# $k-$NN and Linear Classifiers, Learning

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thanks to Matěj Hoffmann, Daniel Novák, Filip Železný, Ondřej Drbohlav

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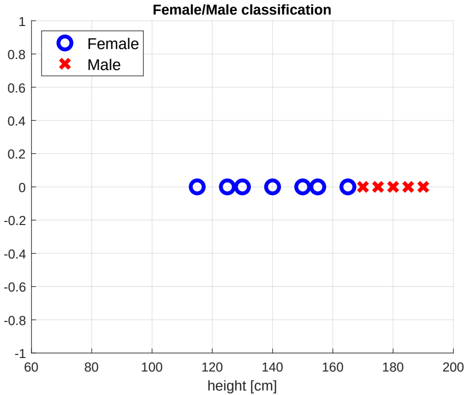
May 10, 2022

# Example: Female/Male classification based on height

Training (multi)set $\mathcal{T} = \{(x_i, s_i)\}_{i=1}^{N}$, $x_i \in \mathbb{N}$, $s_i \in \mathbb{S} = \{F, M\}$

| $i$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Height $x_i$ | 115 | 125 | 130 | 140 | 150 | 155 | 165 | 170 | 175 | 180 | 185 | 190 |
| Gender $s_i$ | F | F | F | F | F | F | F | M | M | M | M | M |



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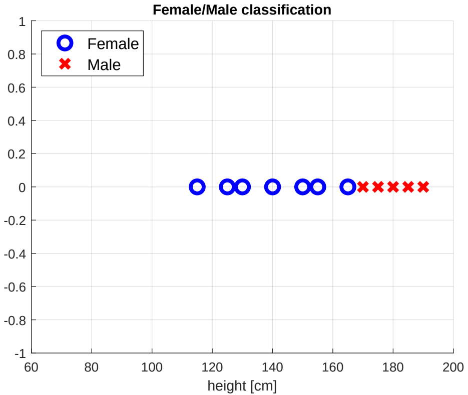


A new point to clasify: $x_Q = 166$

Which class does $x_Q$ belong to? $d_Q = ?$

# Example: F/M classification – $k$-NN

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Query: $x_Q = 166$

1-NN: $d_Q =?$

**A** $d_Q = F$

**B** $d_Q = M$

**C** Both classes equally likely

**D** 1-NN will not provide any decision

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3-NN: $d_Q = ?$

- **A** $d_Q = F$
- **B** $d_Q = M$
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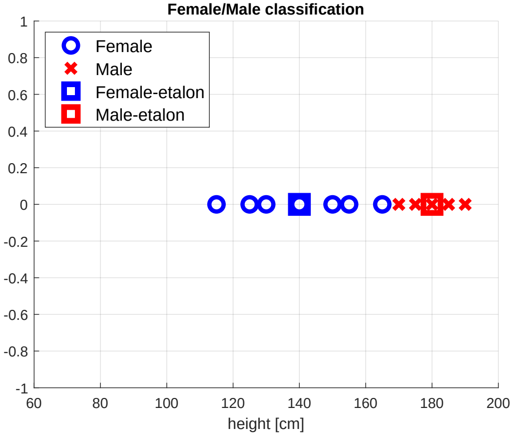
How can we reduce the complexity of $k$-NN method?

# Example: F/M classification – Etalons

Represent each class by a single example called *etalon*! (Or by a very small number of etalons.)




$$e_F = \text{ave}(\{x_i : s_i = F\}) = 140$$
$$e_M = \text{ave}(\{x_i : s_i = M\}) = 180$$

Based on etalons: $d_Q = ?$

- **A** $d_Q = F$
- **B** $d_Q = M$
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- **D** Cannot provide any decision

Classify as $d_Q = \text{argmin}_{s \in S} \text{dist}(x_Q, e_s)$

What type of function is $\text{dist}(x_Q, e_s)$?

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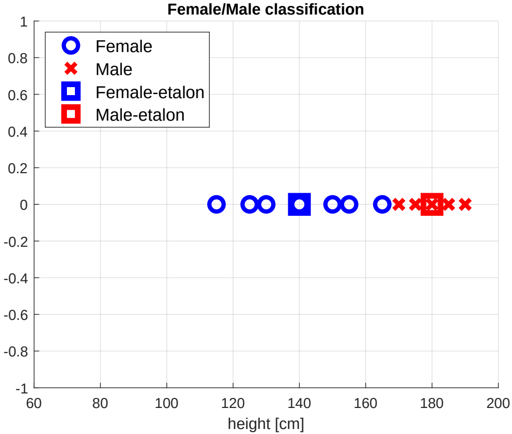


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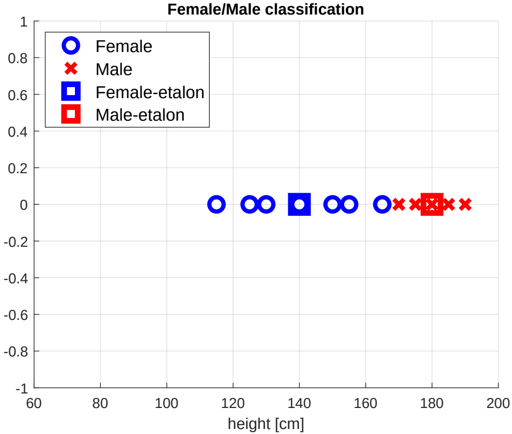


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# Linear discriminant functions

Assuming $\operatorname{dist}(x, e) = (x - e)^2$, then

$$\operatorname*{argmin}_{s \in S} \operatorname{dist}(x, e_s) = \operatorname*{argmin}_{s \in S} (x - e_s)^2 = \operatorname*{argmin}_{s \in S} (\underbrace{x^2}_{\text{const.}} - 2e_s x + e_s^2) =$$

$$= \operatorname*{argmin}_{s \in S} (-2e_s x + e_s^2) = \operatorname*{argmax}_{s \in S} (\underbrace{e_s x - \frac{1}{2} e_s^2}_{\text{linear function of } x})$$

Multiclass classification: each class $s$ has a linear discriminant function $f_s(x) = a_s x + b_s$ and

$$\delta(x) = \operatorname*{argmax}_{s \in S} f_s(x)$$

Binary classification: a single linear discriminant function $g(x)$ is sufficient and

$$\delta(x) = \begin{cases} s_1 & \text{if } g(x) \geq 0 \\ s_2 & \text{if } g(x) < 0 \end{cases}$$

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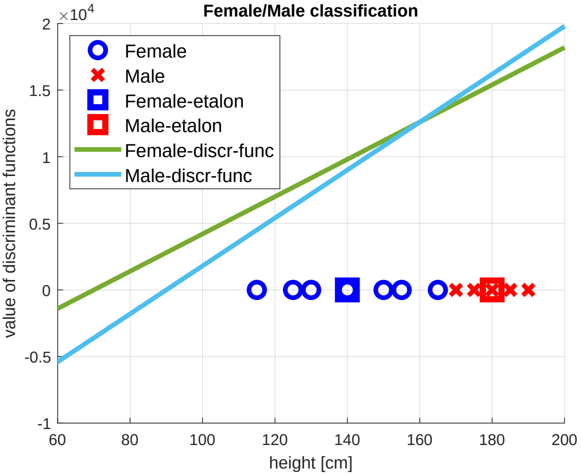


Discriminant functions for 2 classes:

$$f_F(x) = a_F x + b_F = $$
$$= e_F x - \frac{1}{2} e_F^2 = 140x - 9800$$
$$f_M(x) = a_M x + b_M = $$
$$= e_M x - \frac{1}{2} e_M^2 = 180x - 16200$$

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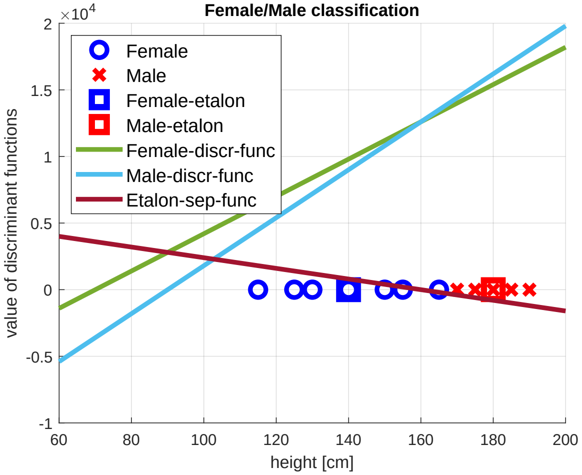


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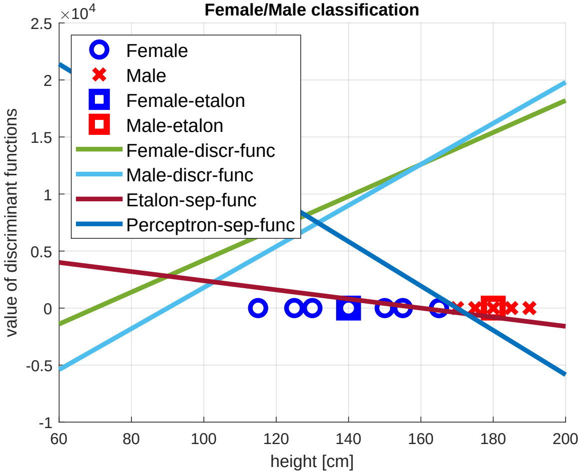
&= e_M x - \frac{1}{2} e_M^2 = 180x - 16200
\end{aligned}
$$

A single discriminant function separating 2 classes:

$$
\begin{aligned}
g(x) &= f_F(x) - f_M(x) = \\
&= -40x + 6400
\end{aligned}
$$

# Example: F/M – Can we do better?



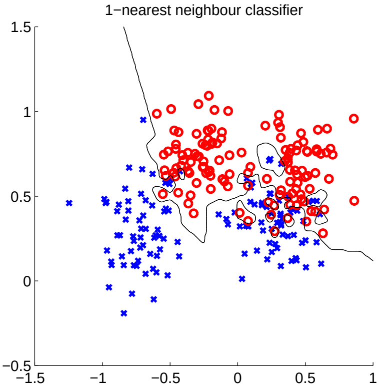

Etalon-based linear classifier makes some errors.

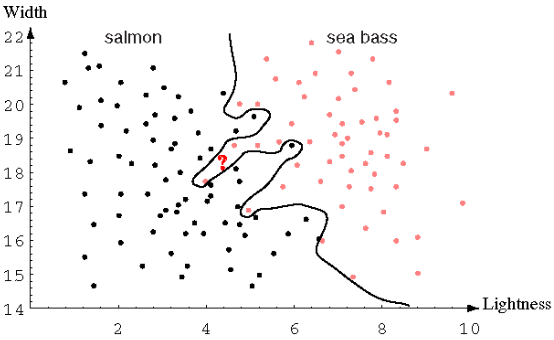
A perceptron algorithm may be used to find a zero-error classifier (if one exists).

# $K$-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.



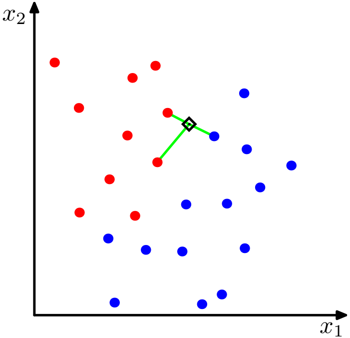



# $K-$ Nearest Neighbor and Bayes $j^* = \text{argmax}_j P(s_j|\vec{x})$

Assume data:

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

We want to classify $\vec{x}$. Draw a sphere centered at $\vec{x}$ containing $K$ points irrespective of class. $V$ is the volume of this sphere. $P(s_j|\vec{x}) = ?$




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

$K_j$ is the number of points of class $s_j$ among the $K$ nearest neighbors.

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

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

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

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

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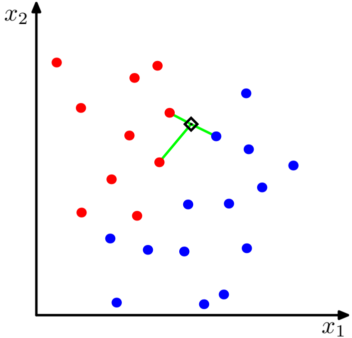


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# $k-NN$ for non-parametric density estimation

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

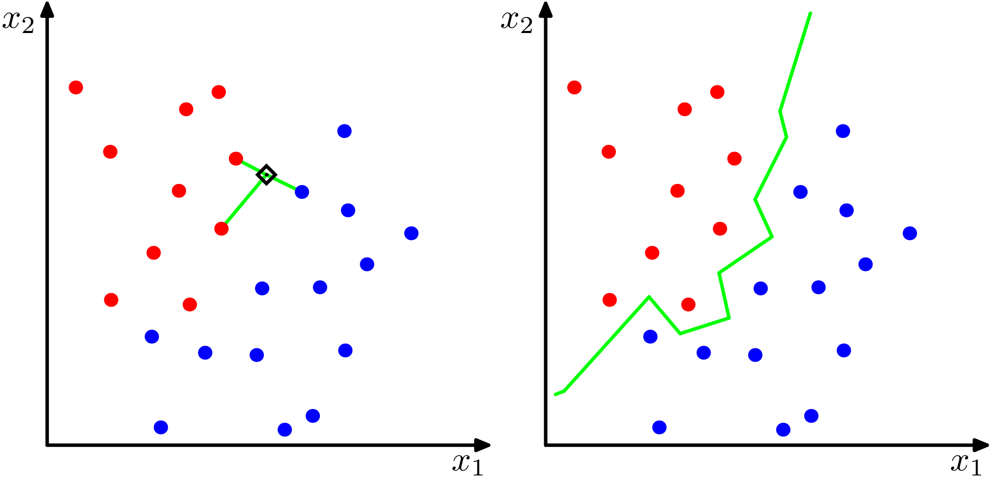
$$V = V_d R_k^d(\vec{x})$$

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

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

volume of $d-$dimensional unit sphere, $\Gamma$ denotes gamma function. $V_1 = 2, V_2 = \pi, V_3 = \frac{4}{3}\pi$

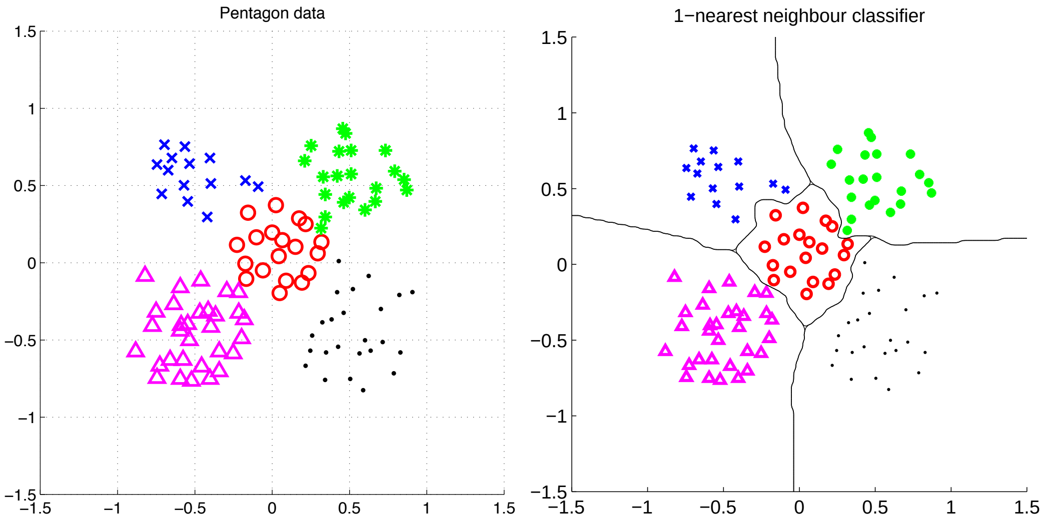
# NN classification example




(a) (b) [1]

[1] Figs from [1]

# NN classification example



# What is *nearest*? Metrics for NN classification ...

A function $D$ which is

- nonnegative,
- reflexive,
- symmetrical,
- satisfying triangle inequality:

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

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

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

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

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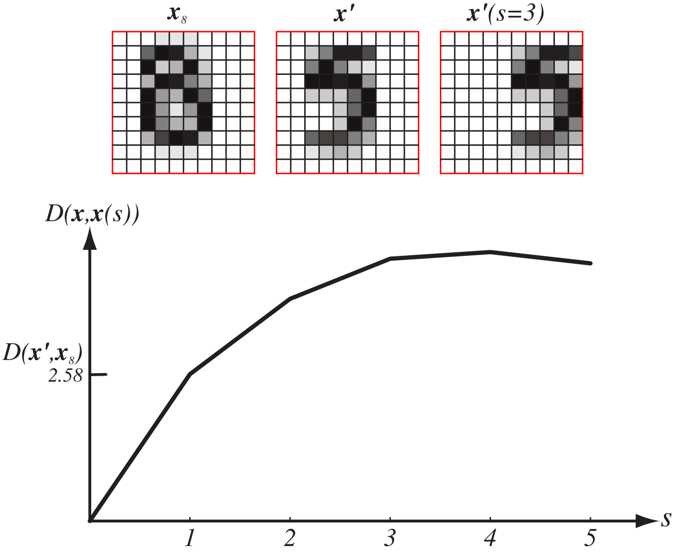
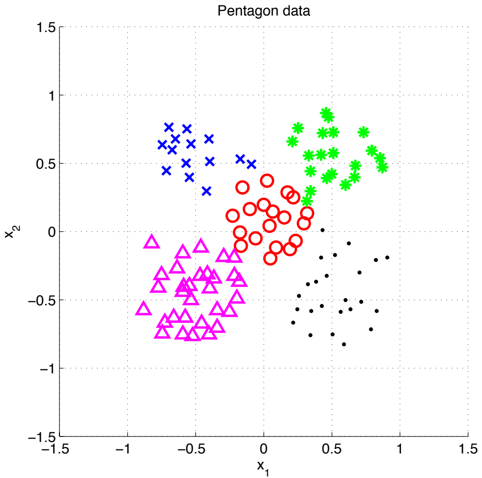
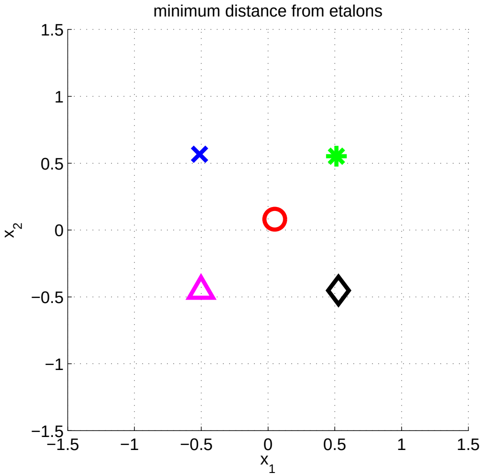



Invariance to geometrical transformations? (figure from [3])

# Etalon based classification

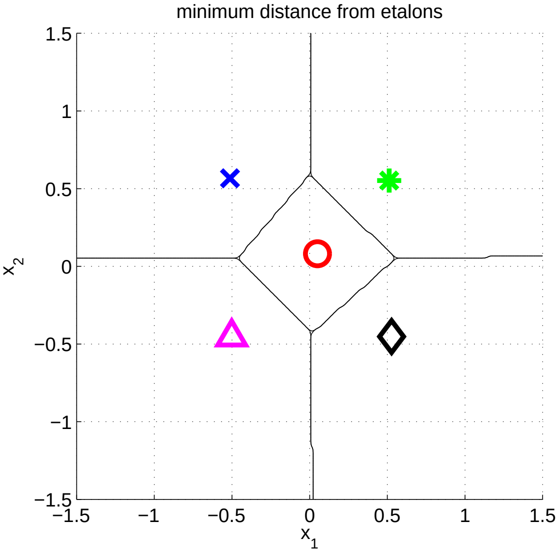



Represent $\vec{x}$ by etalon , $\vec{e}_s$ per each class $s \in S$.

# Separate etalons

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

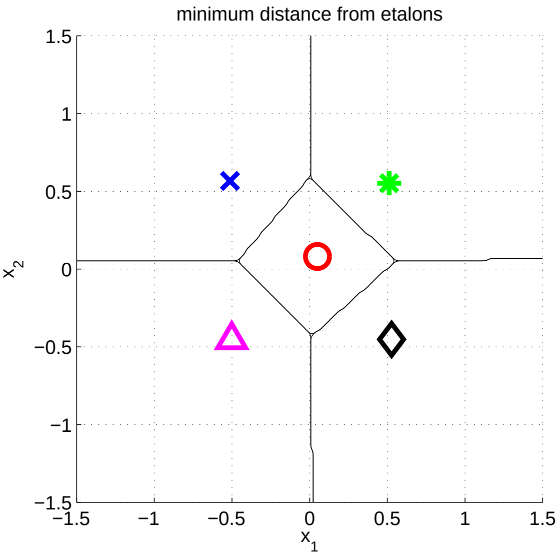


# What etalons?

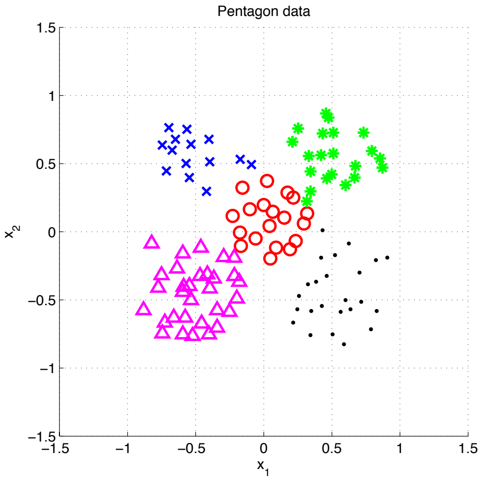
If $\mathcal{N}(\vec{x}|\vec{\mu},\Sigma)$; all classes same covariance matrices, then

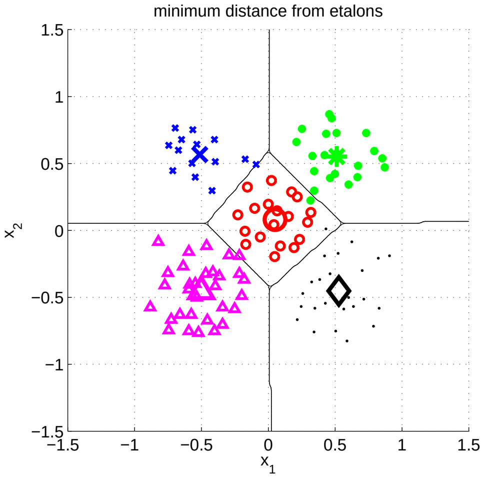
$$\vec{e}_s \stackrel{\text{def}}{=} \vec{\mu}_s = \frac{1}{|\mathcal{X}^s|}\sum_{i\in\mathcal{X}^s} \vec{x}_i^s$$

and separating hyperplanes halve distances between pairs.

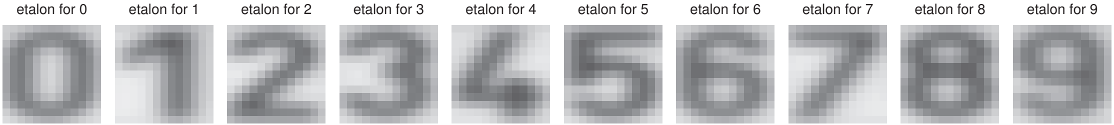


# Etalon based classification, $\vec{e}_s = \vec{\mu}_s$



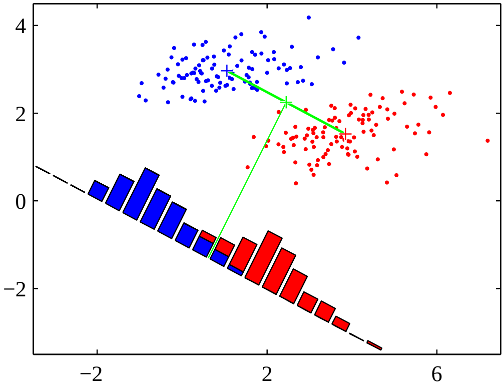



# Digit recognition - etalons $\vec{e}_s = \vec{\mu}_s$




Figures from [6].

# 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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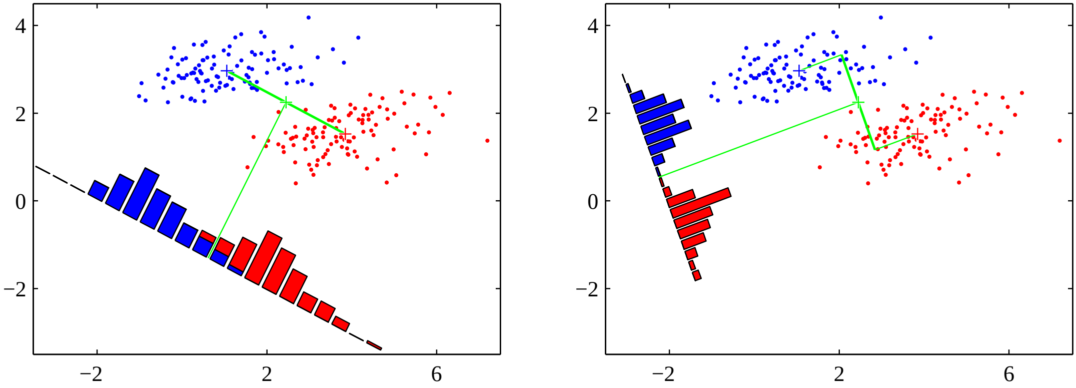


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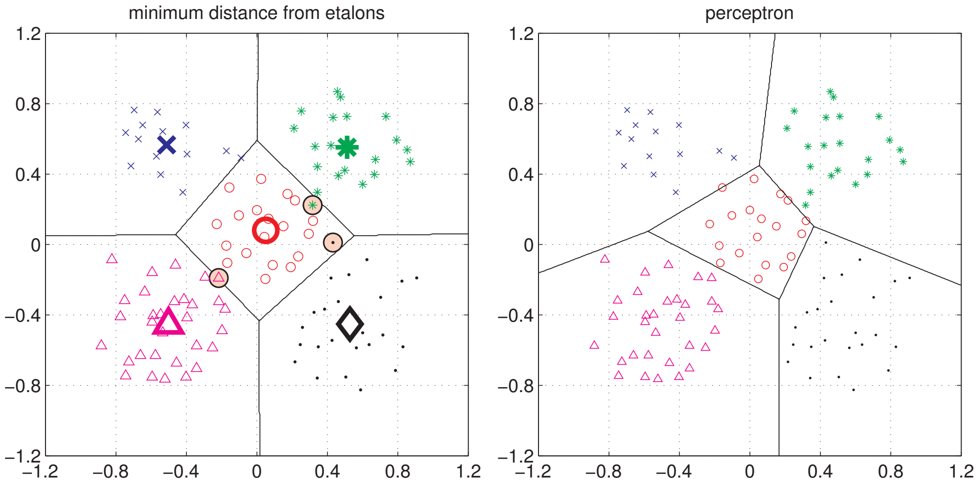



Figures from [6]

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

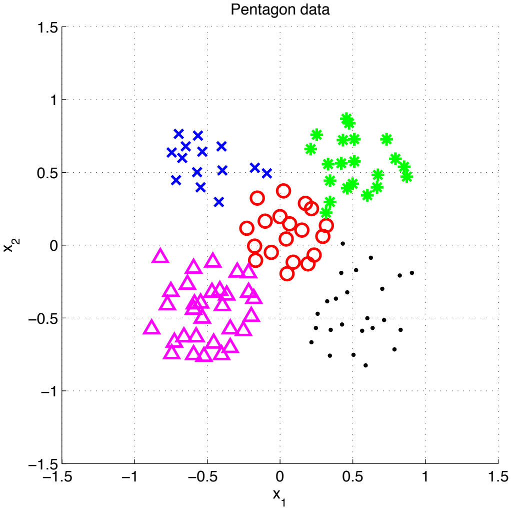
$$s^* = \operatorname*{argmax}_{s \in \mathcal{S}} f(\vec{x}, s)$$

Bayes:

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

Discriminant function:

$$f(\vec{x}, s) = g_s(\vec{x}) = P(\vec{x} \mid s)P(s)$$



# Etalon classifier – Linear classifier

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

Linear function (plus offset)

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

# (1) Linear discriminant function – a 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 [3]

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

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

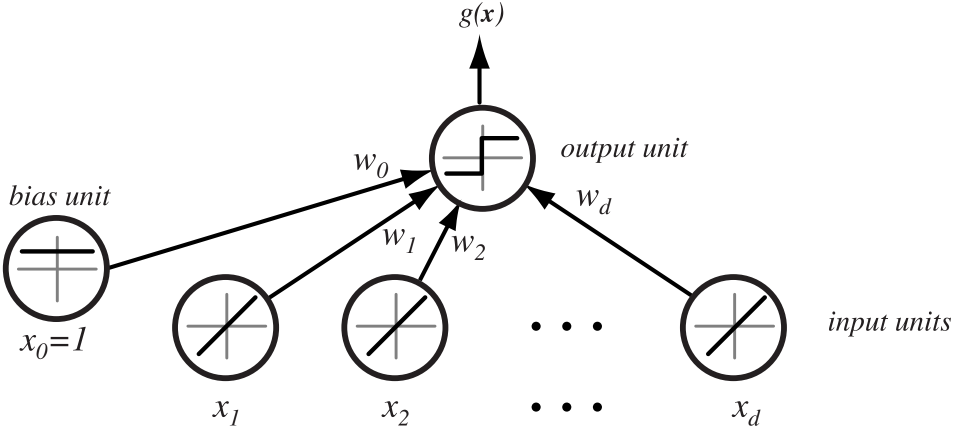


Figure from [3]

# 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:

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

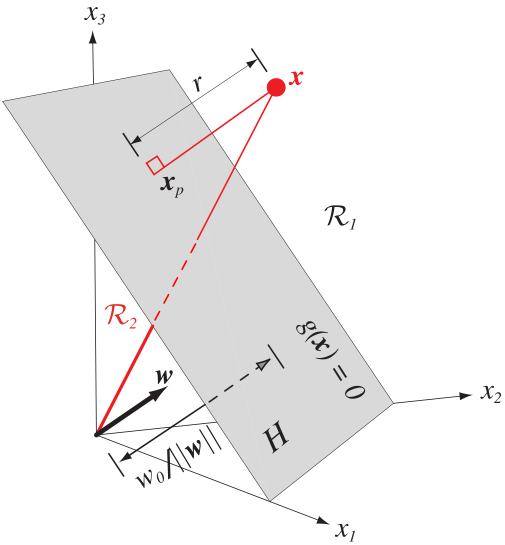


Figure from [3]

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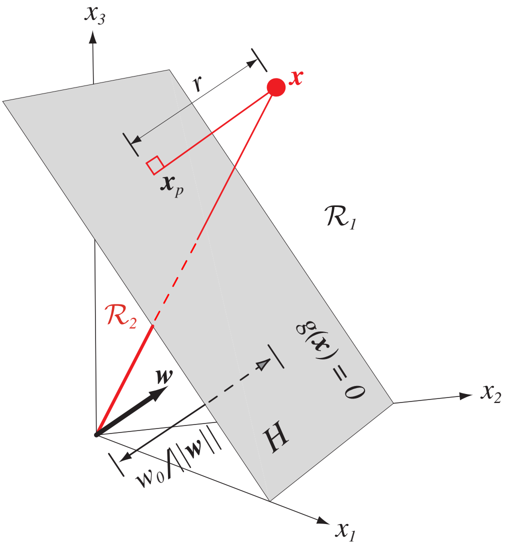


Figure from [3]

# Separating hyperplane from $g_1$ and $g_2$

Etalon classifier, etalons $\vec{\mu}_1, \vec{\mu}_2$

$$
\begin{aligned}
g_1(\vec{x}) &= \vec{\mu}_1^\top \vec{x} - \frac{1}{2}\vec{\mu}_1^\top \vec{\mu}_1 \\
g_2(\vec{x}) &= \vec{\mu}_2^\top \vec{x} - \frac{1}{2}\vec{\mu}_2^\top \vec{\mu}_2
\end{aligned}
$$

Separating hyperplane:

$$g_1(\vec{x}) = g_2(\vec{x})$$

$$(\vec{\mu}_1 - \vec{\mu}_2)^\top \vec{x} = \frac{1}{2}(\vec{\mu}_1^\top \vec{\mu}_1 - \vec{\mu}_2^\top \vec{\mu}_2)$$

# Two classes set-up

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

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

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

for all $\mathbf{x}'$

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

drop the dashes to avoid notation clutter.

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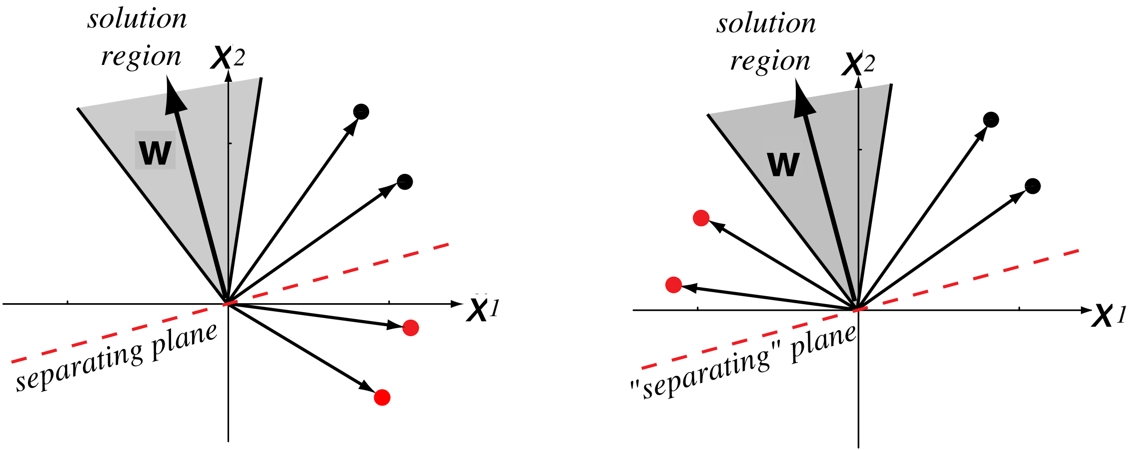
for all $\mathbf{x}'$

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

drop the dashes to avoid notation clutter.

# Solution (graphically)




Four training samples. Left: original, Right: class $s_2$ transformed (sign changed).
Figure from [3] (notation changed)

# Learning $\mathbf{w}$, gradient descent

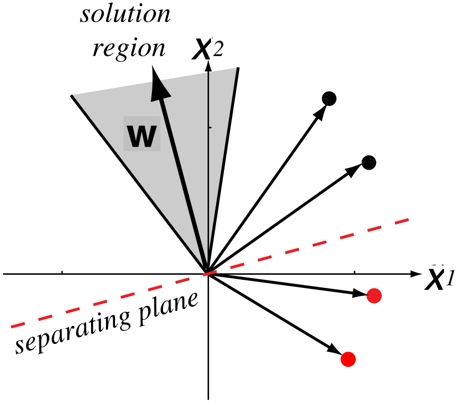
A criterion to be minimized $J(\mathbf{w})$; assume to be known

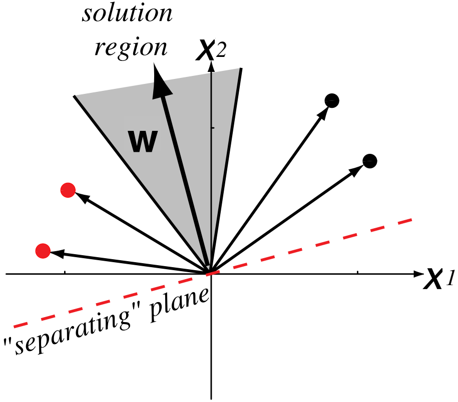
Initialize $\mathbf{w}$, threshold $\theta$, learning rate $\alpha$
$k \leftarrow 0$
**repeat**
  $k \leftarrow k + 1$
  $\mathbf{w} \leftarrow \mathbf{w} - \alpha(k)\nabla J(\mathbf{w})$
**until** $|\alpha(k)\nabla J(\mathbf{w})| < \theta$
return $\mathbf{w}$

# Learning $\mathbf{w}$ – Perceptron criterion

**Goal**: Find a weight vector $\mathbf{w} \in \Re^{D+1}$ (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:

# Learning **w** – Perceptron criterion

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

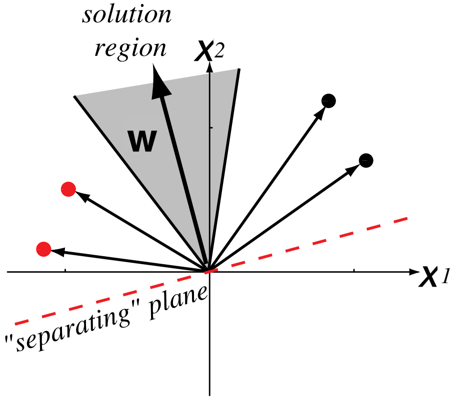
$$\mathbf{w}^\top \mathbf{x}_j > 0 \qquad (\forall j \in \{1, 2, ..., m\})$$

(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 $\mathbf{x}$.

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



# (Batch) Perceptron algorithm

Initialize **w**, threshold $\theta$, learning rate $\alpha$
$k \leftarrow 0$
**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**

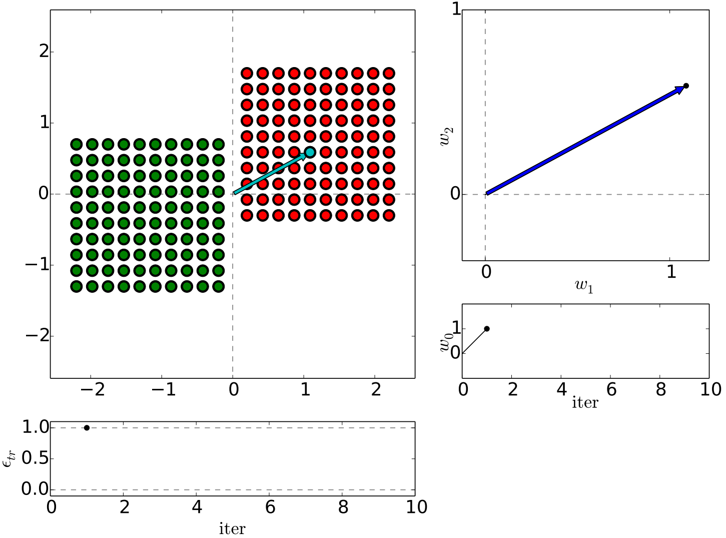
$k \leftarrow (k+1) \bmod n$

**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




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

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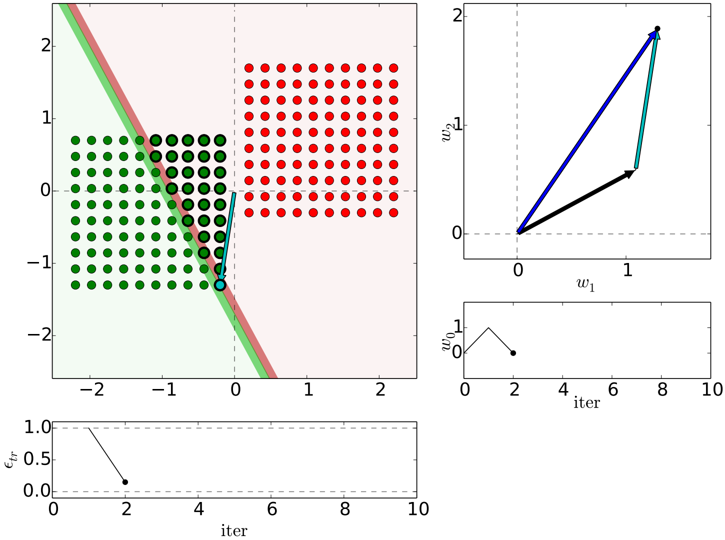
    $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{x}^k$
**until** all $\mathbf{x}$ correctly classified
return $\mathbf{w}$

(Dark) Blue is $\mathbf{w}$ after update step. Reds are $+$, Greens $-$.

# Perceptron iterations/loops

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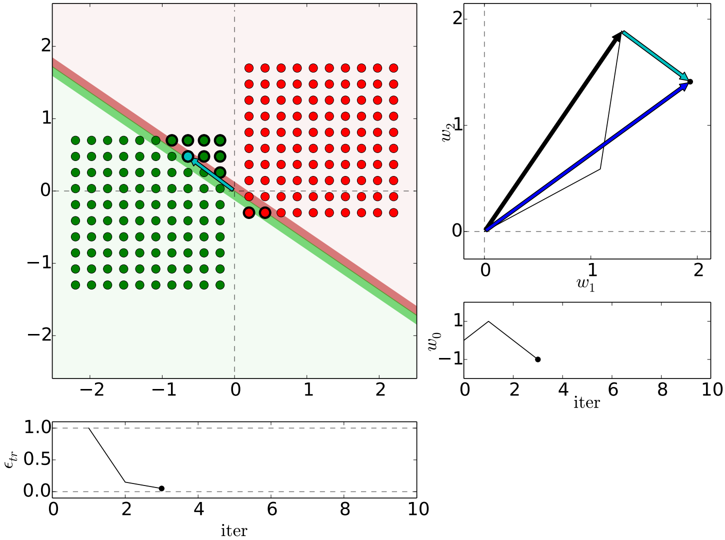


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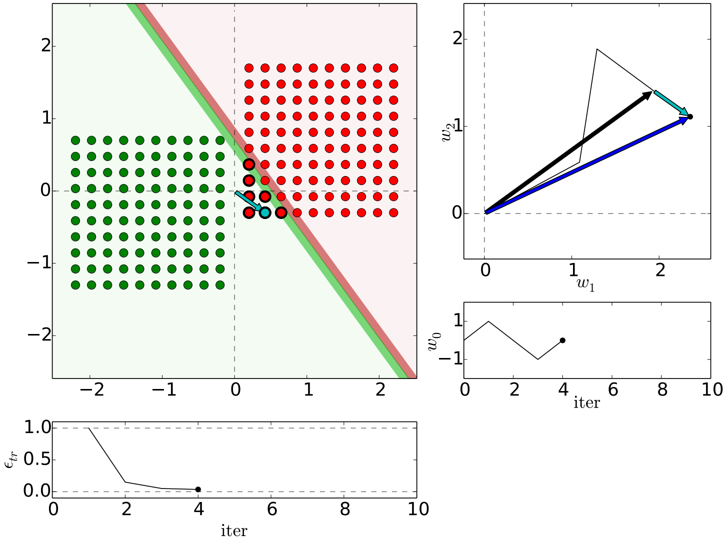
(Dark) Blue is **w** after update step. Reds are $+$, Greens $-$.

# Perceptron iterations/loops

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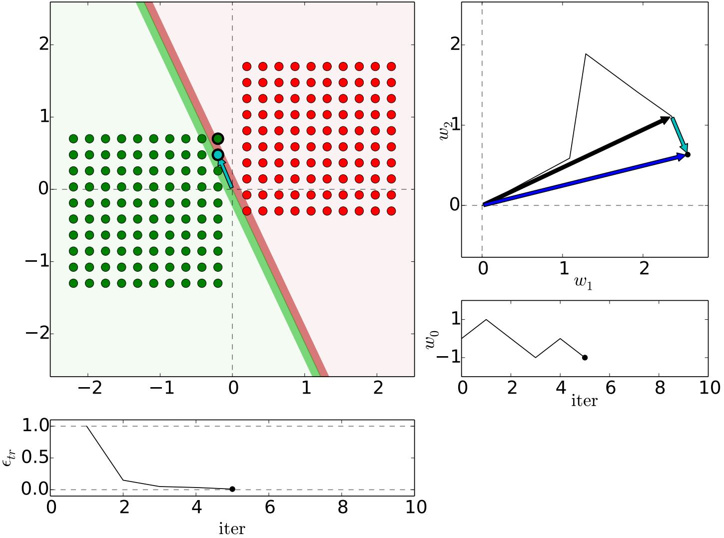


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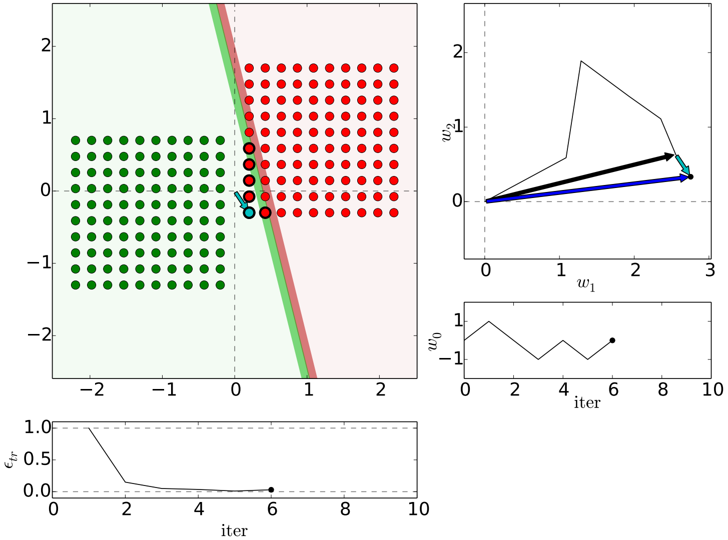
# Perceptron iterations/loops

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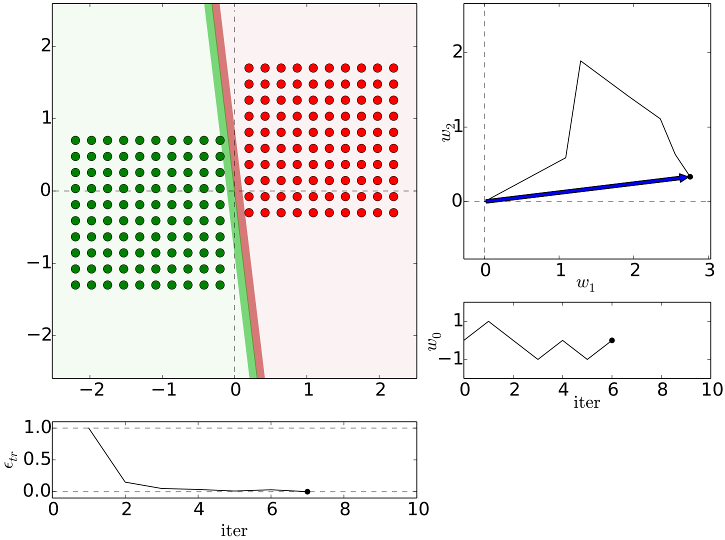
# Perceptron iterations/loops

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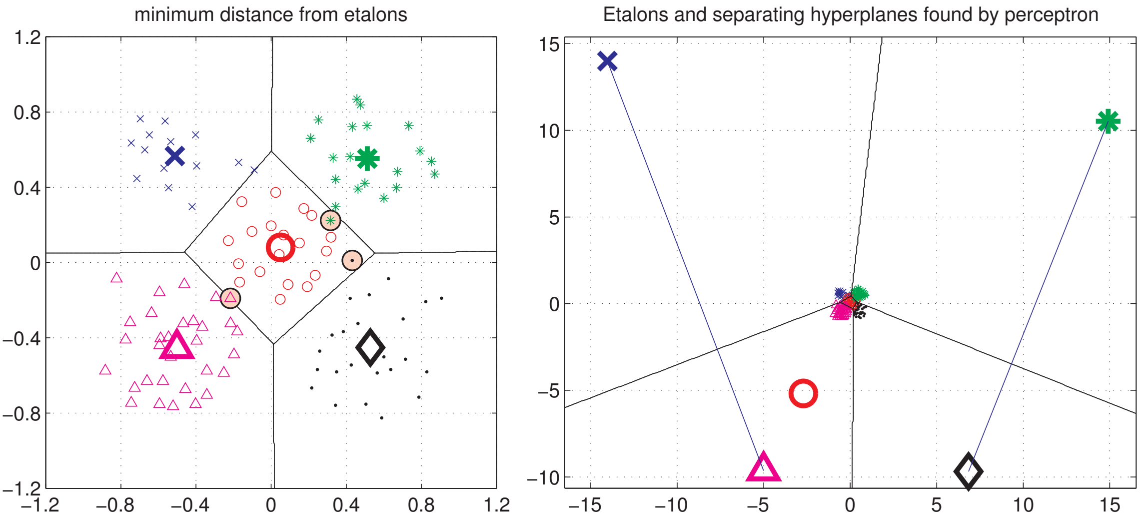
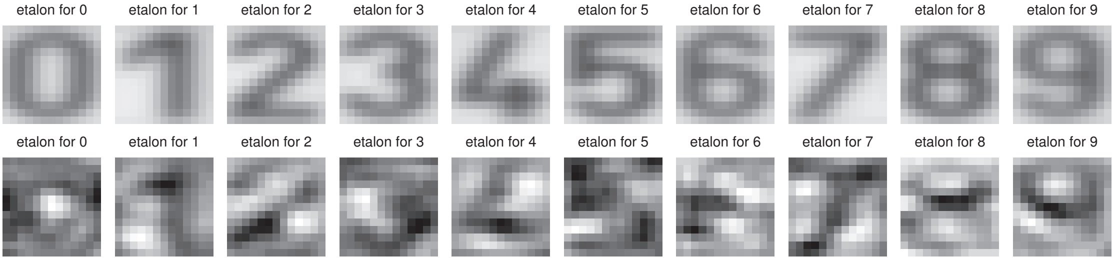
# Etalons: means vs. found by perceptron



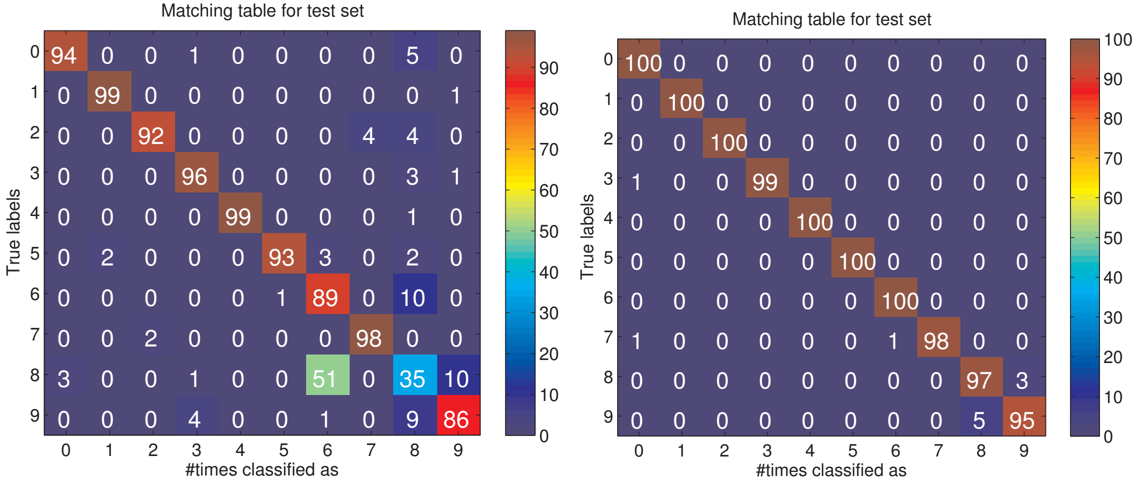

Figures from [6]

# Digit recognition – etalons means vs. perceptron



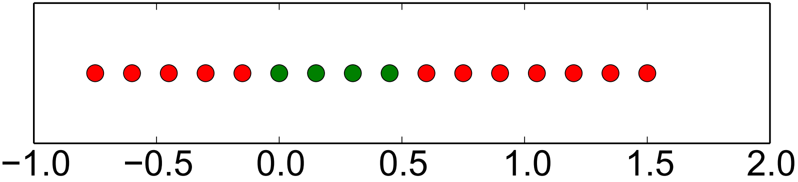

Figures from [6].

# Digit recognition – Performance comparison, parameters fixed




Left: Etalon classification. Right: perceptron classification.

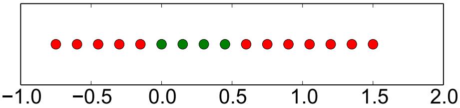
# What if data is not linearly separable?

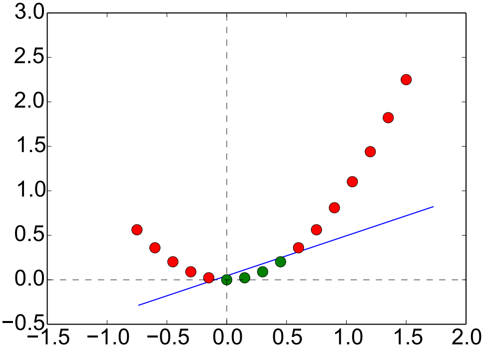



**Dimension lifting**

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

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



# Learning and decision

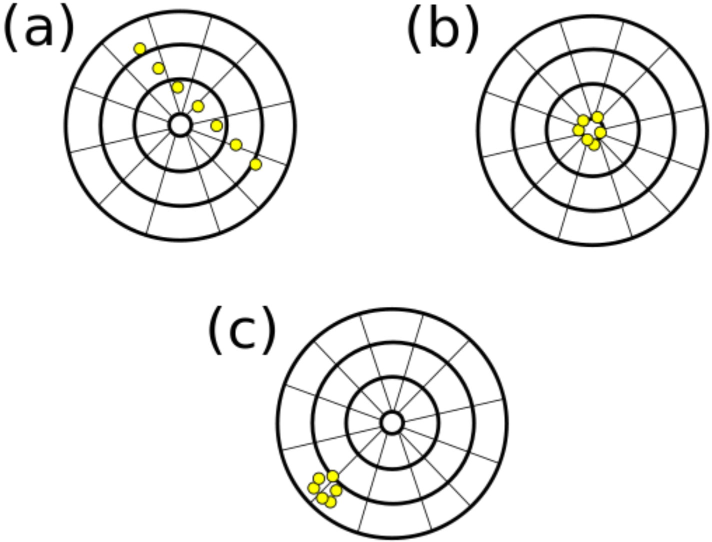
**Learning** stage - learning models/function/parameters from data.

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

What to learn?

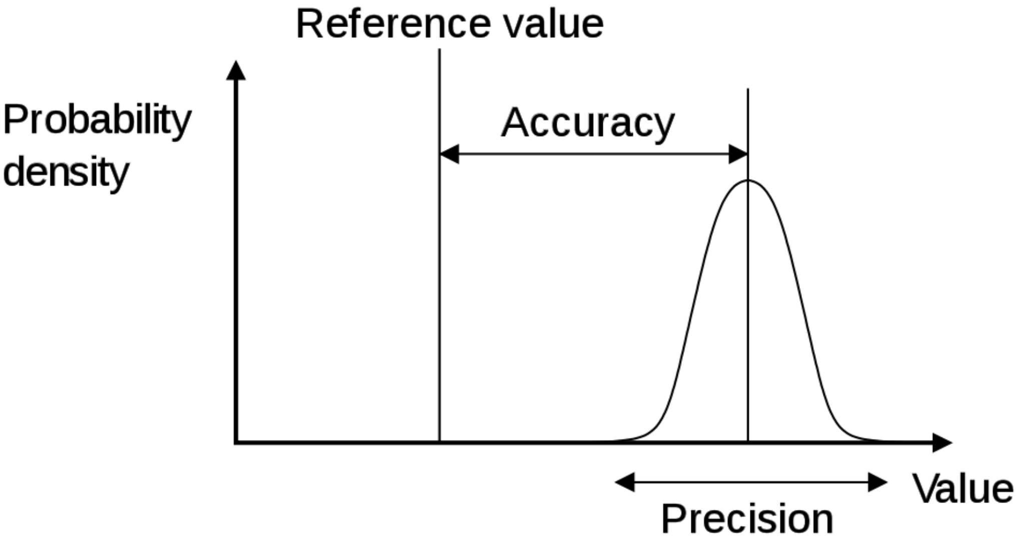
- **Generative model** : Learn $P(\vec{x}, s)$. Decide by computing $P(s|\vec{x})$.
- **Discriminative model** : Learn $P(s|\vec{x})$.
- **Discriminant function** : Learn $g(\vec{x})$ which maps $\vec{x}$ directly into class labels.

# 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 18 of [5], or chapter 4 of [1], or chapter 5 of [3]. Many figures created with the help of [4]. You may also play with demo functions from [6].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[6] Tomáš Svoboda, Jan Kybic, and Hlaváč Václav.
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