k-NN and Linear Classifiers, Learning

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

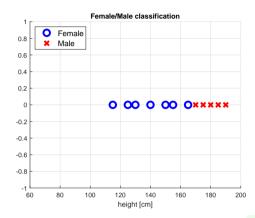
Vision for Robots and Autonomous Systems, Center for Machine Perception
Department of Cybernetics
Faculty of Electrical Engineering, Czech Technical University in Prague

May 23, 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 <i>x_i</i>	115	125	130	140	150	155	165	170	175	180	185	190
Gender si	F	F	F	F	F	F	F	М	М	М	М	М



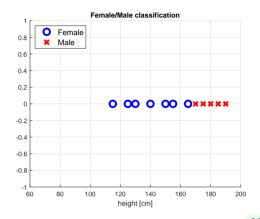
Notes -

Run onedim_linclass_learning

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A new point to clasify: $x_Q = 166$

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

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Notes -

Run onedim_linclass_learning

Example: F/M classification – k-NN

i	1	2	3	4	5	6	7	8	9	10	11	12
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Query: $x_Q = 166$

1-NN: $d_Q = ?$

 $\mathbf{A} d_Q = F$

 $\mathbf{B} \ d_Q = M$

C Both classes equally likely

D 1-NN will not provide any decision

Notes

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For 1-NN: $s_Q = F$ For 3-NN: $s_Q = M$

We can reduce the number of x_i for which we compute $dist(x_Q, x_i) \to \text{Etalons!}$

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3-NN:
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$$\mathbf{A} d_{\mathbf{Q}} = \mathbf{F}$$

$$\mathbf{B} \ d_Q = M$$

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How can we reduce the complexity of k-NN method?

Notes

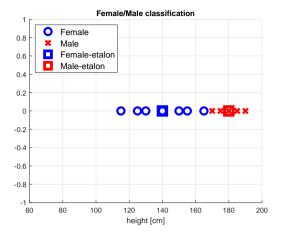
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Example: F/M classification – Etalons

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



$$e_F = ave(\{x_i : s_i = F\}) = 140$$

 $e_M = ave(\{x_i : s_i = M\}) = 180$

Based on etalons: $d_Q = ?$

$$\mathbf{A} d_{\mathcal{Q}} = F$$

$$\mathbf{B} do = M$$

D Cannot provide any decision

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

What type of function is $dist(x_O, e_s)$?

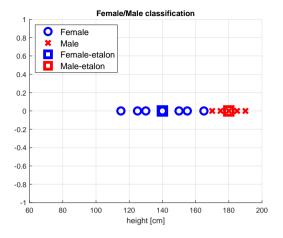
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Notes -

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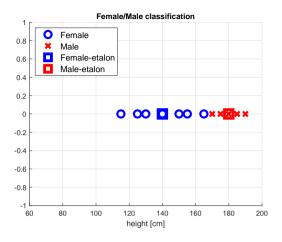
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Notes

Based on etalons: $d_Q = M$

Linear discriminant functions

Assuming dist $(x, e) = (x - e)^2$, then

Multiclass classification: each class s has a linear discriminant function $f_{\epsilon}(x) = a_{\epsilon}x + b_{\epsilon}$ and

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

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

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

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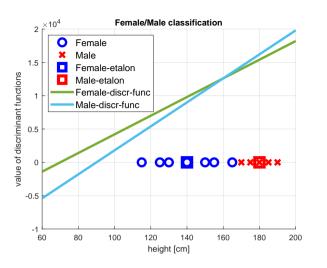
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Notes -

Example: F/M – Linear discriminant functions based on etalons



Discriminant functions for 2 classes:

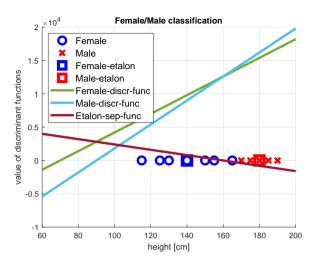
$$f_F(x) = a_F x + b_F =$$

$$= e_F x - \frac{1}{2}e_F^2 = 140x - 9800$$

$$f_M(x) = a_M x + b_M =$$

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

Example: F/M – Linear discriminant functions based on etalons



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A single discriminant function separating 2 classes:

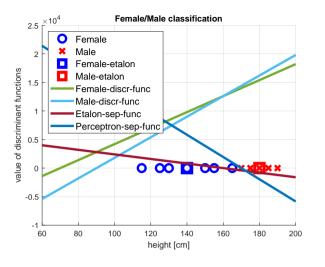
$$g(x) = f_F(x) - f_M(x) =$$

= -40x + 6400

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Notes

Example: F/M – Can we do better?



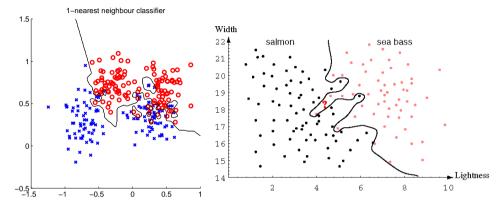
Etalon-based linear classifier makes some errors.

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.



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

Assume data:

ightharpoonup N points \vec{x} in total.

▶ N_j points in s_j class. Hence, $\sum_i N_j = N$.

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

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

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

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

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

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

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

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Notes -

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

k - NN for non-parametric density estimation

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

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

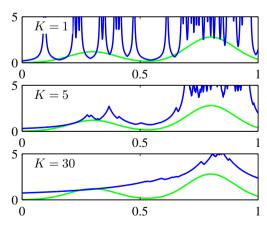
 $R_k(\vec{x})$ - distance from \vec{x} to its k-th nearest neighbour point (radius)

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

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

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Notes -

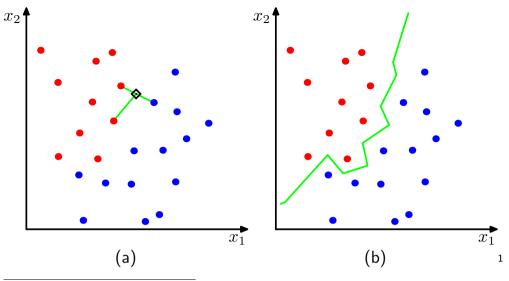


More details, including a computational example, in [?].

A K-NN belongs to non-parametric methods for density estimation, see section 2.5 from [1]. (Figure from [1])

Try yourself, https://scikit-learn.org/stable/modules/density.html#kernel-density

NN classification example



¹Figs from [1]

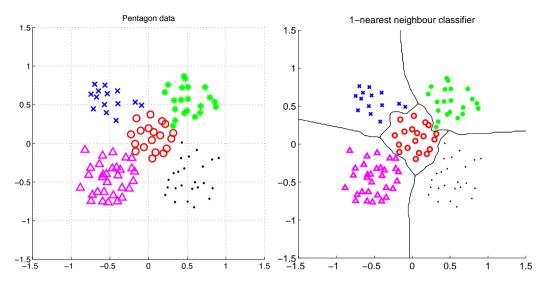
- Notes

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Left: k = 3.

Right: Decision boundary for k = 1.

NN classification example



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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:

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

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

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

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

Notes -

Note, the minimum distance calculation can be reformulated into maximum similarity obtained by a dot product between the feature vector and the training examples.

When taking \vec{x} as all the intensities, a "5" shifted 3 pixels left is farther from its etalon than 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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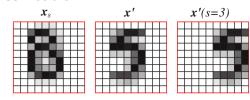
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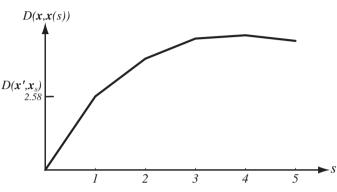
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Invariance to geometrical transformations? (figure from [2]) 13/42

- Notes

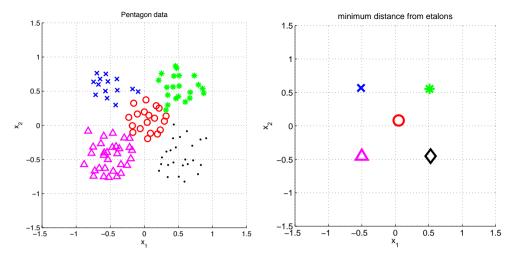
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Etalon based classification



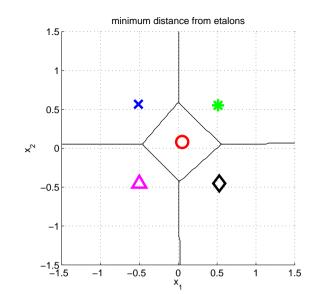
Represent \vec{x} by etalon , \vec{e}_s per each class $s \in S$.

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Notes -

Separate etalons

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



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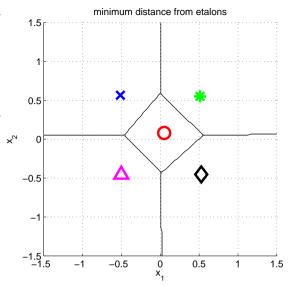
Notes -

What etalons?

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

$$ec{e}_s \stackrel{ ext{def}}{=} ec{\mu}_s = rac{1}{|\mathcal{X}^s|} \sum_{i \in \mathcal{X}^s} ec{x}_i^s$$

and separating hyperplanes halve distances between pairs.

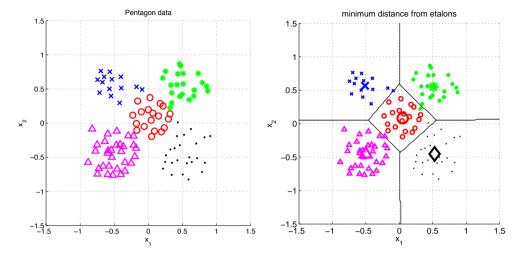


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Notes

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

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

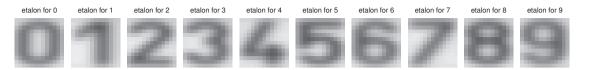


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Notes -

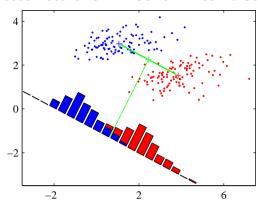
Some wrongly classified samples. We like the simple idea. Are there better etalons? How to find them?

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



Figures from [5].

Better etalons - Fischer linear discriminant



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

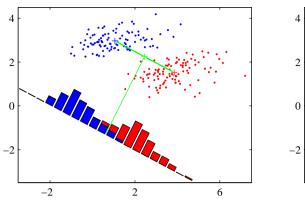
Figures from [1]

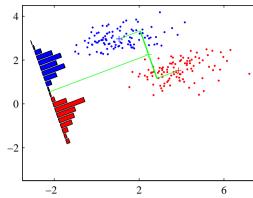
Notes -

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Searching for a (in this case 1D) projection of the data to minimize intra-class variance and maximize inter-class variance.

Better etalons - Fischer linear discriminant





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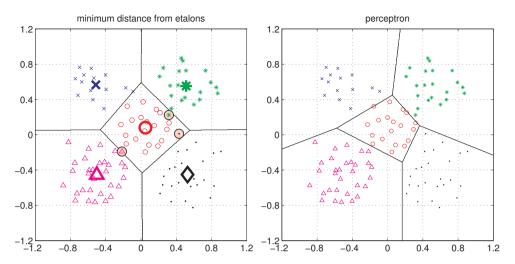
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Figures from [1]

Notes

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Better etalons?



Figures from [5]

Notes -

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

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

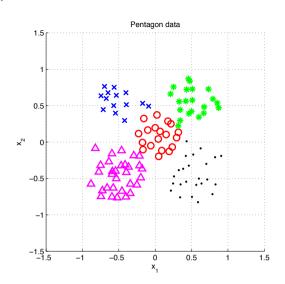
$$s^* = \operatorname*{argmax}_{s \in \mathcal{S}} f(\vec{x}, s)$$

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:

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



Notes

Normal distribution for general dimensionality D:

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

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How about learning $f(\vec{x},s)$ directly without explicit modeling of underlying probabilities? What about $f(\vec{x},s) = \vec{w}_s^{\top} \vec{x} + w_{s0}$

Etalon classifier - Linear classifier

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

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.

(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 [2] 23/42

Notes -

g(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} ?

One could mention the metaphor of the biological neuron here.

(1) Linear discriminant function – a two class case

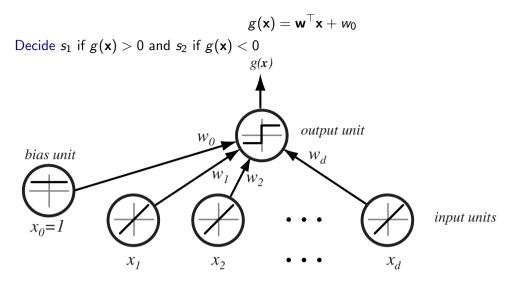


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Separating hyperplane

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

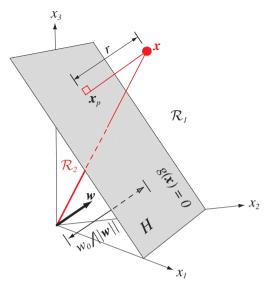
 $\mathbf{w}^{\mathsf{T}}(\mathbf{x}_1 - \mathbf{x}_2) = 0$

g(x) gives an algebraic measure of the distance from x to the hyperplane.

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

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

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



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Figure from [2]

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.

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

Separating hyperplane

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

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

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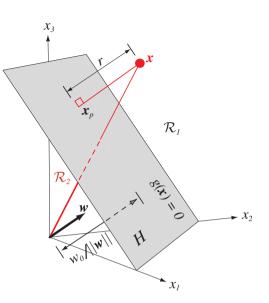


Figure from [2]

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Separating hyperplane from g_1 and g_2

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

$$g_1(\vec{x}) = \vec{\mu}_1^{\top} \vec{x} - \frac{1}{2} \vec{\mu}_1^{\top} \vec{\mu}_1$$

$$g_2(\vec{x}) = \vec{\mu}_2^{\top} \vec{x} - \frac{1}{2} \vec{\mu}_2^{\top} \vec{\mu}_2$$

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 -

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

Two classes set-up

Transform the training data $\mathcal{T} = \{(\mathbf{x}_j, s_j)\}_{j=1}^N$:

1. |S| = 2: let's denote the two states/classes by +1 and -1:

$$s_j = \left\{ egin{array}{ll} +1 & ext{if } \mathbf{x}_j ext{ is from class 1,} \\ -1 & ext{if } \mathbf{x}_j ext{ is from class 2.} \end{array}
ight.$$

2. Use homogeneous coordinates and invert x: of the "negative" class

$$\left[\begin{array}{c} \mathbf{x}_j' = \mathbf{s}_j \left[\begin{array}{c} 1 \\ \mathbf{x}_j \end{array}\right], \ \mathbf{w}' = \left[\begin{array}{c} w_0 \\ \mathbf{w} \end{array}\right] \end{array}\right]$$

Then, we search for \mathbf{w}' such that for all \mathbf{x}' ;

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

(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 x depends on the class it belongs to! Keep in mind.

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, $\mathbf{w}' = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$

Then, we search for \mathbf{w}' such that for all \mathbf{x}'_i

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

(Drop the dashes to avoid notation clutter.)

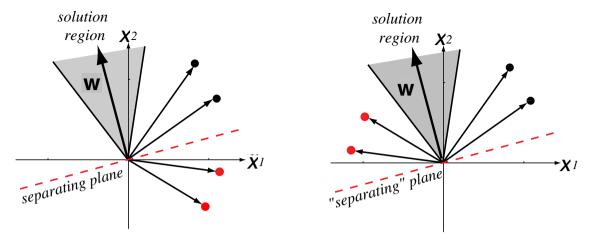
Notes -

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It means, the sign of x depends on the class it belongs to! Keep in mind.

Solution (graphically)



Four training samples. Left: original, Right: class s_2 transformed (sign changed). 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?

What is the meaning of solution region? There are multiple possible solution vectors within that region...

Learning 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}
```

Notes -

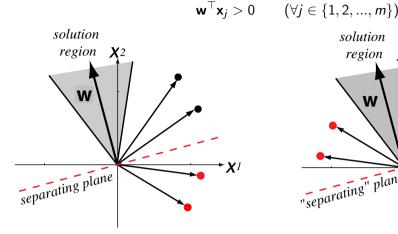
This is a general scheme, we do not know $J(\mathbf{w})$, yet.

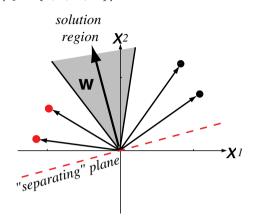
We're looking into error-based classification methods: missclassified examples are used to tune the classifier...

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:





Perceptron) Criterion to be minimized:

Notes

What are the possible choices for $J(\mathbf{w})$?

- First choice: number of missclassified examples. Problem: this function is a piecewise constant function of **w**, with discontinuities wherever a change in **w** causes the decision boundary to move across one of the data points. Gradient is zero almost everywhere, so gradient descent methods cannot be applied.
- Better choice: perceptron criterion function. This error function is piecewise linear (piecewise as some data points may change how they are classified; linear depends on the actual weight vector).

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

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

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

Learning w - Perceptron criterion

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

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

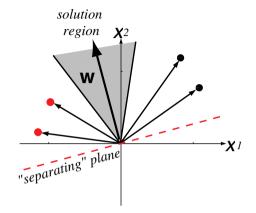
(Perceptron) Criterion to be minimized:

$$J(\mathbf{w}) = \sum_{\mathbf{x} \in \mathcal{T}} - \min(0, \mathbf{w}^{\top} \mathbf{x}) =$$

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

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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Notes

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

(Batch) Perceptron algorithm

```
Initialize \mathbf{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 \mathbf{w}
```

Notes -

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

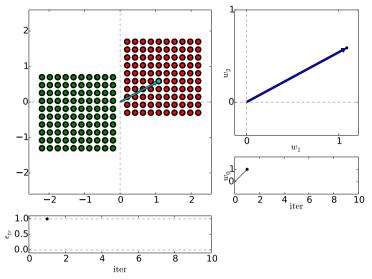
Fixed-increment single-sample Perceptron

```
n patterns/samples, we are looping over all patterns repeatedly Initialize \mathbf{w} k \leftarrow 0 \mathbf{repeat} k \leftarrow (k+1) \bmod n \mathbf{if} \ \mathbf{x}^k \ \text{missclassified}, \ \mathbf{then} \ \mathbf{w} \leftarrow \mathbf{w} + \mathbf{x}^k \mathbf{until} \ \text{all} \ \mathbf{x} \ \text{correctly classified} \mathbf{return} \ \mathbf{w}
```

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Notes -

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



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

Initialize \mathbf{w}

 $k \leftarrow 0$

repeat

 $k \leftarrow (k+1) \mod n$ if \mathbf{x}^k missclassified, then

 $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{x}^k$

until all x correctly classified
return w

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

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Notes

Keep in mind the \pm normalization of \mathbf{x} .

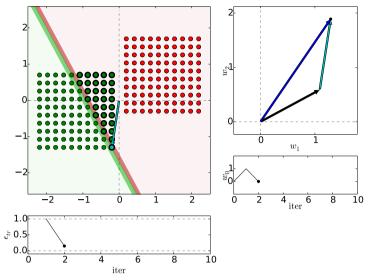
$$s_j = \left\{ egin{array}{ll} +1 & ext{if } \mathbf{x}_j ext{ is from class 1,} \ -1 & ext{if } \mathbf{x}_j ext{ is from class 2.} \end{array}
ight.$$

$$\mathbf{x}_{j}' = s_{j} \begin{bmatrix} 1 \\ \mathbf{x}_{j} \end{bmatrix}, \mathbf{w}' = \begin{bmatrix} w_{0} \\ \mathbf{w} \end{bmatrix}$$

(as discussed few slides ago)

Red \mathbf{x} are +, green are -

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



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32 / 42

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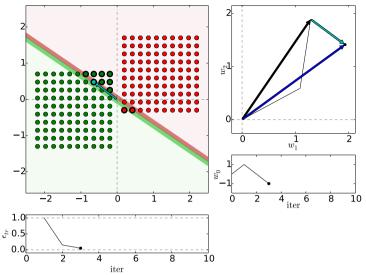
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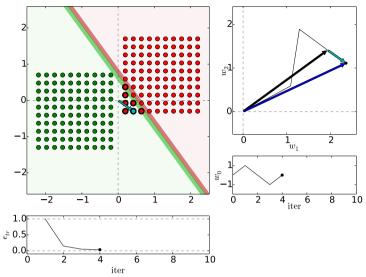
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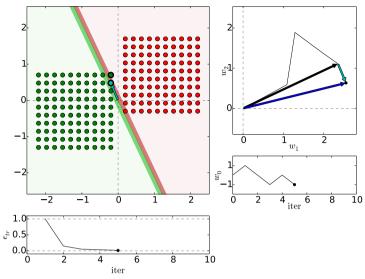
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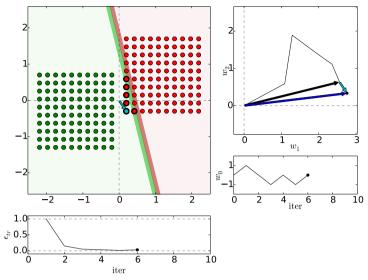
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32 / 42

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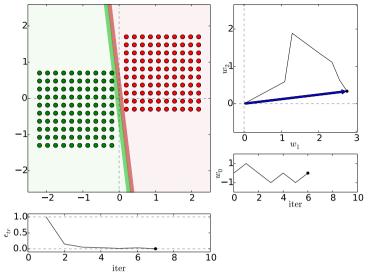
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32 / 42

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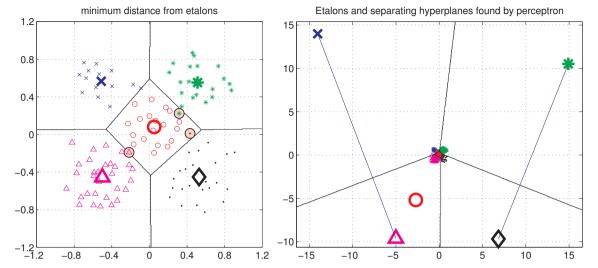
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Etalons: means vs. found by perceptron



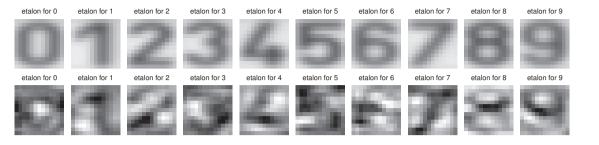
Figures from [5]

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Notes

Again, the "etalons" from perceptron are "far out" because the weight vector kept growing.

Digit recognition – etalons means vs. perceptron

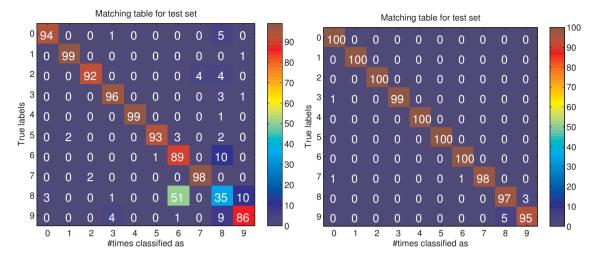


Figures from [5].

Notes -

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

Digit recognition - Performance comparison, parameters fixed



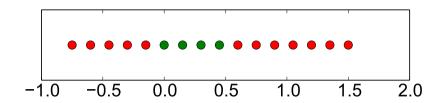
Left: Etalon classification. Right: perceptron classification.

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Notes -

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

What if data is not linearly separable?



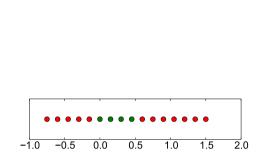
Dimension lifting

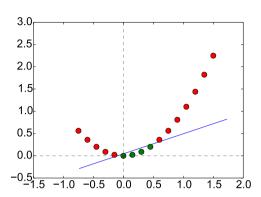
$$\mathbf{x} = [x, x^2]^\top$$

Notes -

Kernel methods are here to serve this purpose – in more sophisticated ways.

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





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Notes -

Learning and decision

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

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

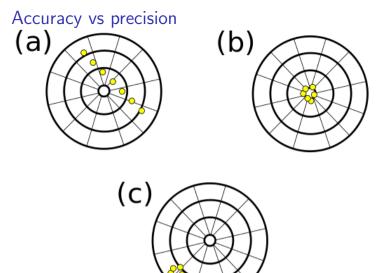
What to learn?

- ► 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:

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



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

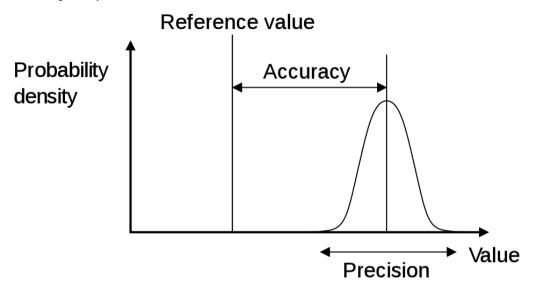
• Both together: Genauigkeit

In Czech:

• Accuracy: Věrnost, přesnost.

• Precision: Rozptyl.

Accuracy vs precision

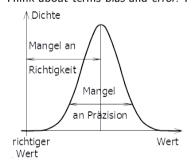


https://en.wikipedia.org/wiki/Accuracy_and_precision

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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 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.

Springer Science+Bussiness Media, New York, NY, 2006.

https://www.microsoft.com/en-us/research/uploads/prod/2006/01/Bishop-Pattern-Recognition-and-Machine-Learning-2006.pdf

[2] Richard O. Duda, Peter E. Hart, and David G. Stork.

Pattern Classification.

John Wiley & Sons, 2nd edition, 2001.

[3] Vojtěch Franc and Václav Hlaváč.

Statistical pattern recognition toolbox.

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

References II

[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, 1st edition, September 2007.

http://visionbook.felk.cvut.cz/.