$k-$NN and Linear Classifiers, Learning

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thanks to Daniel Novák and Filip Železný, Ondřej Drbohlav

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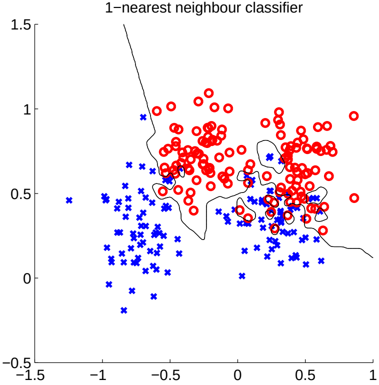
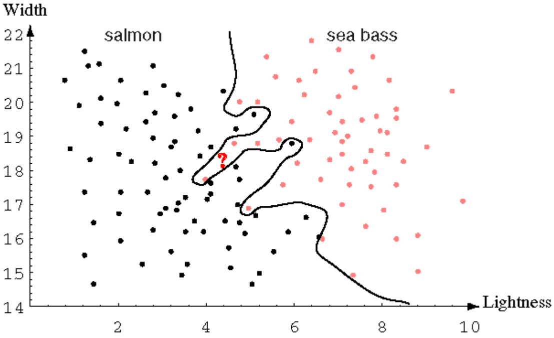
K-Nearest neighbors classification

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 $j^* = \text{argmax}_j \, P(s_j|\vec{x})$

Assume data:

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

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

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

$$\begin{aligned} P(s_j) &= \frac{N_j}{N} \\ P(\vec{x}) &= \frac{K}{NV} \\ P(\vec{x}|s_j) &= \frac{K_j}{N_j V} \\ P(s_j|\vec{x}) &= \frac{P(\vec{x}|s_j)P(s_j)}{P(\vec{x})} = \frac{K_j}{K} \end{aligned}$$

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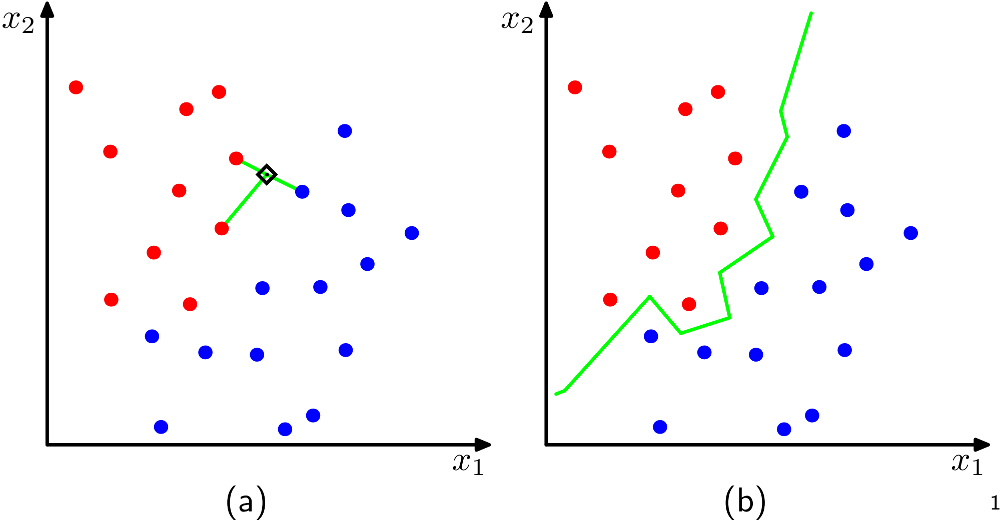
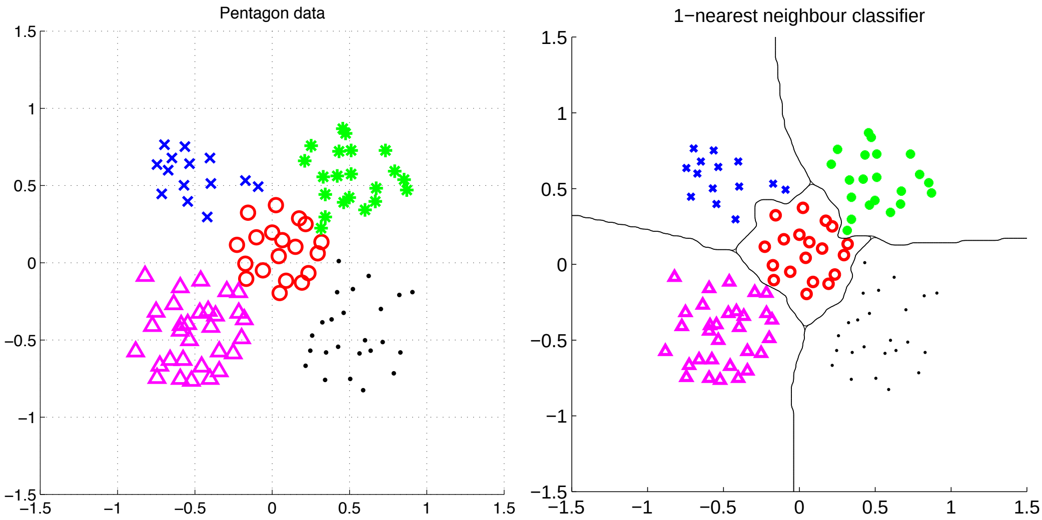
NN classification example



[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:

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

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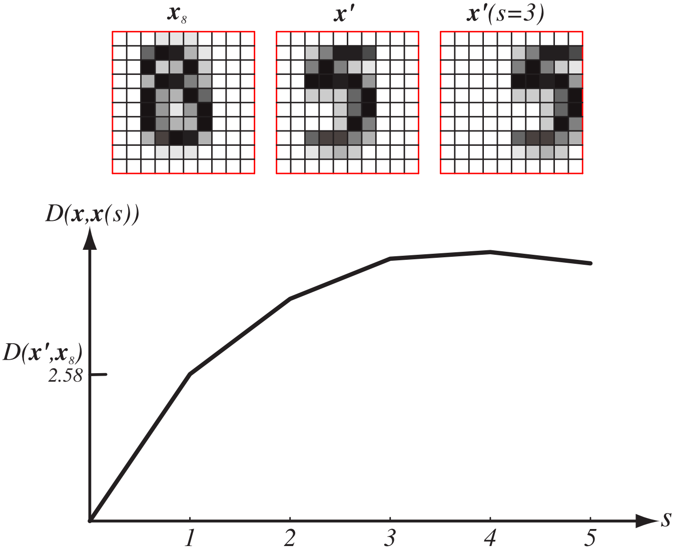
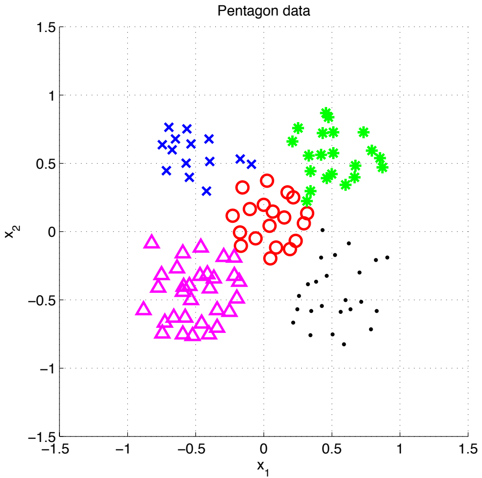
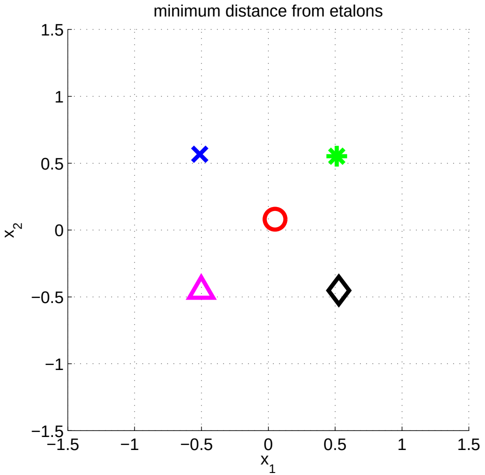


Invariance to geometrical transformations? (figure from [2])

Etalon based classification

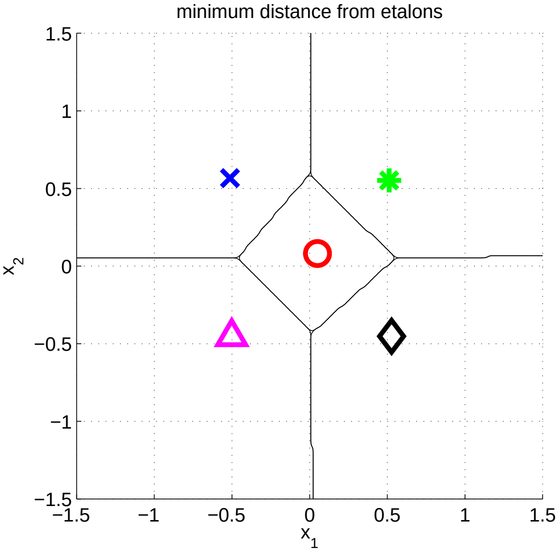




Represent $\vec{x}$ by etalon , $\vec{e}_s$ per each class $s \in S$

Separate etalons

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

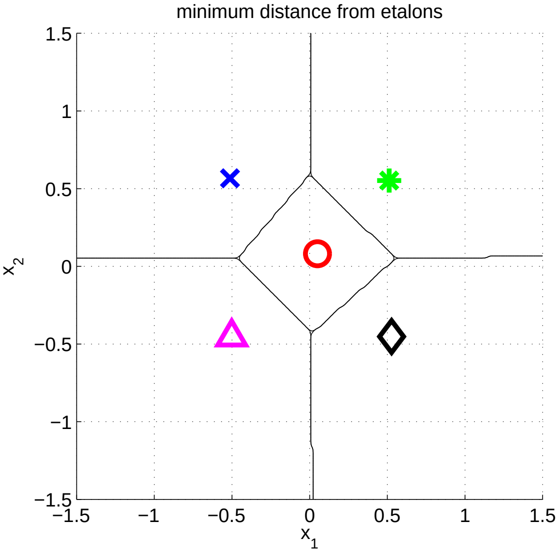


What etalons?

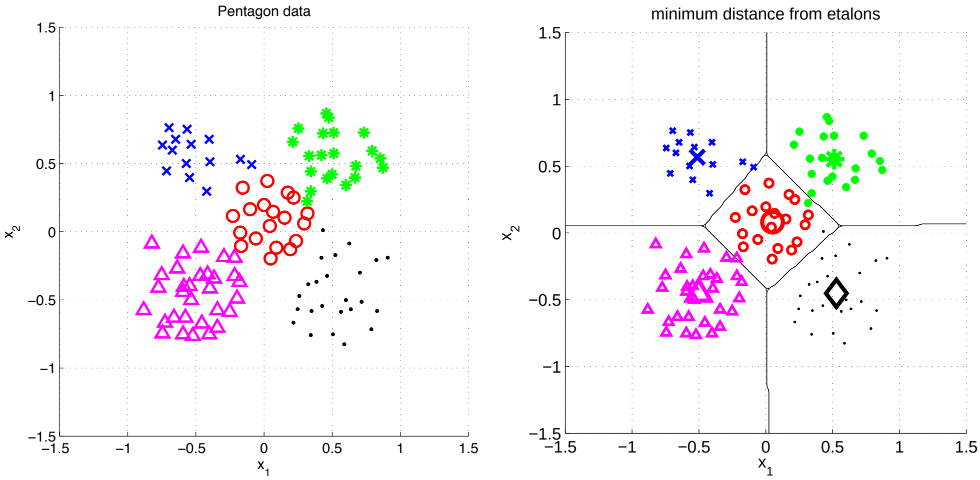
If $\mathcal{N}(\vec{x}|\vec{\mu},\Sigma)$; all classes same covariance matrices, then

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

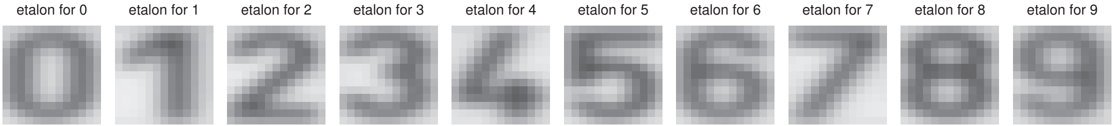
and separating hyperplanes halve distances between pairs.



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

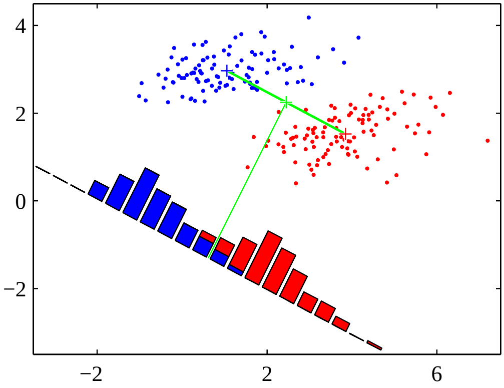


Digit recognition - etalons $\vec{e}_s = \vec{\mu}_s$



Figures from [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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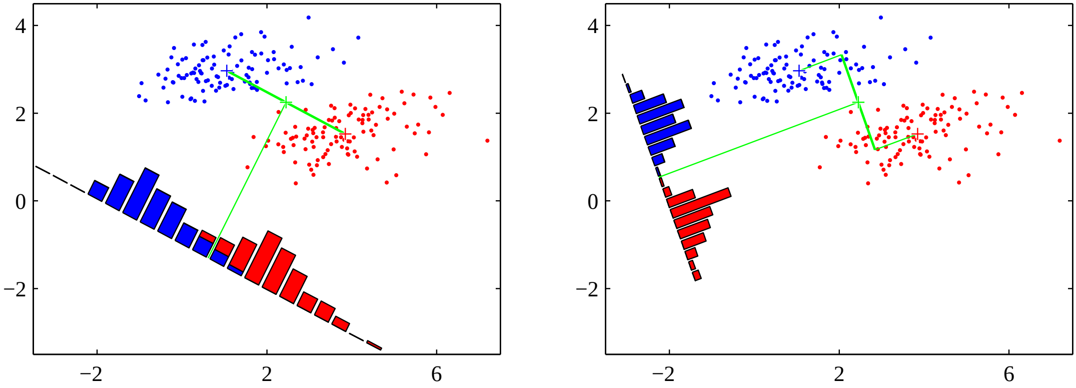

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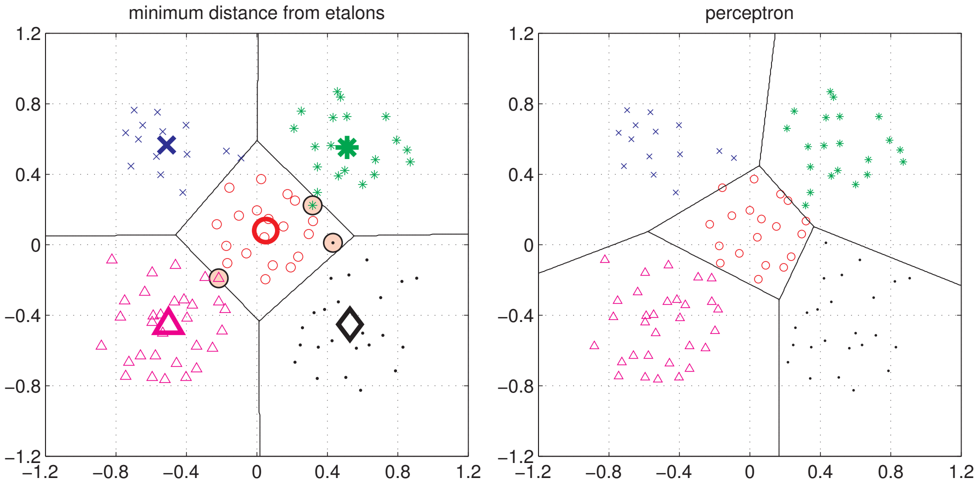

Figures from [5]

Etalon classifier – Linear classifier

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

Linear function (plus offset)

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

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.

(1) 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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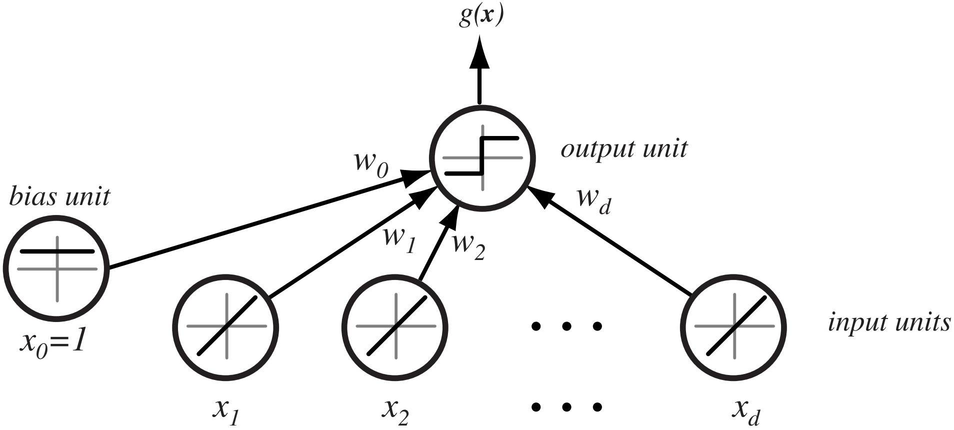


Figure from [2]

Separating hyperplane

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

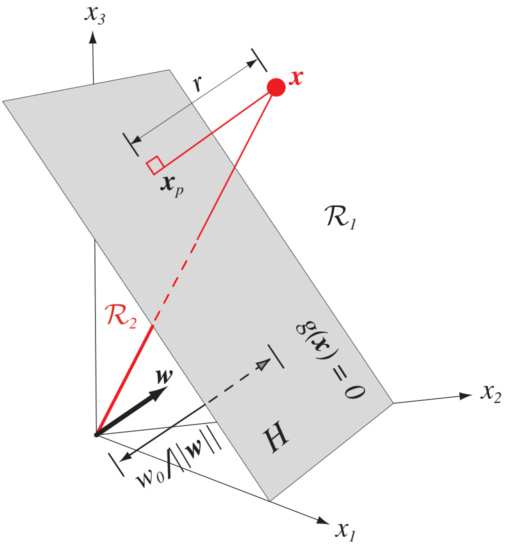
$$\mathbf{w}^\top (\mathbf{x}_1 - \mathbf{x}_2) = 0$$

$g(\mathbf{x})$ 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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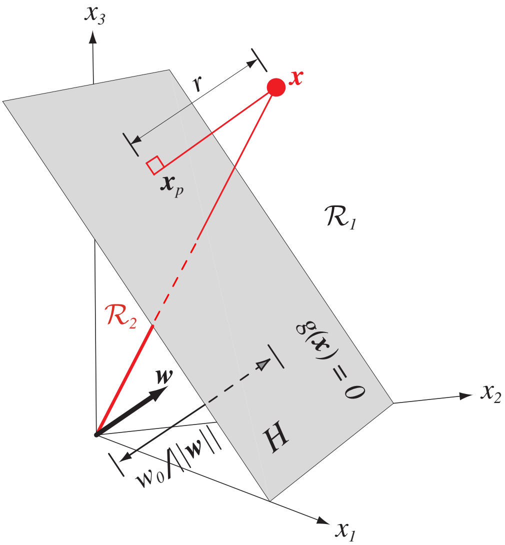

Figure from [2]

Separating hyperplane from g_1 and g_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)

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

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

for all $\mathbf{x}'$

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

drop the dashes to avoid notation clutter.

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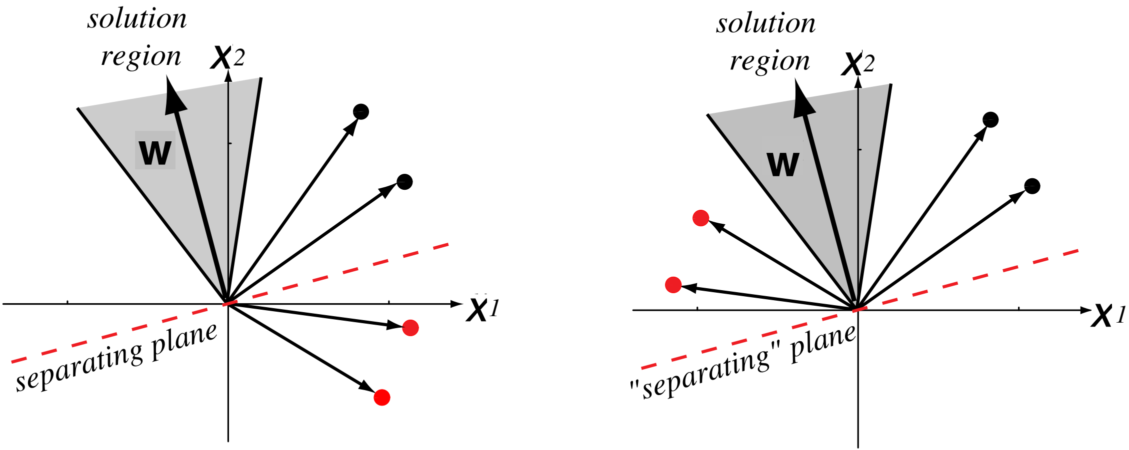
Solution (graphically)



Four training samples. Left: orginal, Right: sign corrected

Figure from [2] (notation changed)

Learning $\mathbf{w}$, gradient descent

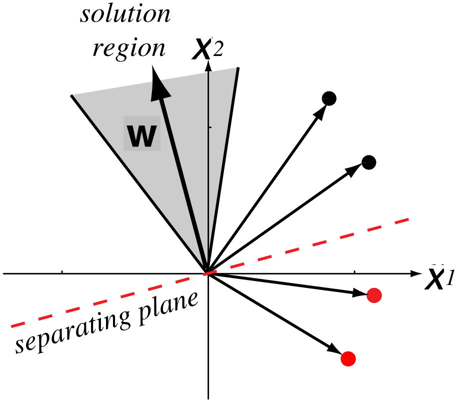
A criterion to be minimized $J(\mathbf{w})$; assume to be known

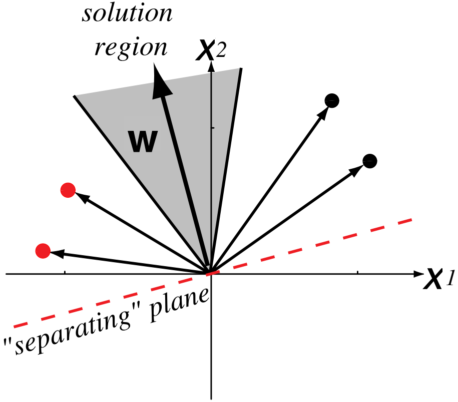
Initialize $\mathbf{w}$, threshold θ, learning rate α
$k \leftarrow 0$
repeat
  $k \leftarrow k + 1$
  $\mathbf{w} \leftarrow \mathbf{w} - \alpha(k)\nabla J(\mathbf{w})$
until $|\alpha(k)\nabla J(\mathbf{w})| < \theta$
return $\mathbf{w}$

Learning **w** - Perceptron criterion

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

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





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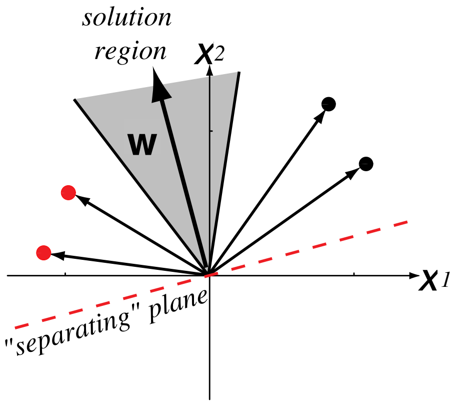
(Perceptron) Criterion to be minimized:

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

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

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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

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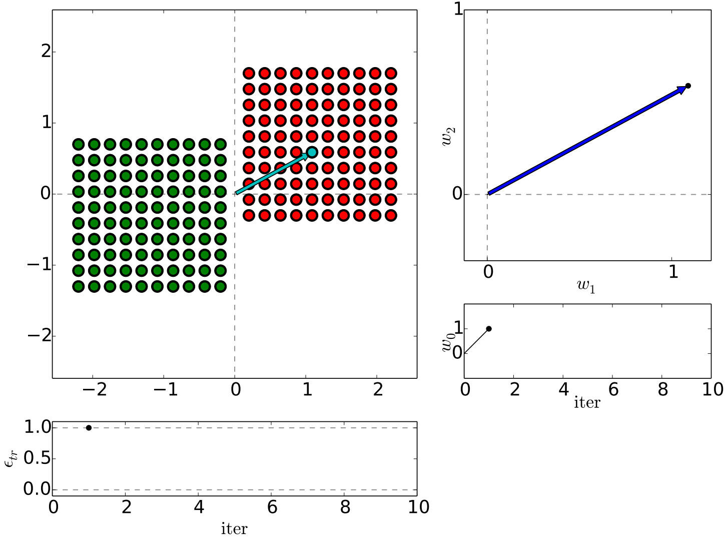
until all $\mathbf{x}$ correctly classified
return $\mathbf{w}$

Perceptron iterations/loops



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

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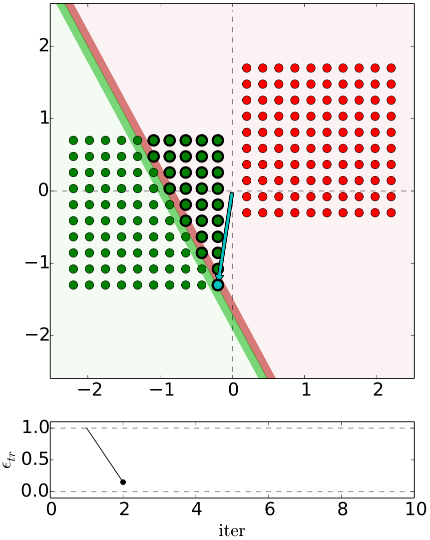

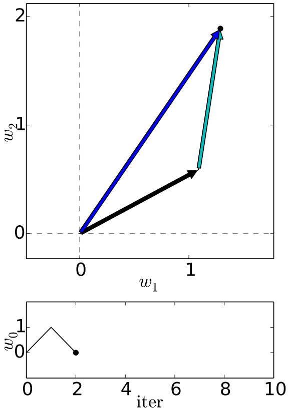

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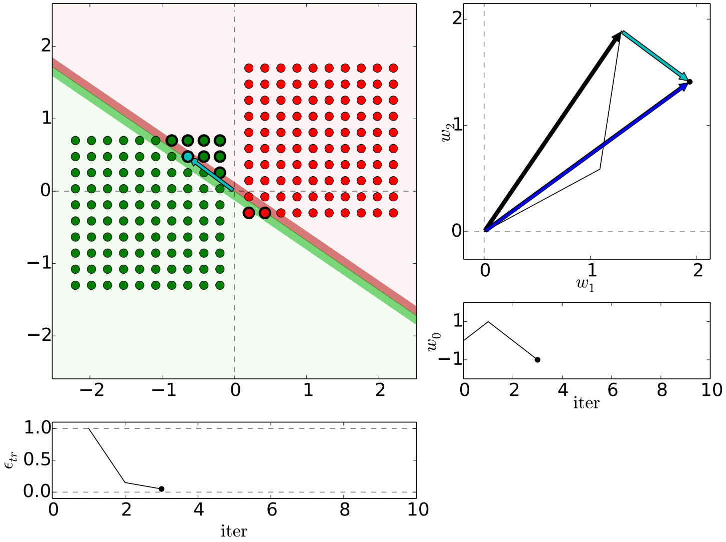

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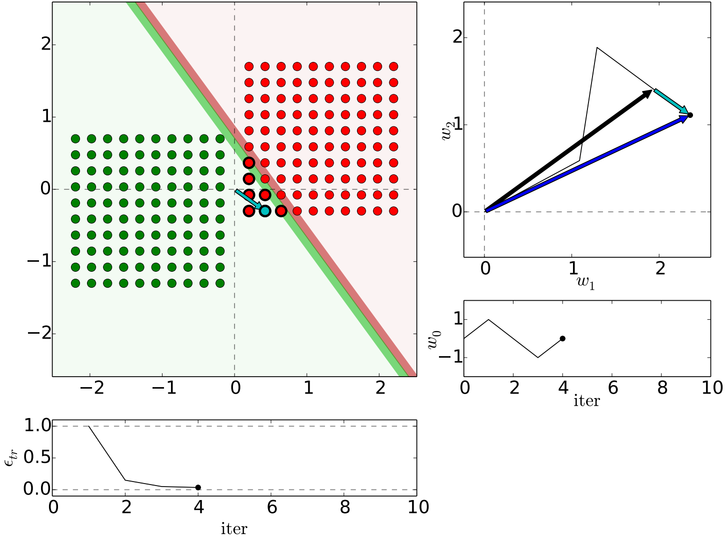

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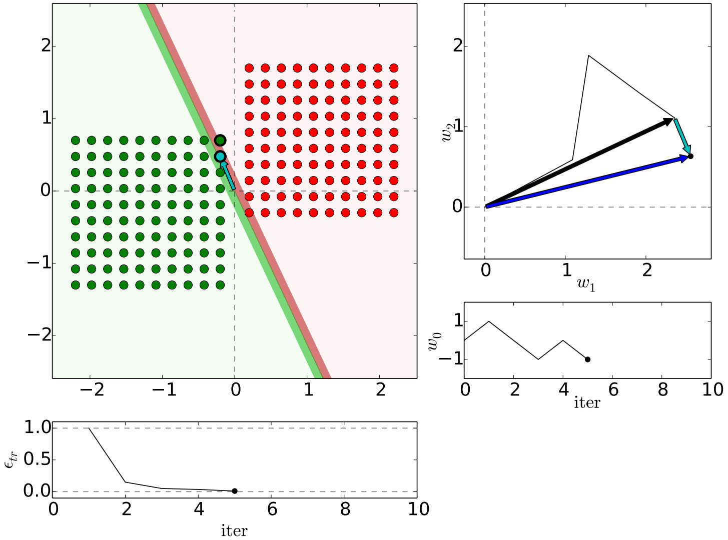

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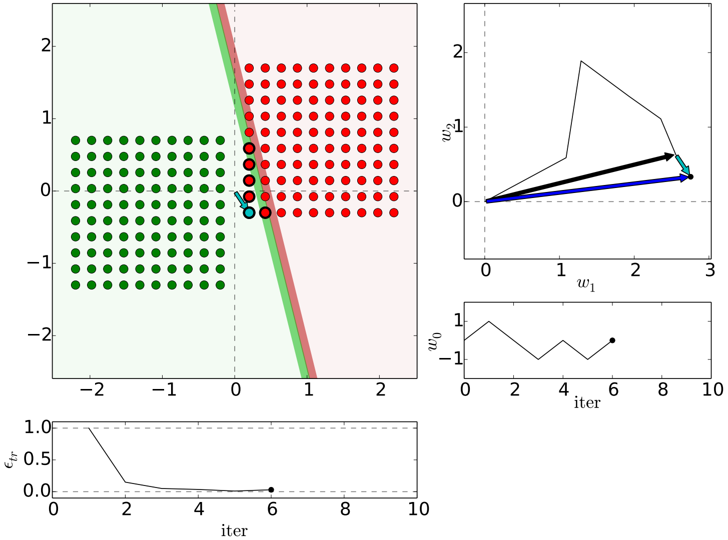

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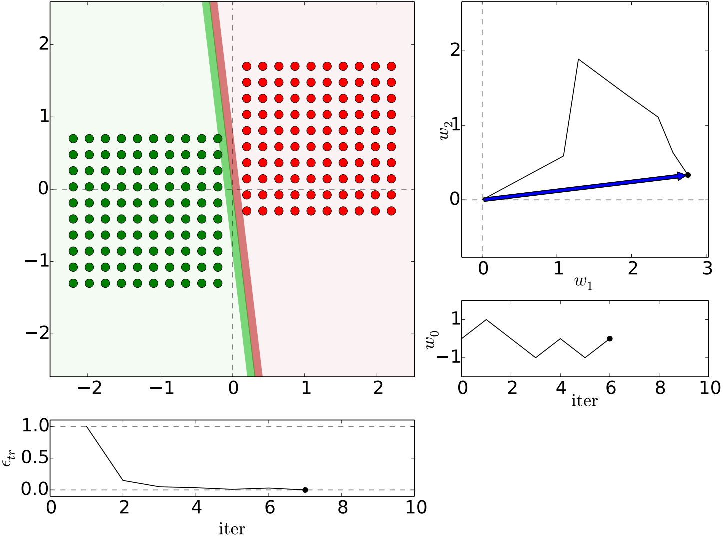

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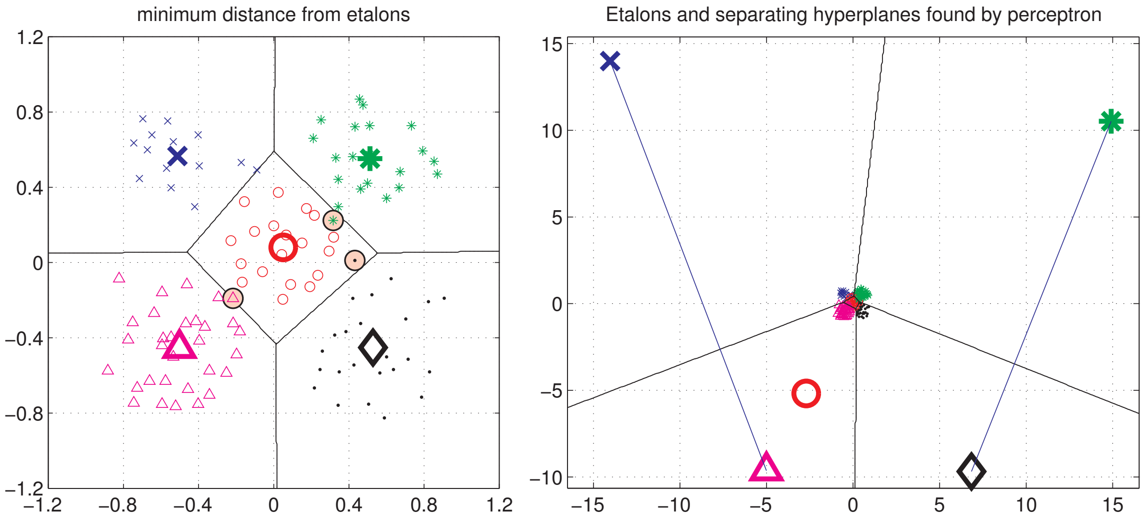
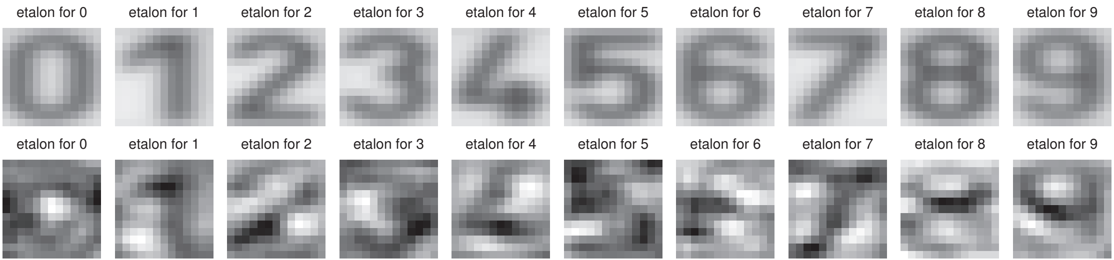
Etalons: means vs. found by perceptron



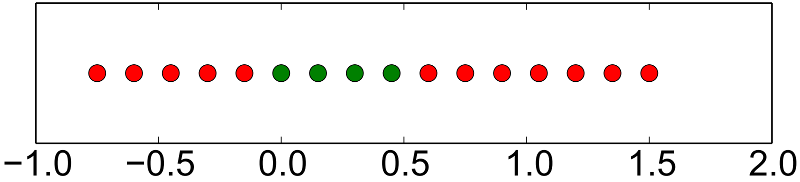
Figures from [5]

Digit recognition - etalons means vs. perceptron



Figures from [5]

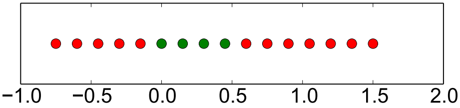
What if not lin separable?

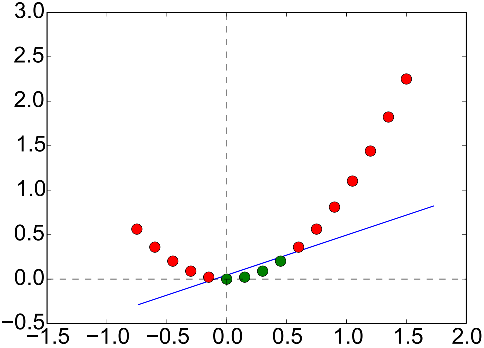


Dimension lifting

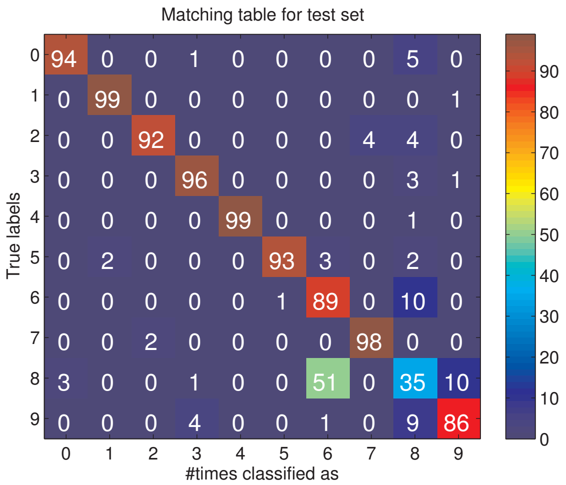
$$\mathbf{x} = [x, x^2]^\top$$

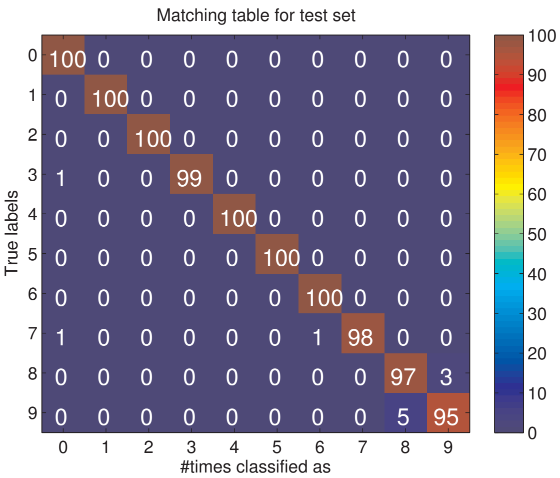
Dimension lifting, $\mathbf{x} = [x, x^2]^\top$



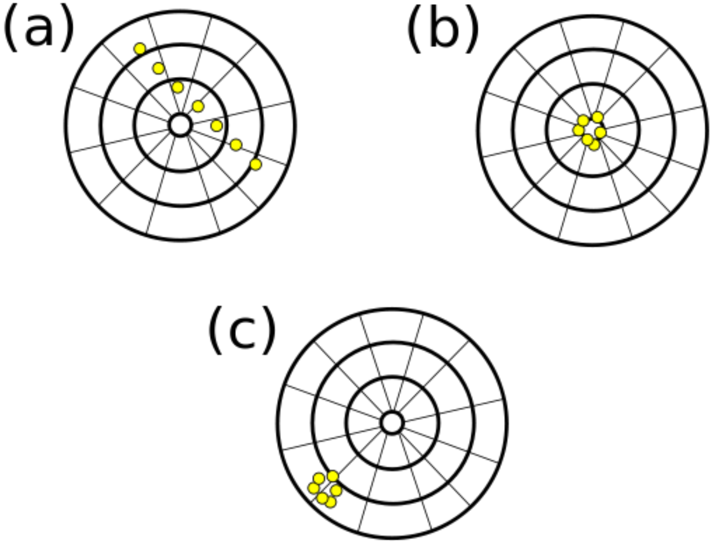


Performance comparison, parameters fixed



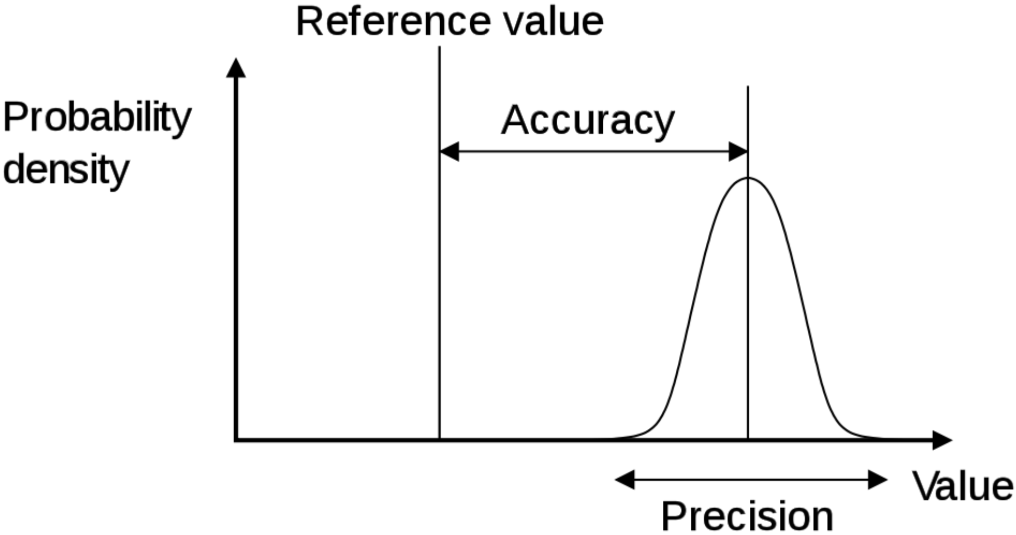


Accuracy vs precision



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