$k-$NN and Linear Classifiers, Learning

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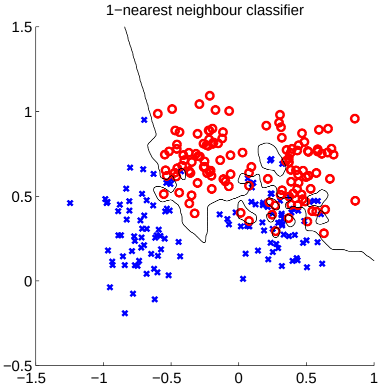
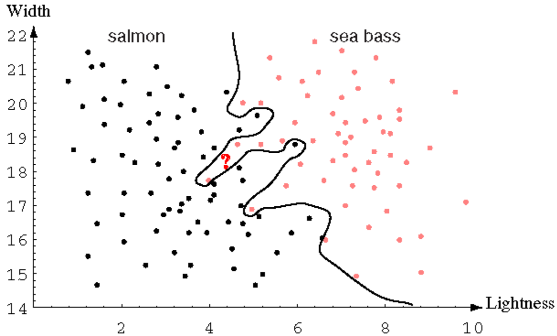
Notes

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.





Notes

Some properties:

- A *nonparametric* method – does not assume anything about the distribution (that it is Gaussian etc.)
- Can be used for classification or regression. Here: classification.
- Training: Only store feature vectors and their labels.
- Very simple and suboptimal. With unlimited nr. prototypes, error never worse than twice the Bayes rate (optimum).
- *instance-based* or *lazy* learning – function only approximated locally; computation only during inference.
- Limitations
  - Curse of dimensionality - for every additional dimension, one needs exponentially more points to cover the space.
  - Comp. complexity - has to look through all the samples all the time. Some speed-up is possible. E.g., storing data in a K-d tree.
  - Noise. Missclassified examples will remain in the database....

$K-$ 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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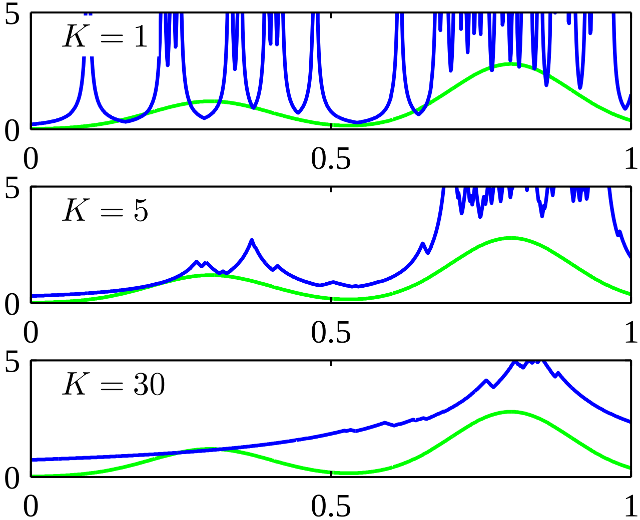

A $K-$NN classifier can be understood as a non-parametric density estimator. (Figure from [1])

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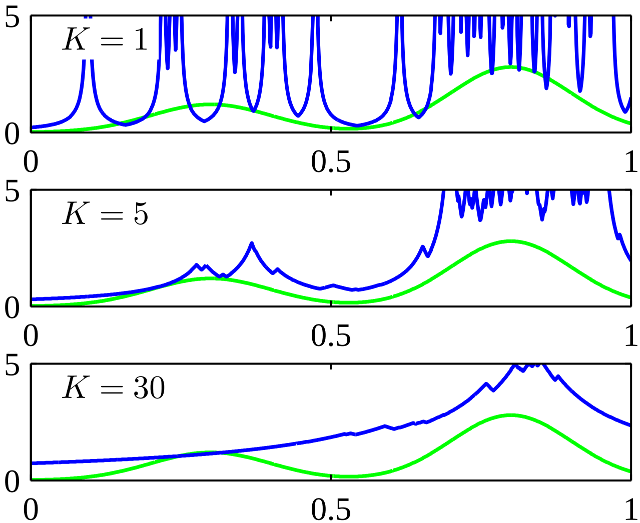

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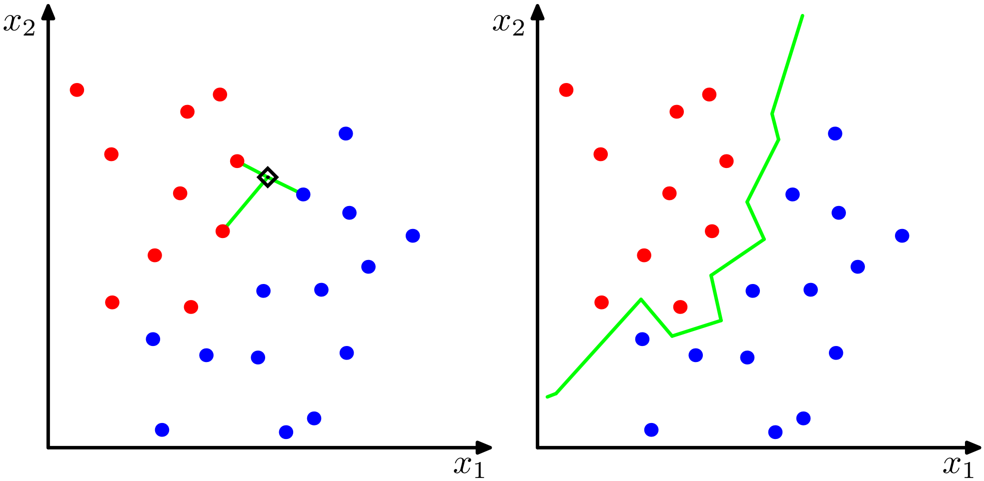
NN classification example



(a) (b) [1]

[1] Figs from [1]

Notes

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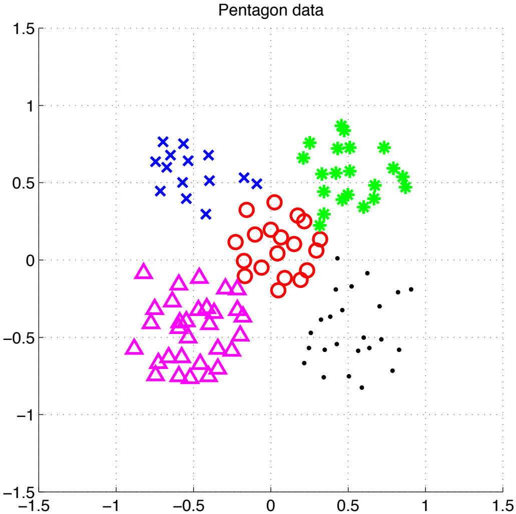

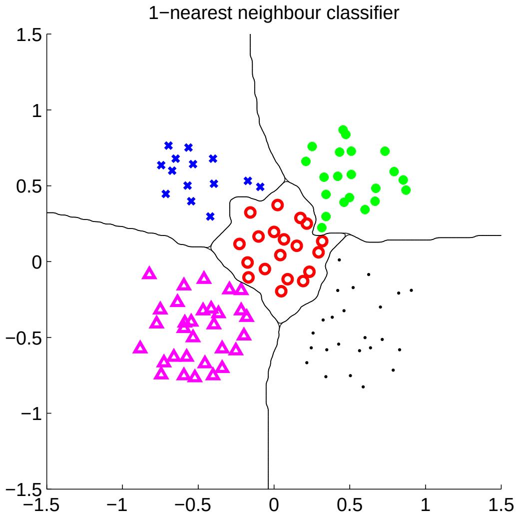

Notes

Fast on "learning", very slow on decision.

There are ways for speeding it up, search for NN editing - making training data sparser, keeping only representative points.

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

Notes

When taking $\vec{x}$ as all the intenties, "5" shifted 3 pixels left is farther from its etalon thant to etalon of "8". One could consider preprocessing:

1. shift query image to all possible positions and compute min distances
2. take the min(min(distance))
3. perform NN classification

Costly ...

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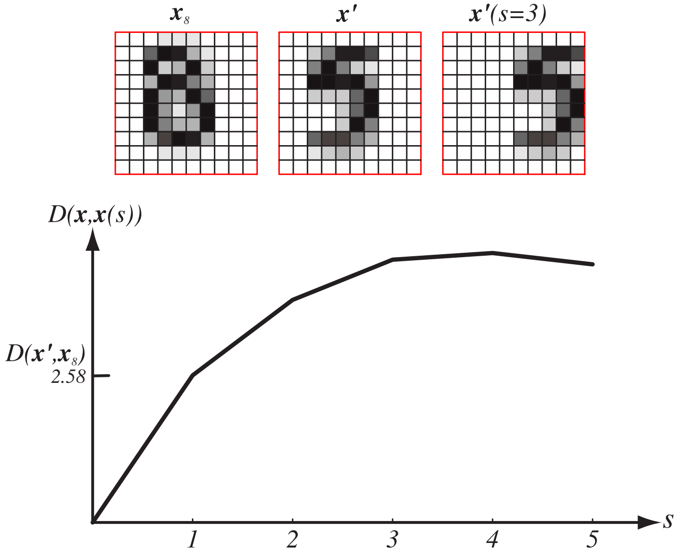

Invariance to geometrical transformations? (figure from [2])

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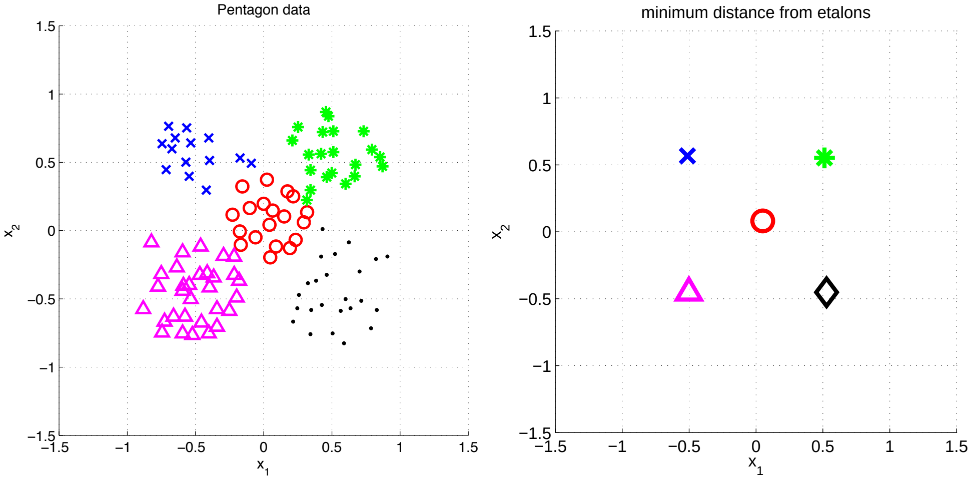
Etalon based classification

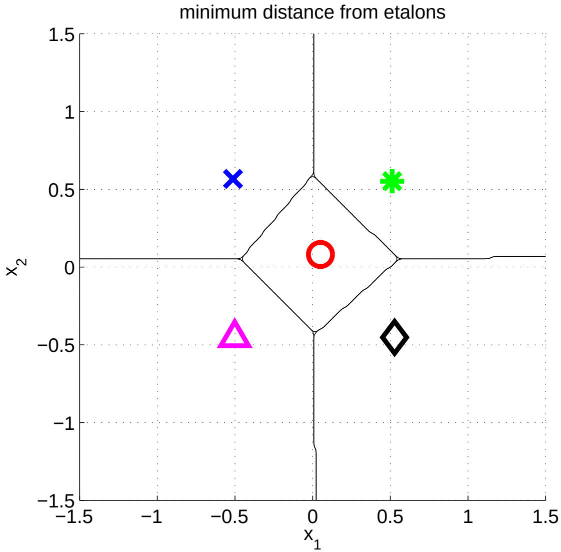


Represent $\vec{x}$ by etalon , $\vec{e}_s$ per each class $s \in S$

Notes

Separate etalons

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



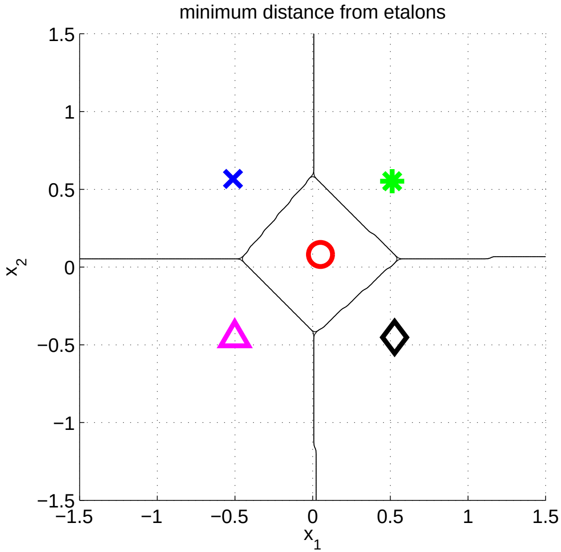
Notes

What etalons?

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

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

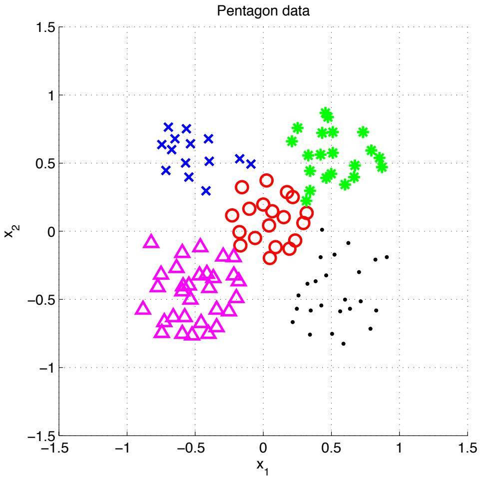
and separating hyperplanes halve distances between pairs.

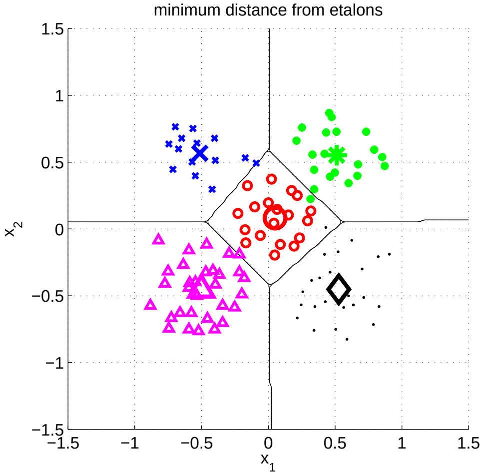


Notes

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

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

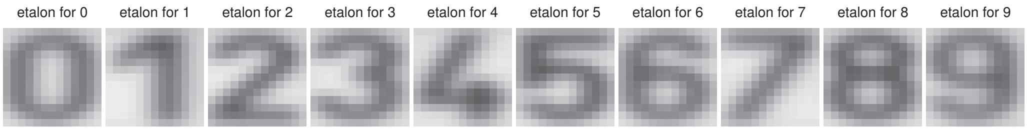




Notes

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

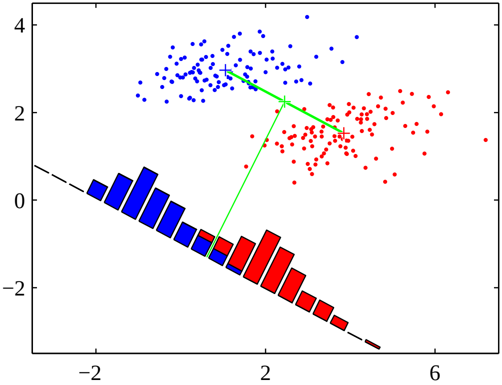
Digit recognition - etalons $\vec{e}_s = \vec{\mu}_s$



Figures from [5]

Notes

Better etalons – Fischer linear discriminant



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

Figures from [1]

Notes

Searching for a projection of the data to minimize intra-class variance and maximize inter-class variance.

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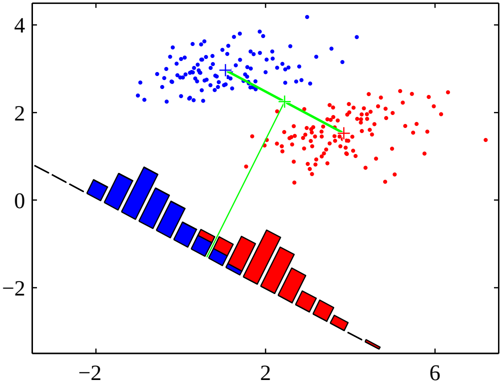

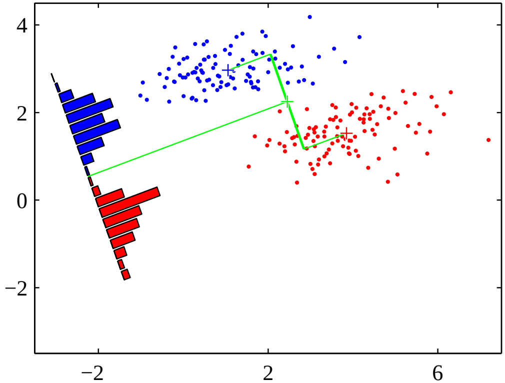

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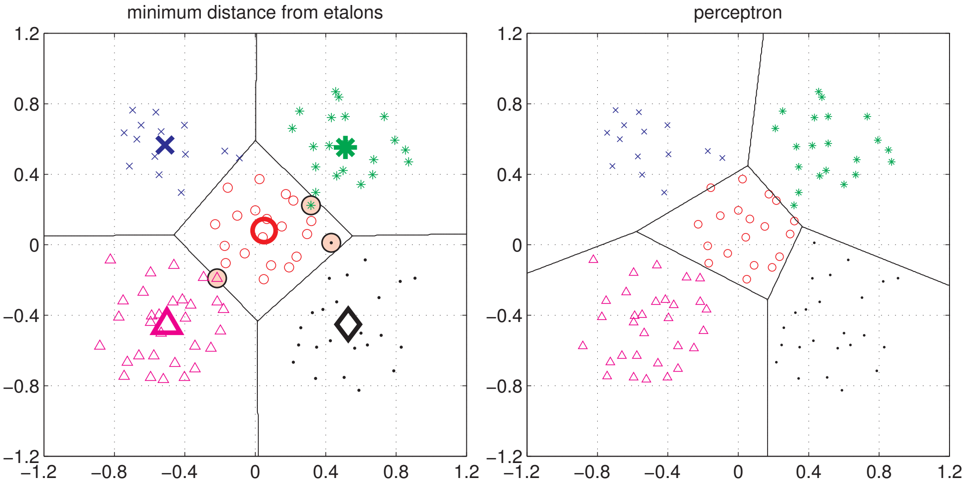
Better etalons?



Figures from [5]

Notes

This is just to show that there is an etalon classifier that make no mistake on the data. But how to find the best etalons?

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)

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

Notes

The result is a *linear discriminant function* – hence etalon classifier is a linear classifier.
We classify into the class with highest value of the discriminant function.
$\mathbf{w}_s$ is a generalized etalon. How do we find it? Such that it is better than just the mean of the class members in the training set.

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.

Notes

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:

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

(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]

Notes

$g(\mathbf{x}) = 0$ is the *separating hyperplane*. Its dimension is one less that that of the input space – for 2D space, it is a line. (This is a bit counterintuitive - "hyper" normally means above, more...)

What is the geometric meaning of the weight vector $\mathbf{w}$?

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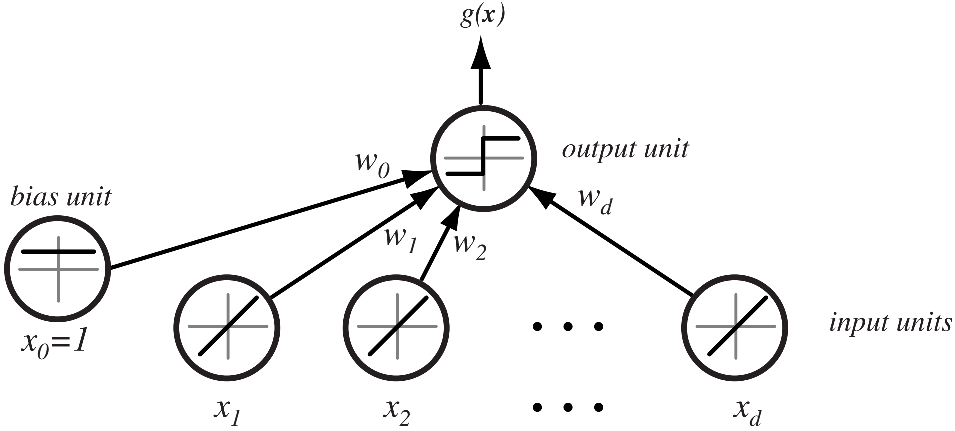

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Separating hyperplane

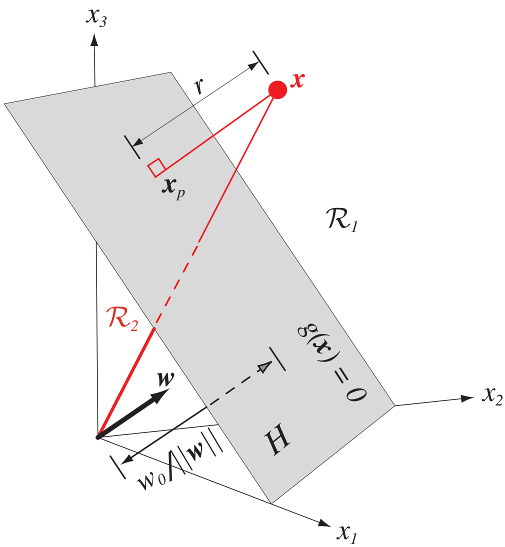
$$\mathbf{w}^\top \mathbf{x}_1 + w_0 = \mathbf{w}^\top \mathbf{x}_2 + w_0$$
$$\mathbf{w}^\top (\mathbf{x}_1 - \mathbf{x}_2) = 0$$

$g(\mathbf{x})$ 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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Notes

(any) vector $(\mathbf{x}_1 - \mathbf{x}_2)$ lies on the separating hyperplane, $\mathbf{w}$ is perpendicular to it
Summary: A linear discriminant function divides the feature space by a hyperplane decision surface.

- The orientation of the surface is detemined by the normal vector $\mathbf{w}$.
- The location of the surface is determined by the bias term w_0.

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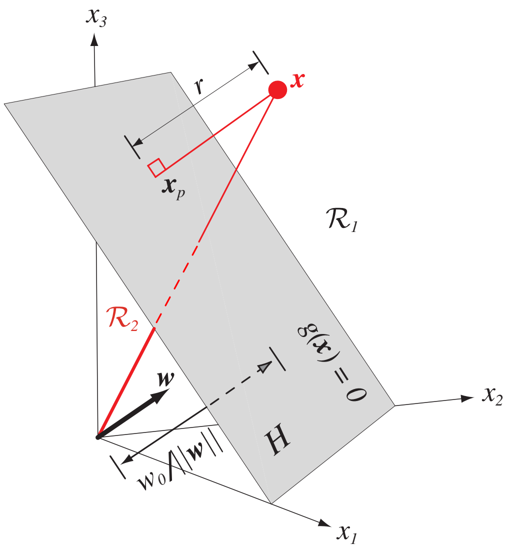

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Separating hyperplane from g_1 and g_2

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

Separating hyperplane:

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

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

Notes

Think about case where $\|\vec{\mu}_1\| = \|\vec{\mu}_2\|$ and reason about simplified equation of the separating hyperplane.

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.

Notes

There are two steps here:

1. Transformation to homogenous notation with augmented feature vector and augmented weight vector.
2. "Normalization" that simplifies treatment of the two-class case: labels can be ignored. Just look for a weight vector $\mathbf{w}$ such that $\mathbf{w}^\top \mathbf{x} > 0$

It means, the sign of $\mathbf{x}$ depends on the class it belongs to! Keep in mind.

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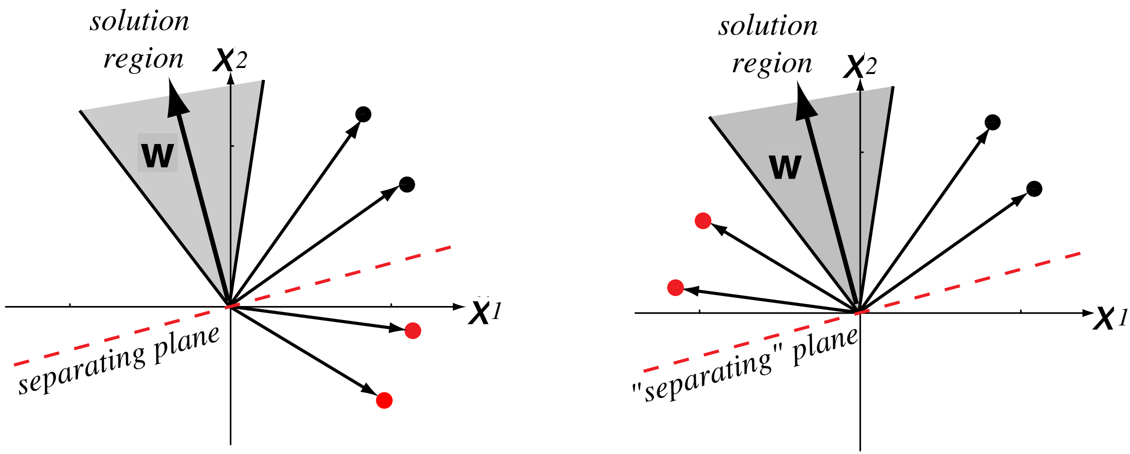
Solution (graphically)



Fou

training samples. Left: orginal, Right: sign corrected

Figure from [2] (notation changed)

Notes

Four training samples (black for class/category w_1, red for w_2). Left: Raw data Right: "Normalized data". Class w_2 member replaced by their negatives... Simplifies the situation: labels can be ignored. Just look for a weight vector $\mathbf{w}$ such that $\mathbf{w}^\top \mathbf{x} > 0$
Before: defining the linear discriminant function.
Now: How can we obtain it from (labeled) data?

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 $\mathbf{w}$

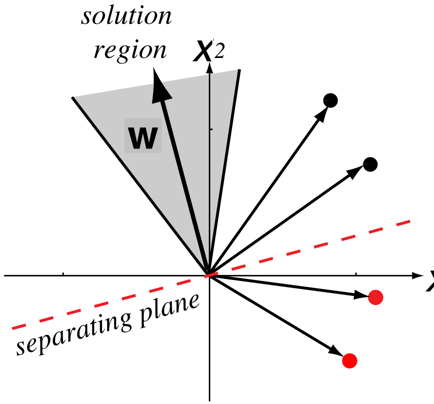
Notes

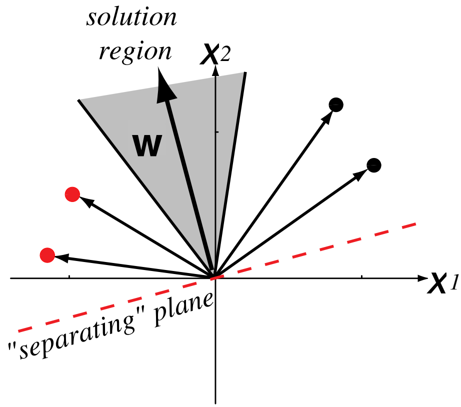
This is a general scheme, we do not know $J(\mathbf{w})$, yet.
We're looking into *error-based classification* methods: missclassified examples are used to tune the classifier...
We already discussed (stochastic) Gradient descent when talking about $Q-$function learning

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 $\mathbf{x}$.

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

Notes

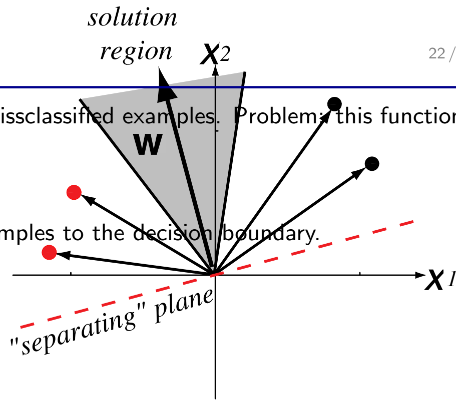
What are the possible choices for $J(\mathbf{w})$? First choice: number of missclassified examples. Problem: this function is piecewise constant.

Better choice: perceptron criterion function.

Mind that $\mathbf{w}^\top \mathbf{x}_j \leq 0$ for $\mathbf{x} \in \mathcal{X}$

Geometrically: $J(\mathbf{w}) \propto$ sum of the distance of the missclassified samples to the decision boundary.

What is $\nabla J(\mathbf{w})$ equal to?



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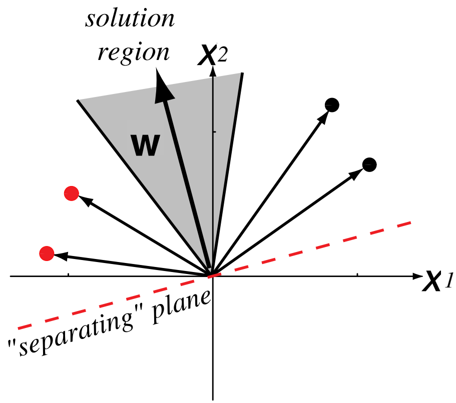
$$J(\mathbf{w}) = \sum_{\mathbf{x} \in \mathcal{X}} -\mathbf{w}^\top \mathbf{x}$$

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

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



Notes

What are the possible choices for $J(\mathbf{w})$? First choice: number of missclassified examples. Problem: this function is piecewise constant.
Better choice: perceptron criterion function.
Mind that $\mathbf{w}^\top \mathbf{x}_j \leq 0$ for $\mathbf{x} \in \mathcal{X}$
Geometrically: $J(\mathbf{w}) \propto$ sum of the distance of the missclassified samples to the decision boundary.
What is $\nabla J(\mathbf{w})$ equal to?

(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 $\mathbf{w}$

Notes

Next weight vector $\sim$ adding some multiple of the sum of the missclassified samples to the present weight vector.

Fixed-increment single-sample Perceptron

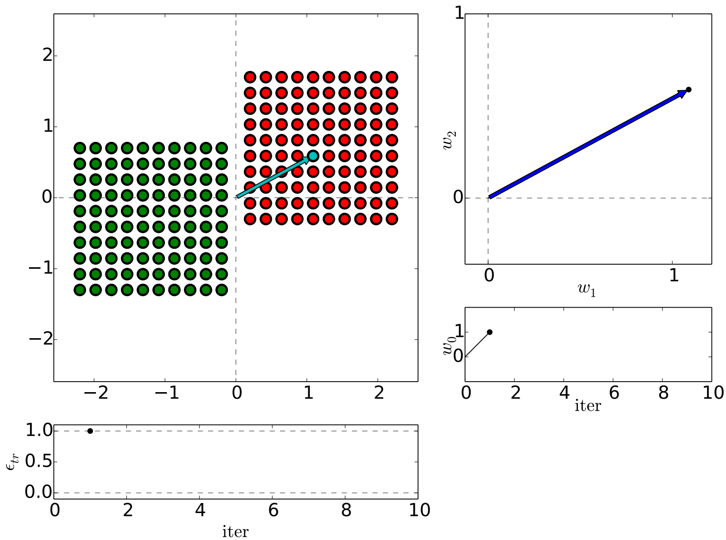
n patterns/samples, we are looping over all patterns repeatedly

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 $\mathbf{w}$

Notes

As we are looping over all patterns repeatedly, it is not an on-line algorithm

Perceptron iterations/loops



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

Initialize **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 **x** correctly classified
return **w**

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

Notes

Keep in mind the $\pm$ normalization of **x**.

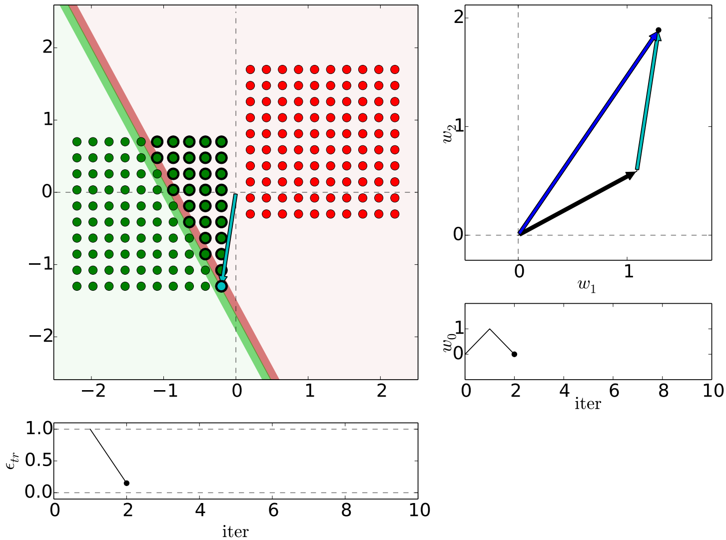
$$g(\mathbf{x}) = \begin{cases} s = 1\,, & \text{if} \quad \mathbf{w}^\top \mathbf{x} + w_0 > 0\,, \\ s = -1\,, & \text{if} \quad \mathbf{w}^\top \mathbf{x} + w_0 < 0\,. \end{cases}$$

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

(as discussed few slides ago)
Red **x** are $+$, green are $-$

Track the iteration steps. After each update **x**, draw a separating line for the next and verify.

Perceptron iterations/loops



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 $\mathbf{w}$

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

Notes

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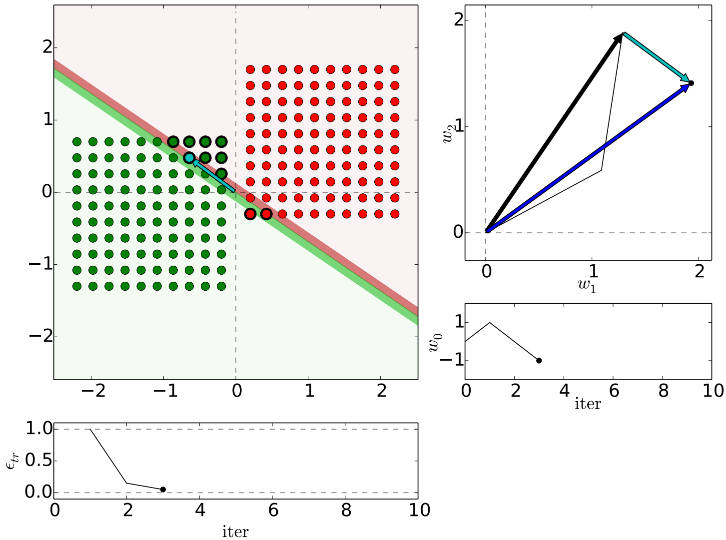

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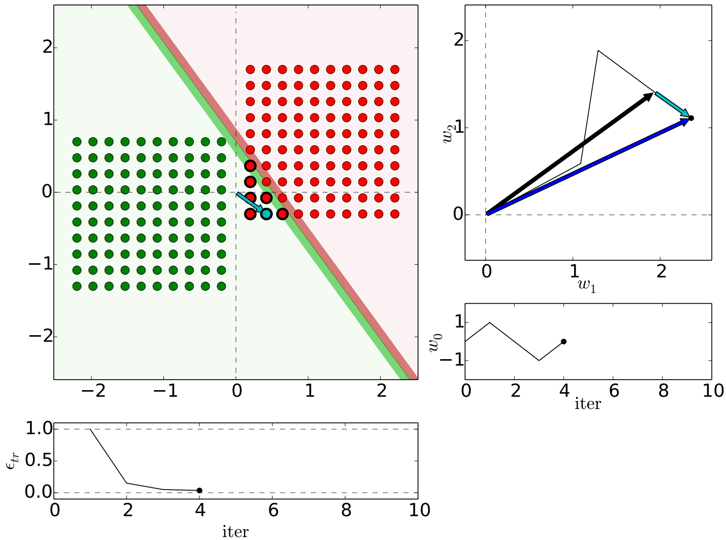

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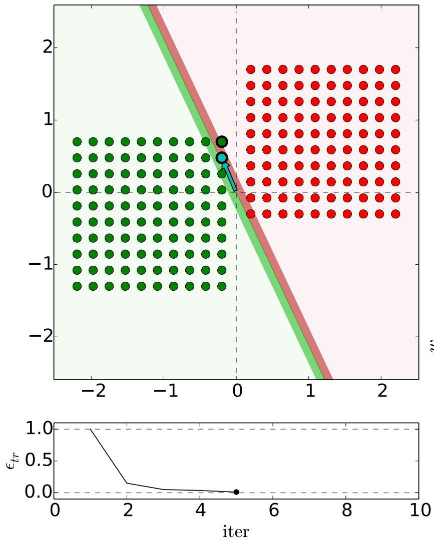

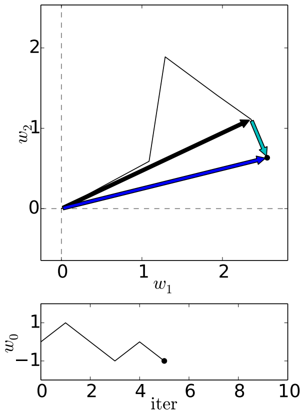

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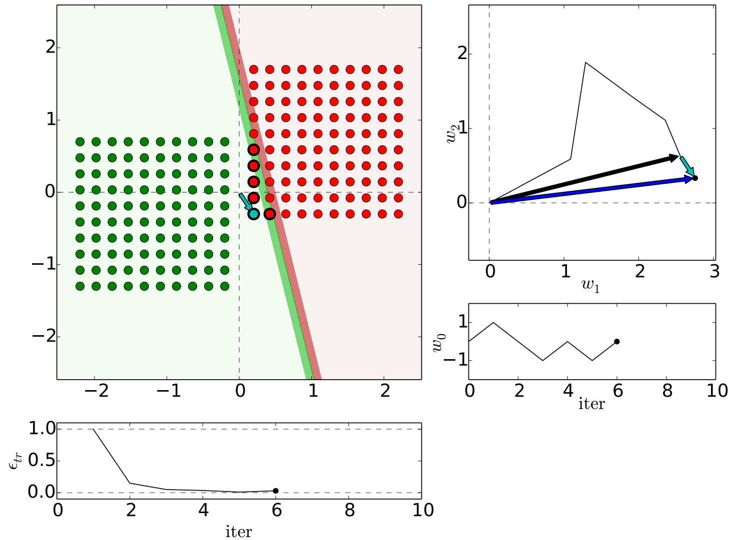
Perceptron iterations/loops



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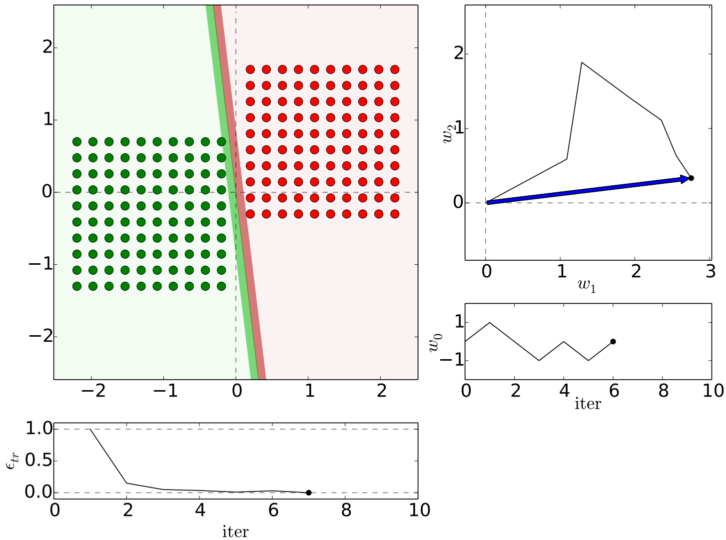
Perceptron iterations/loops



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(as discussed few slides ago)

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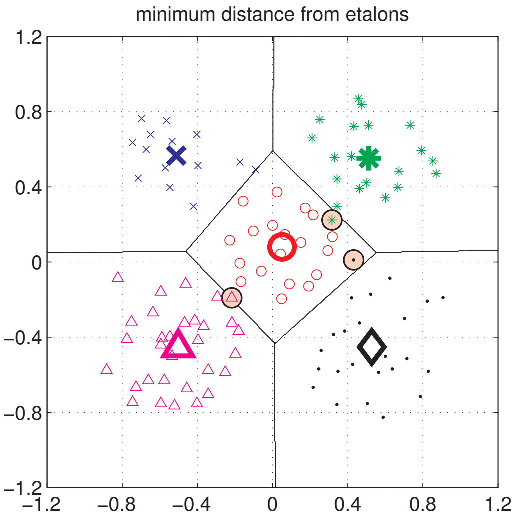
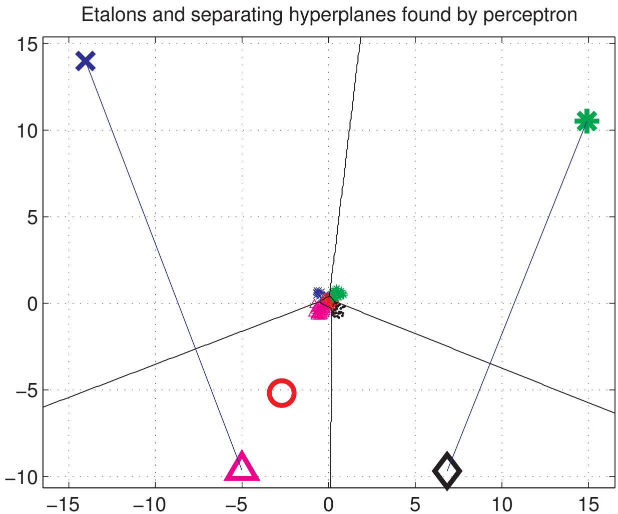
Etalons: means vs. found by perceptron

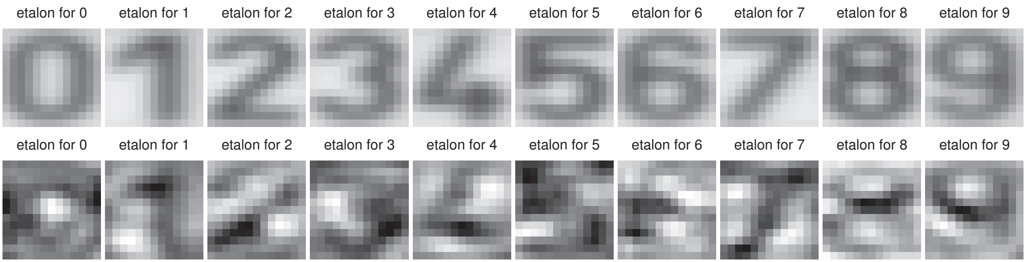




Figures from [5]

Notes

Digit recognition - etalons means vs. perceptron

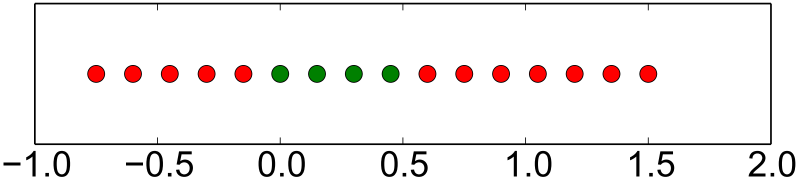


Figures from [5]

Notes

"Prototypes" resulting from the perceptron algorithm are harder to interpret because they are not means – instead, they are optimized for separating the classes.

What if not lin separable?

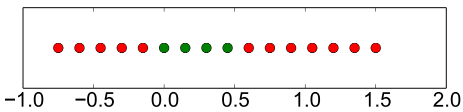


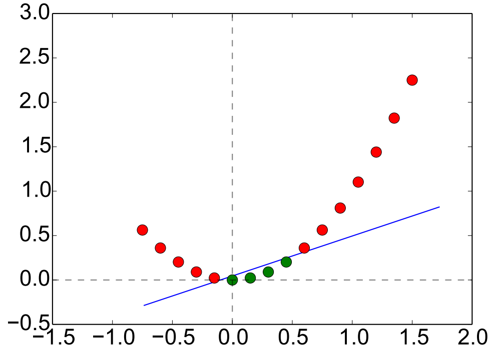
Dimension lifting

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

Notes

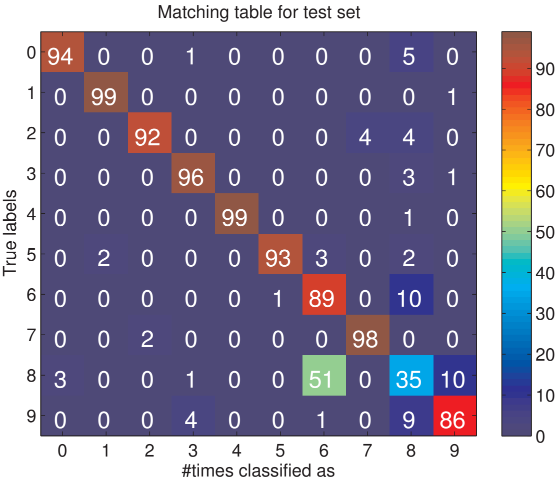
Dimension lifting, $\mathbf{x} = [x, x^2]^\top$

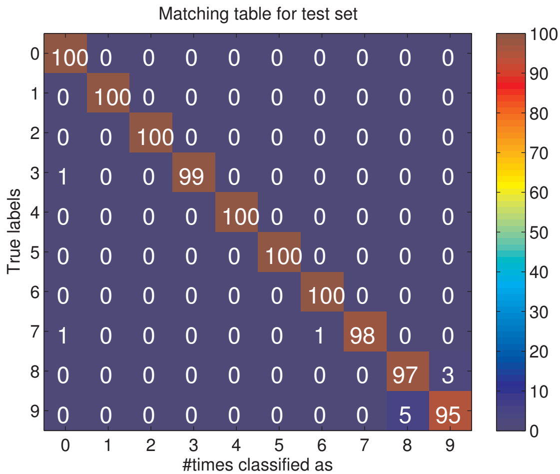




Notes

Performance comparison, parameters fixed

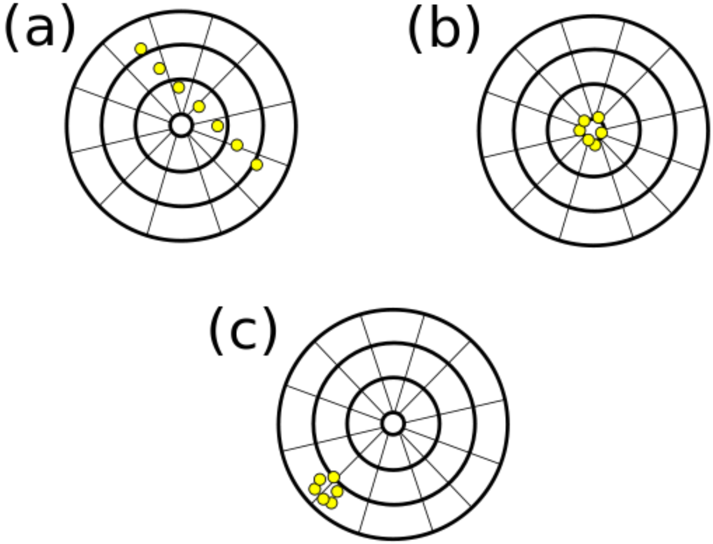




Notes

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

Accuracy vs precision



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

Notes

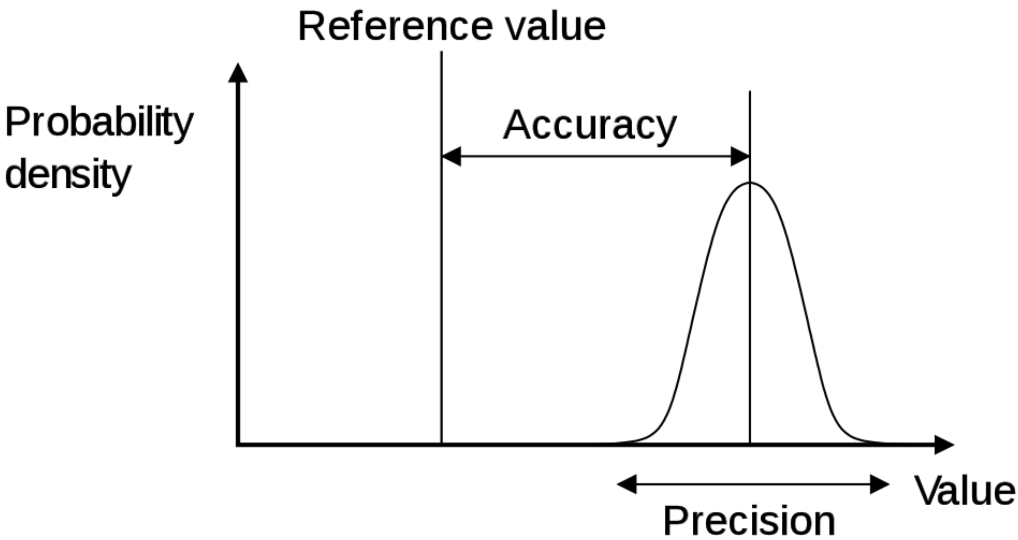
Accuracy: how close (is your model) to the truth. Precision: how consistent/stable
In German:

- Accuracy: Richtigkeit
- Precision: Präzision
- Both together: Genauigkeit

In Czech:

- Accuracy: Věrnost, přesnost.
- Precition: Rozptyl,

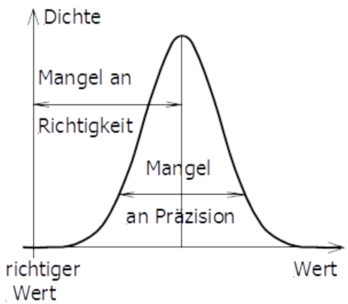
Accuracy vs precision



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

Notes

Accuracy: how close (is your model) to the truth. Precision: how consistent/stable.
Think about terms *bias* and *error*. I



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].

[1] Christopher M. Bishop.
Pattern Recognition and Machine Learning.
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[2] Richard O. Duda, Peter E. Hart, and David G. Stork.
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Notes

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.
Image Processing, Analysis and Machine Vision — A MATLAB Companion.
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Notes