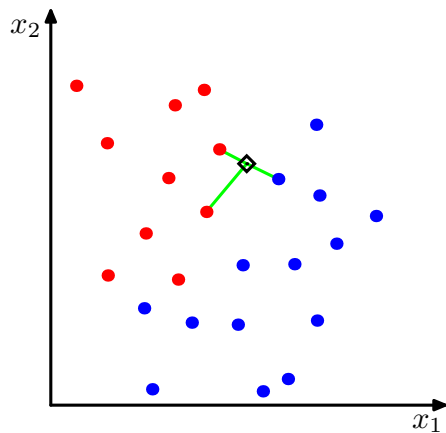
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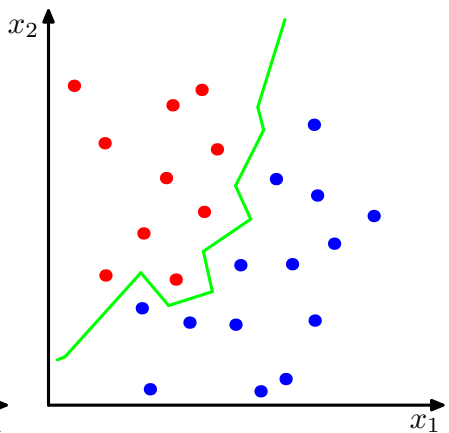
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NN classification example



(a)

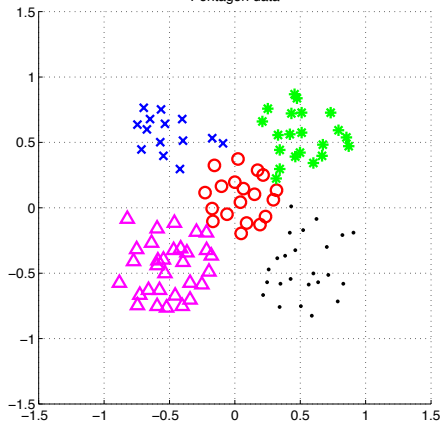


(b)

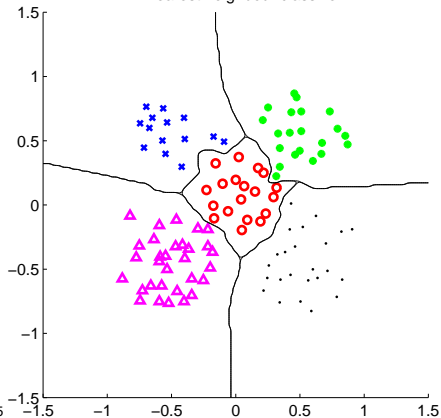
1

NN classification example

Pentagon data



1-nearest neighbour classifier



Metrics for NN classification

$$D(\mathbf{a}, \mathbf{b}) \geq 0$$

$$D(\mathbf{a}, \mathbf{b}) = 0 \text{ iff } \mathbf{a} = \mathbf{b}$$

$$D(\mathbf{a}, \mathbf{b}) = D(\mathbf{b}, \mathbf{a})$$

$$D(\mathbf{a}, \mathbf{b}) + D(\mathbf{b}, \mathbf{c}) \geq D(\mathbf{a}, \mathbf{c})$$

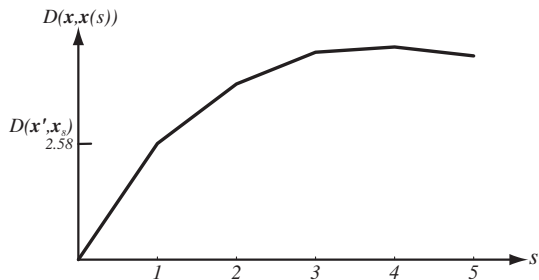
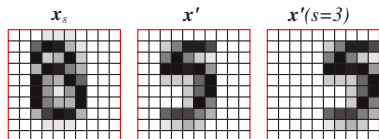
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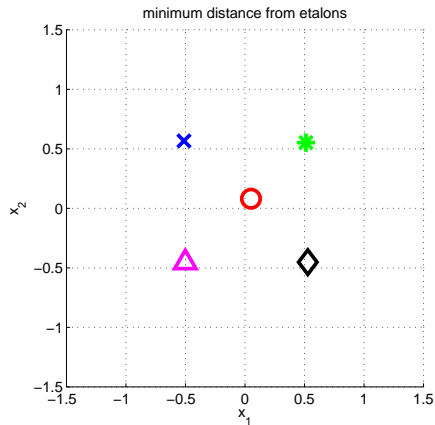
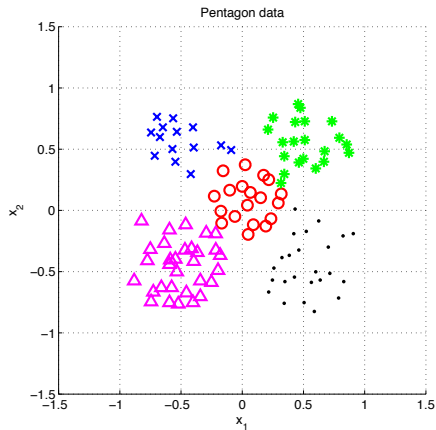
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Invariance to geometrical transformations?

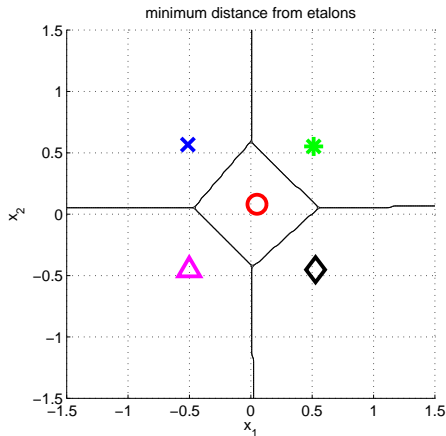
Etalon based classification



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

Separate etalons

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

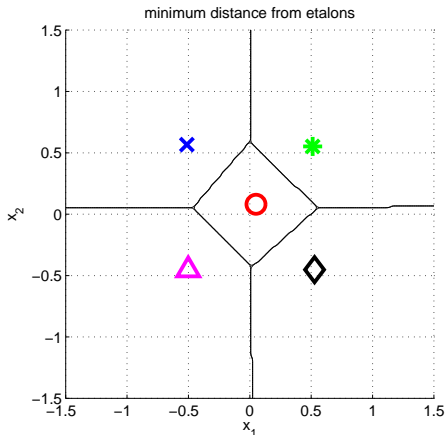


What etalons?

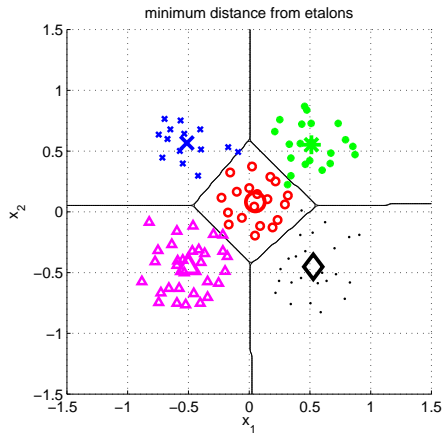
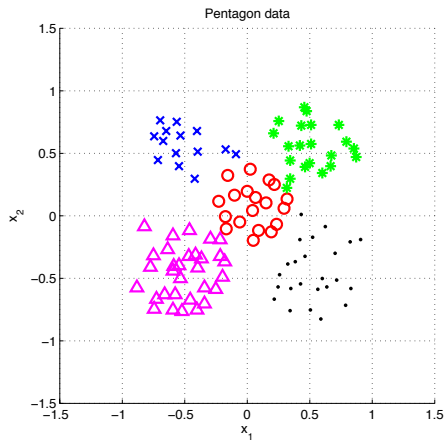
If $\mathcal{N}(\vec{x}|\vec{\mu}, \Sigma)$; all classes same covariance matrices, then

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

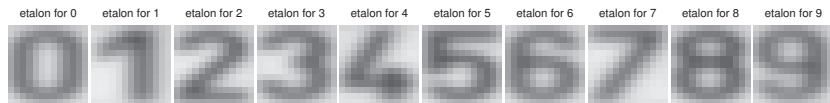
and separating hyperplanes halve distances between pairs.



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

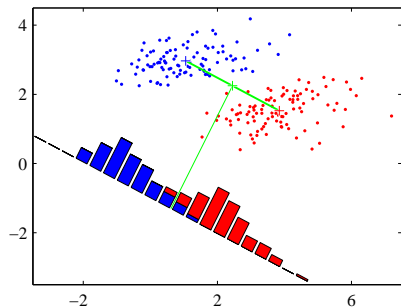


Digit recognition - etalons $\vec{e}_s = \vec{\mu}_s$



Figures from [5]

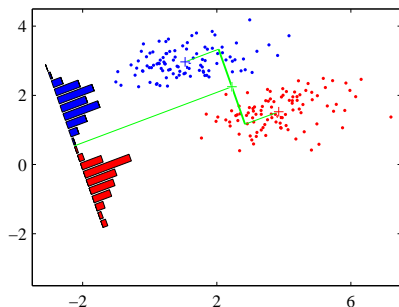
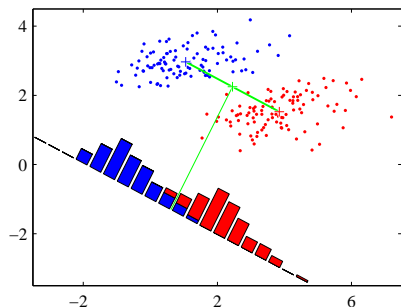
Better etalons – Fischer linear discriminant



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

Figures from [1]

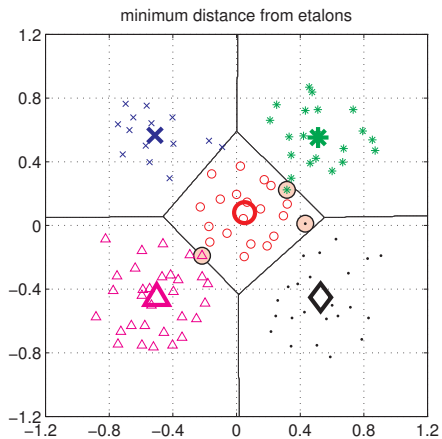
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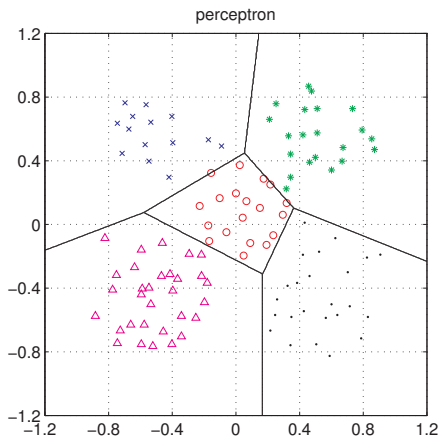
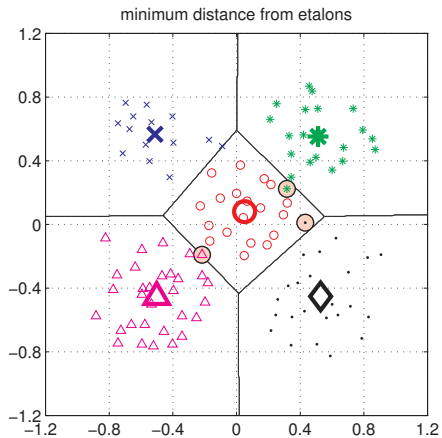
Figures from [1]

Better etalons?



Figures from [5]

Better etalons?



Figures from [5]

Etalon classifier – Linear classifier

$$\begin{aligned} s^* &= \arg \min_{s \in S} (\|\vec{x} - \vec{e}_s\|^2 + o_s) = \arg \min_{s \in S} (\vec{x}^T \vec{x} - 2 \vec{e}_s^T \vec{x} + \vec{e}_s^T \vec{e}_s + o_s) = \\ &= \arg \min_{s \in S} \left(\vec{x}^T \vec{x} - 2 (\vec{e}_s^T \vec{x} - \frac{1}{2} (\vec{e}_s^T \vec{e}_s + o_s)) \right) = \\ &= \arg \min_{s \in S} (\vec{x}^T \vec{x} - 2 (\vec{e}_s^T \vec{x} + b_s)) = \\ &= \boxed{\arg \max_{s \in S} (\vec{e}_s^T \vec{x} + b_s)} = \arg \max_{s \in S} g_s(\vec{x}). \end{aligned} \quad b_s = -\frac{1}{2} (\vec{e}_s^T \vec{e}_s + o_s)$$

Linear function (plus offset)

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

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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

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

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

Figure from [2]

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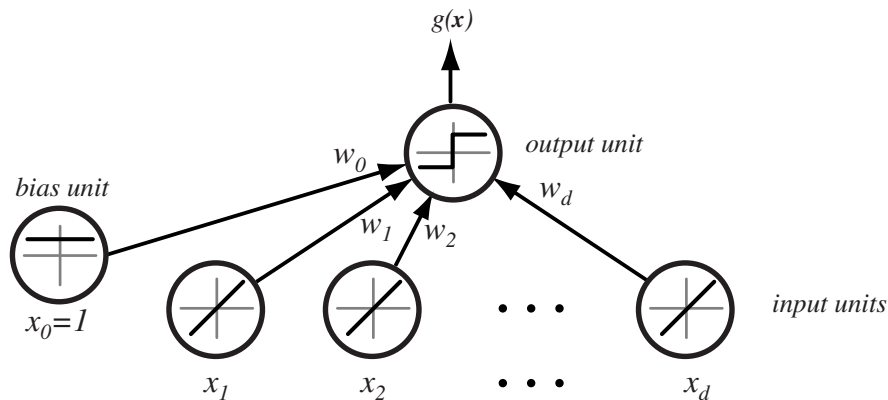


Figure from [2]

Separating hyperplane

$$\mathbf{w}^\top \mathbf{x}_1 + w_0 = \mathbf{w}^\top \mathbf{x}_2 + w_0$$

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

$g(\mathbf{x})$ gives an algebraic measure of the distance from \mathbf{x} to the hyperplane.

$$\mathbf{x} = \mathbf{x}_p + r \frac{\mathbf{w}}{\|\mathbf{w}\|}$$

as $g(\mathbf{x}_p) = 0$,
and $g(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$, then:

$$g(\mathbf{x}) = r \|\mathbf{w}\|$$

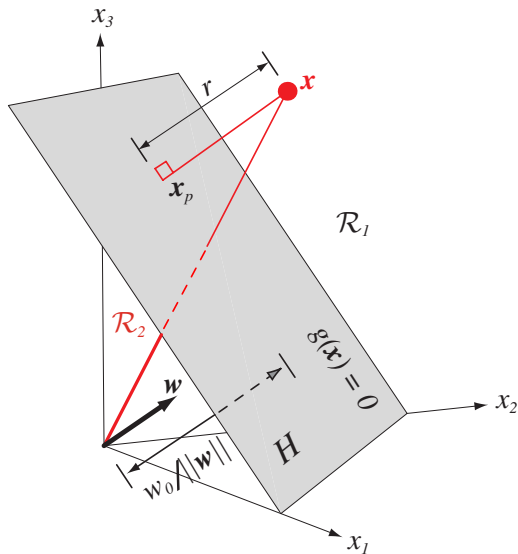


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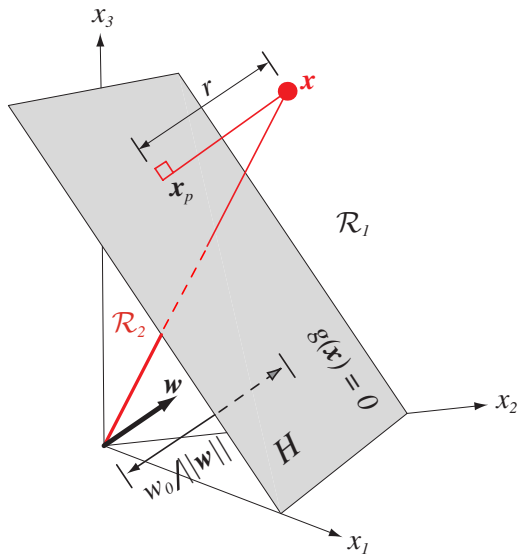


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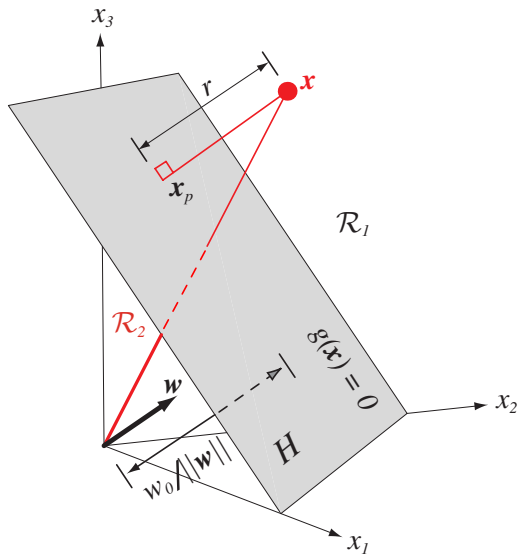


Figure from [2]

Multiclass case

each class has its own discriminant function

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

and the classification s^* is along the max.

Two classes set-up

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

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

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

for all \mathbf{x}'

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

drop the dashes to avoid notation clutter.

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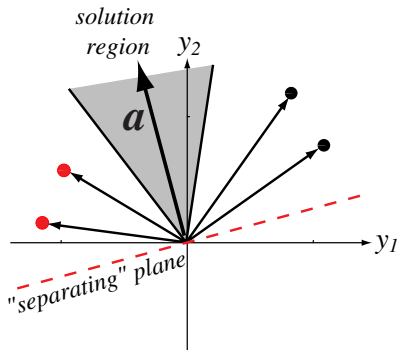
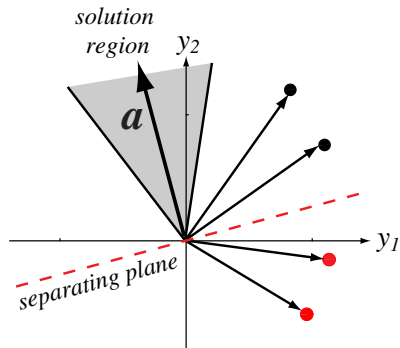
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Solution (graphically)



notation in the book: substitute $\mathbf{a} \leftarrow \mathbf{w}$ and $y_1, y_2 \leftarrow x_1, x_2$

Figure from [2]

Dif

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 \mathbf{w} - Perceptron criterion

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

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

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

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

(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} .

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

Learning \mathbf{w} - Perceptron criterion

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

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

(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} .

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

(Batch) Perceptron algorithm

Initialize \mathbf{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 \mathbf{w}

Fixed-increment single-sample Perceptron

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

Initialize \mathbf{w}

$k \leftarrow 0$

repeat

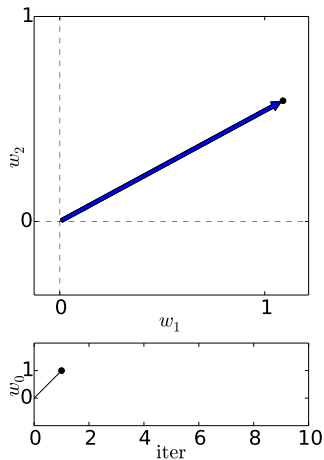
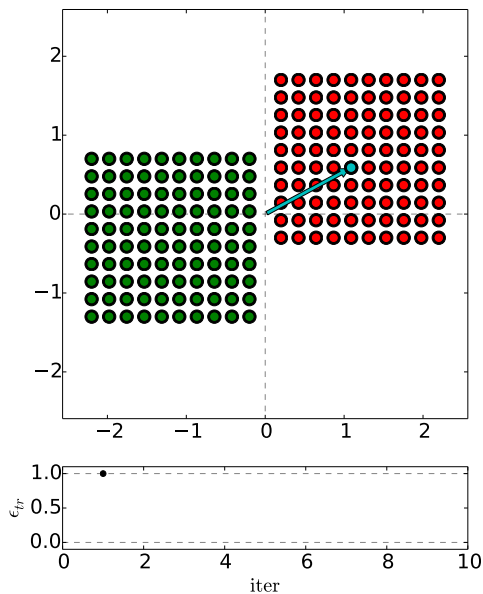
$k \leftarrow (k + 1) \bmod n$

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

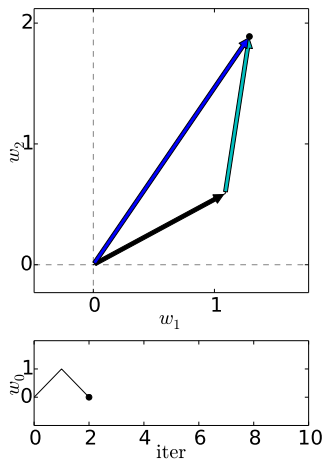
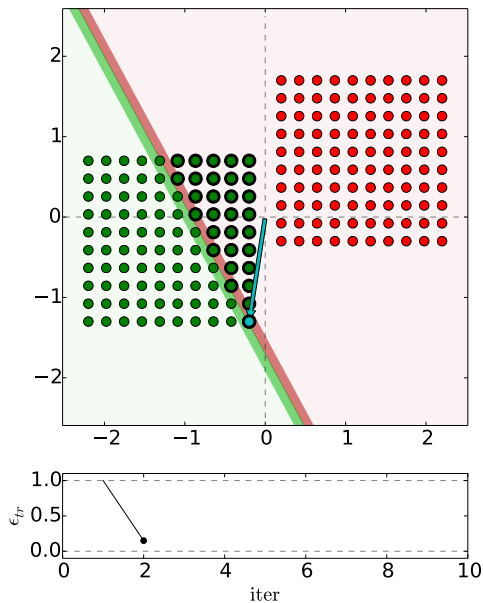
until all \mathbf{x} correctly classified

return \mathbf{w}

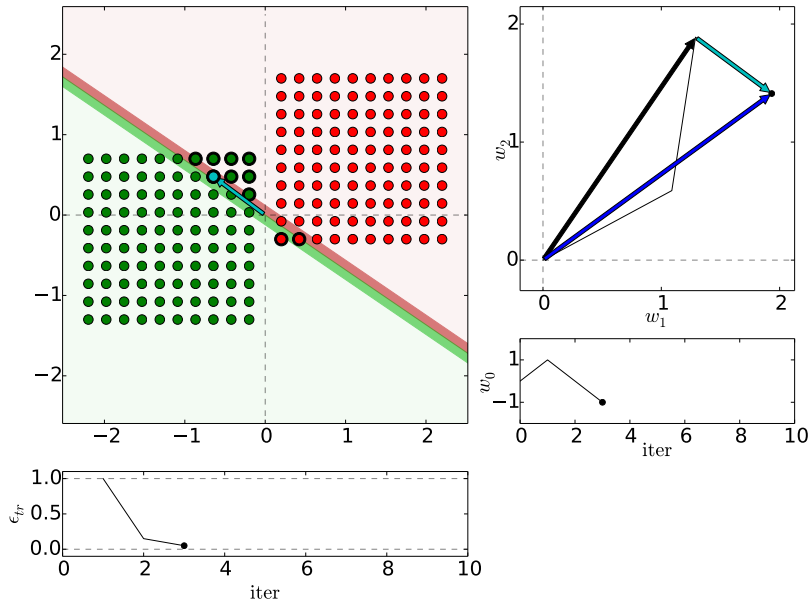
Perceptron iterations/loops



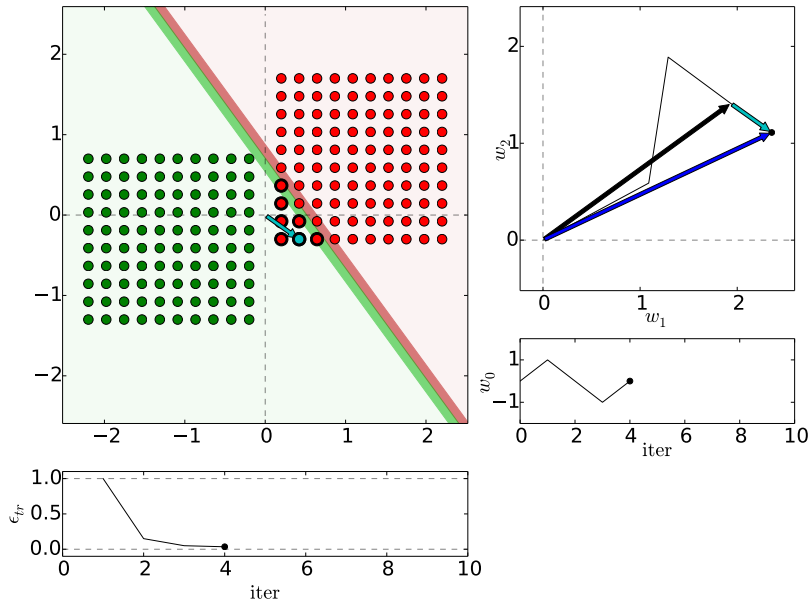
Perceptron iterations/loops



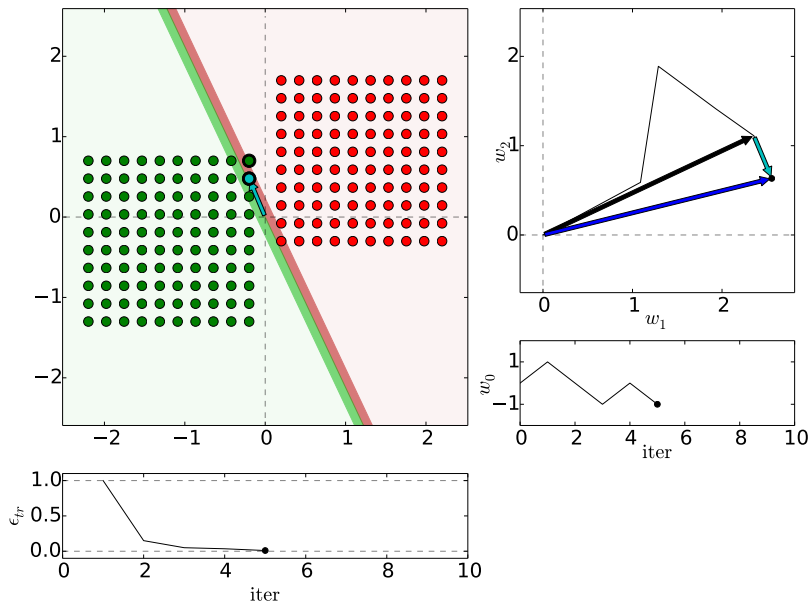
Perceptron iterations/loops



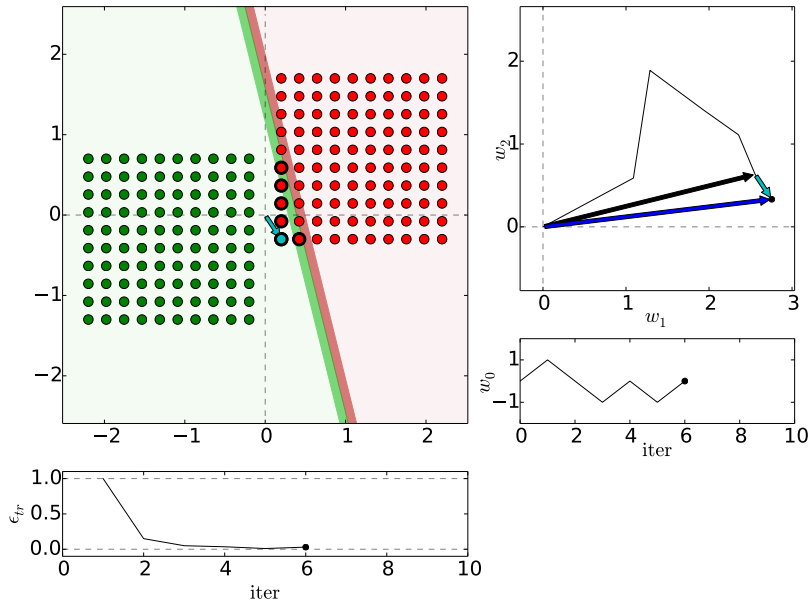
Perceptron iterations/loops



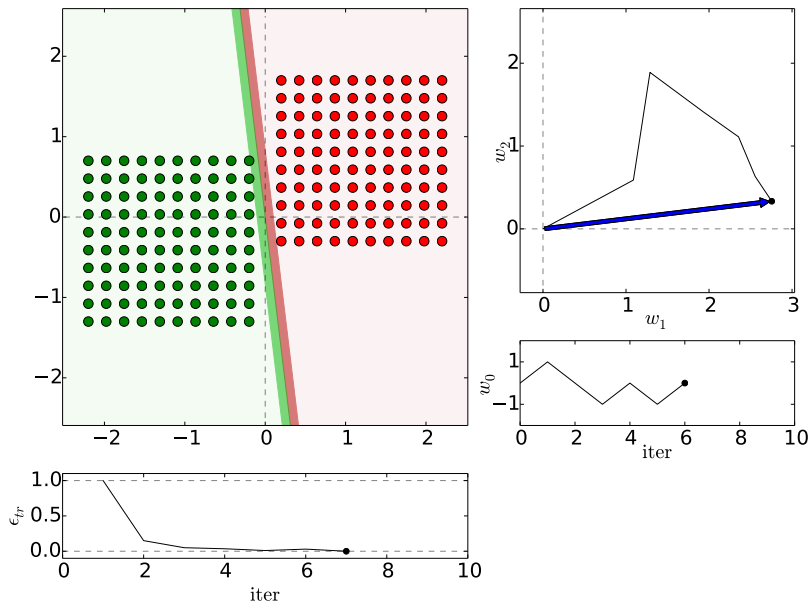
Perceptron iterations/loops



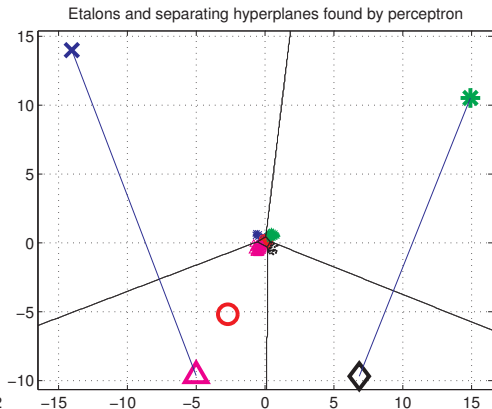
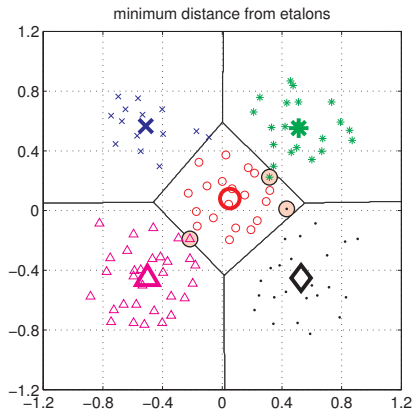
Perceptron iterations/loops



Perceptron iterations/loops

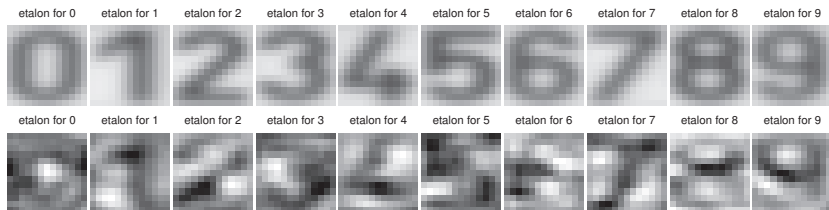


Etalons: means vs. found by perceptron



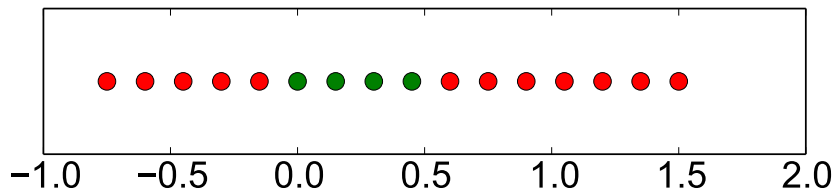
Figures from [5]

Digit recognition - etalons means vs. perceptron



Figures from [5]

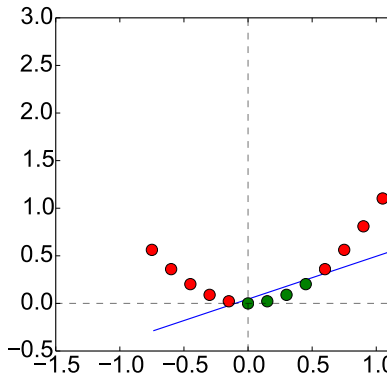
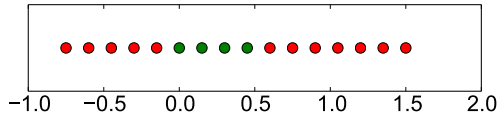
What if not lin separable?



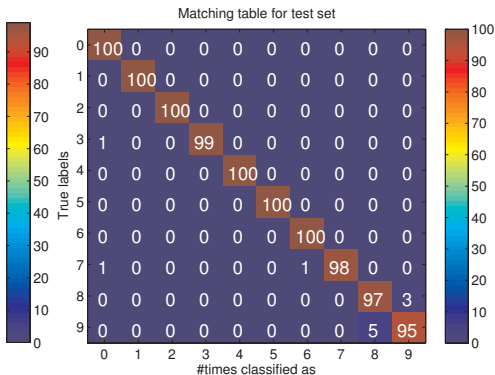
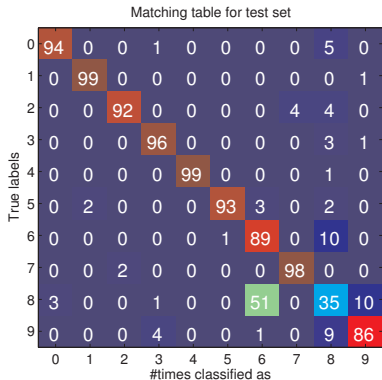
Dimension lifting

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

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

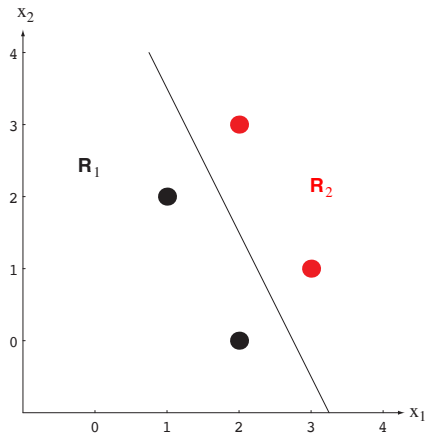


Performance comparison, parameters fixed



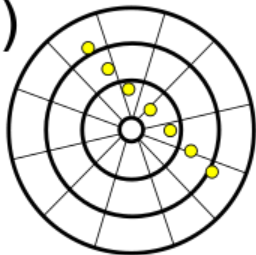
LSQ approach to linear classification

$$X\mathbf{w} = \mathbf{b}$$

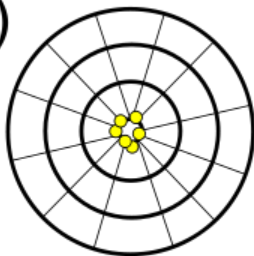


Accuracy vs precision

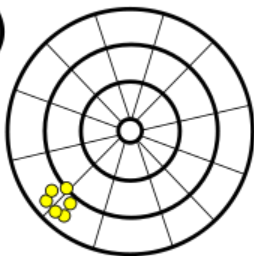
(a)



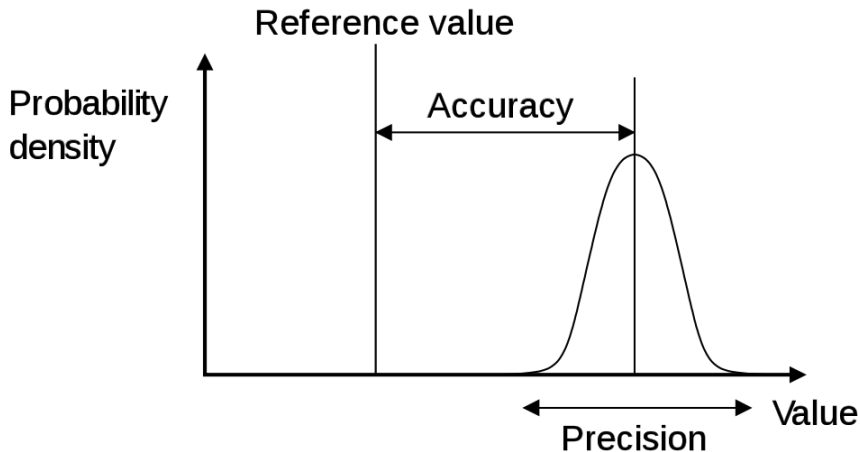
(b)



(c)



Accuracy vs precision



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

References I

Further reading: Chapter 18 of [4], or chapter 4 of [1], or chapter 5 of [2]. Many Matlab figures created with the help of [3]. You may also play with demo functions from [5].

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