Linear Models for Regression and Classification, Learning

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

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May 18, 2024

Contents

Supervised learning

A training multi-set of examples is available. Correct answers (hidden state, class, the quantity we want to predict) are *known* for all training examples.

Classification :

- Nominal dependent variable
- Examples: predict spam/ham based on email contents, predict 0/1/.../9 based on the image of a number, etc.

Regression :

- Quantitative/continuous dependent variable
- Examples: predict temperature in Prague based on date and time, predict height of a person based on weight and gender, etc.

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Learning: minimization of empirical risk

- Given the set of parametrized strategies $\delta\colon \mathcal{X} \to \mathcal{D}$, penalty/loss function $\ell\colon \mathcal{S} \times \mathcal{D} \to \mathbb{R}$, the quality of each strategy δ could be described by the risk

$$R(\delta) = \sum_{s \in \mathcal{S}} \sum_{x \in \mathcal{X}} P(x, s)\ell(s, \delta(x)),$$

  but P is unknown.

- We thus use the empirical risk R_{emp}, i.e., average loss on training (multi)set $\mathcal{T} = \{(x^{(i)}, s^{(i)})\}_{i=1}^{N}$, $x \in \mathcal{X}$, $s \in \mathcal{S}$:

$$R_{\mathrm{emp}}(\delta) = \frac{1}{N} \sum_{(x^{(i)}, s^{(i)}) \in \mathcal{T}} \ell(s^{(i)}, \delta(x^{(i)})).$$

- Optimal strategy $\delta^* = \operatorname{argmin}_{\delta} R_{\mathrm{emp}}(\delta)$.
- We assume data $\mathcal{T}$ are from distribution $P(x, s)$.

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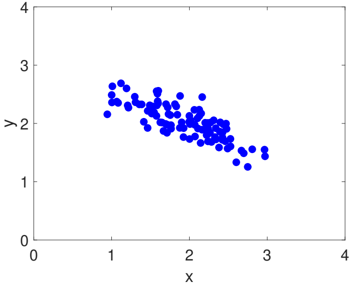
Quiz: Line fitting

We would like to fit a line of the form $\widehat{y} = w_0 + w_1 x$ to the following data:



The parameters of a line with the best fit will likely be

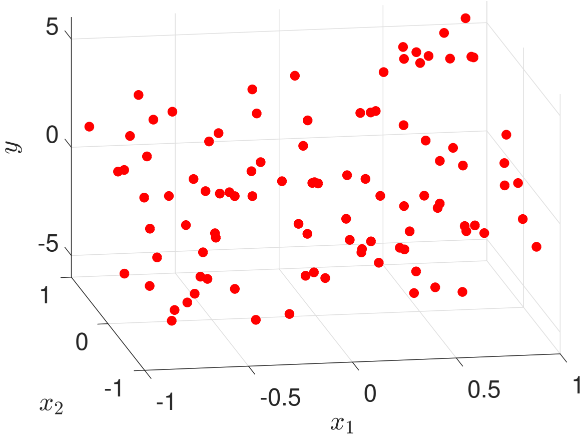
A $w_0 = -1,\ w_1 = -2$

B $w_0 = -\frac{1}{2},\ w_1 = 1$

C $w_0 = 3,\ w_1 = -\frac{1}{2}$

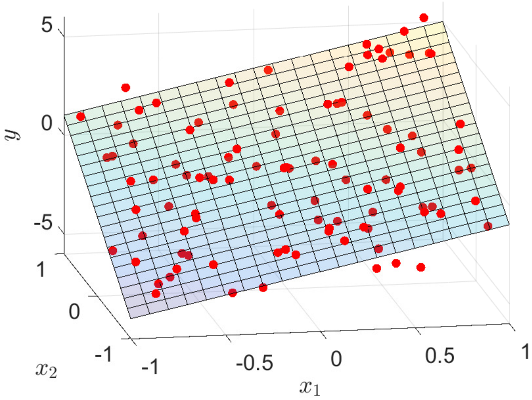
D $w_0 = 2,\ w_1 = \frac{1}{3}$

Linear regression: Illustration



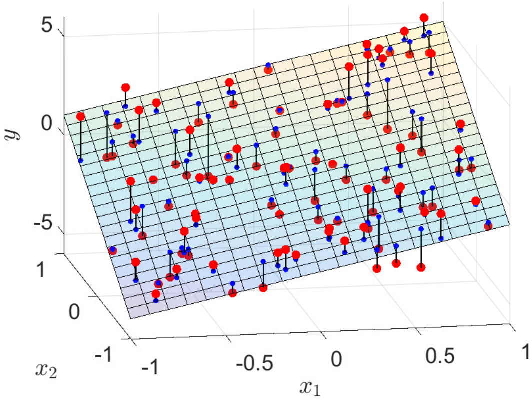
Given a dataset of input vectors $\vec{x}^{(i)}$ and the respective values of output variable $y^{(i)}$ ...

Linear regression: Illustration



. . . we would like to find a linear model of this dataset . . .

Linear regression: Illustration



... minimizing the errors between target values and the model predictions.

Regression

Reformulating Linear algebra in a machine learning language.

Regression task is a supervised learning task, i.e.

- a training (multi)set $\mathcal{T} = \{(\vec{x}^{(1)}, y^{(1)}), \ldots, (\vec{x}^{(N)}, y^{(N)})\}$ is available, where
- the labels $y^{(i)}$ are *quantitative*, often *continuous* (as opposed to classification tasks where $y^{(i)}$ are nominal).
- Its purpose is to model the relationship between independent variables (inputs) $\vec{x} = (x_1, \ldots, x_D)$ and the dependent variable (output) y.

Linear Regression

Linear regression uses a particular regression model which assumes (and learns) linear relationship between the inputs and the output:

$$\widehat{y} = \delta(\vec{x}) = w_0 + w_1 x_1 + \ldots + w_D x_D = w_0 + \langle \vec{w}, \vec{x} \rangle = w_0 + \vec{w}^\top \vec{x},$$

where

- $\widehat{y}$ is the model *prediction* (*estimate* of the true value y),
- $\delta(\vec{x})$ is the decision strategy (a linear model in this case),
- $w_0, \ldots, w_D$ are the coefficients of the linear function (weights), w_0 is the *bias*,
- $\langle \vec{w}, \vec{x} \rangle$ is a *dot product* of vectors $\vec{w}$ and $\vec{x}$ (scalar product),
- which can be also computed as a matrix product $\vec{w}^\top \vec{x}$ if $\vec{w}$ and $\vec{x}$ are *column vectors*, i.e. matrices of size $[D \times 1]$.

Notation remarks

Homogeneous coordinates :

- If we add "1" as the first element of $\vec{x}$ so that $\vec{x} = (1, x_1, \ldots, x_D)$, and
- if we include the bias term w_0 in the vector $\vec{w}$ so that $\vec{w} = (w_0, w_1, \ldots, w_D)$, then

$$\widehat{y} = \delta(\vec{x}) = w_0 \cdot 1 + w_1 x_1 + \ldots + w_D x_D = \langle \vec{w}, \vec{x} \rangle = \vec{w}^\top \vec{x}.$$

Matrix notation: If we organize the data $\mathcal{T}$ into matrices $\mathbf{X}$ and $\mathbf{Y}$, such that

$$\mathbf{X} = \begin{pmatrix} 1 & \ldots & 1 \\ \vec{x}^{(1)} & \ldots & \vec{x}^{(N)} \end{pmatrix} \quad \text{and} \quad \mathbf{Y} = \left(y^{(1)}, \ldots, y^{(N)}\right),$$

then we can write a batch computation of predictions for all data in $\mathbf{X}$ as

$$\widehat{\mathbf{Y}} = \left(\delta(\vec{x}^{(1)}), \ldots, \delta(\vec{x}^{(N)})\right) = \left(\vec{w}^\top \vec{x}^{(1)}, \ldots, \vec{w}^\top \vec{x}^{(N)}\right) = \vec{w}^\top \mathbf{X}.$$

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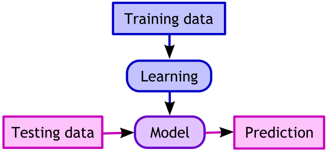
Two operation phases of ML models

Any ML model has 2 operation phases:

1. learning (training, fitting) of δ and
2. application of δ (testing, making predictions).



The strategy δ can be viewed as a function of 2 variables: $\delta(\vec{x}, \vec{w})$.

Model application (Inference): Given $\vec{w}$, we can manipulate $\vec{x}$ to make predictions:

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Model learning: Given $\mathcal{T}$, we can tune the model parameters $\vec{w}$ to fit the model to the data:

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where usually $J(\vec{w}, \mathcal{T}) = \dfrac{1}{|\mathcal{T}|} \sum_{(\vec{x},y)\in\mathcal{T}} \ell(y, \delta(\vec{x}, \vec{w}))$. How to train the model?

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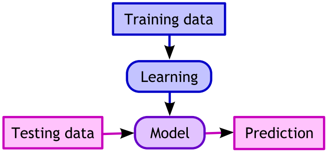

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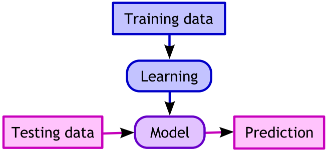

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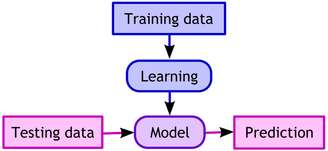

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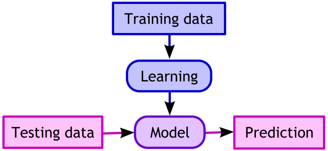

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Example: Simple (univariate) linear regression

Simple regression

- $\vec{x}^{(i)} = x^{(i)}$, i.e., the examples are described by a single feature (they are 1-dimensional).
- Find parameters w_0, w_1 of a linear model $\hat{y} = w_0 + w_1 x$
  given a training (multi)set $\mathcal{T} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$.

How many lines can be fit to N linearly independent training examples?

- $N = 1$ (1 equation, 2 parameters) $\Rightarrow \infty$ linear functions with zero error
- $N = 2$ (2 equation, 2 parameters) $\Rightarrow$ 1 linear function with zero error
- $N \geq 3$ (> 2 equation, parameters) $\Rightarrow$ no linear function with zero error
  $\Rightarrow$ but we can fit a line which minimizes the "size" of error $y - \widehat{y}$:

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The least squares method

Choose such parameters $\vec{w}$ which minimize the *mean squared error* (MSE)

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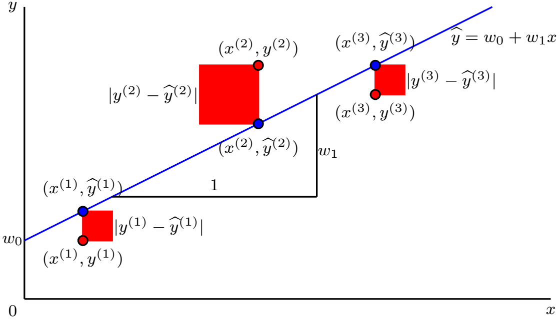
$$= \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \delta_{\vec{w}}(\vec{x}^{(i)})\right)^2 .$$



Is there a (closed-form) solution? Explicit solution:

$$w_1 = \frac{\sum_{i=1}^{N}(x^{(i)} - \bar{x})(y^{(i)} - \bar{y})}{\sum_{i=1}^{N}(x^{(i)} - \bar{x})^2} = \frac{s_{xy}}{s_x^2} = \frac{\text{covariance of } X \text{ and } Y}{\text{variance } X} \qquad w_0 = \bar{y} - w_1\bar{x}$$

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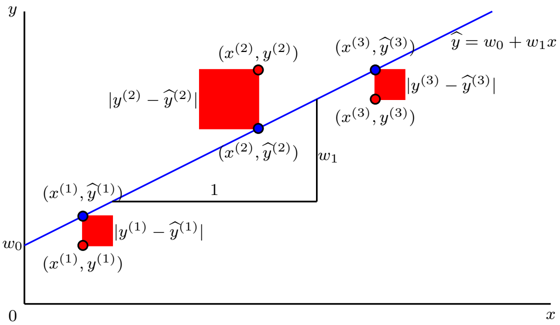

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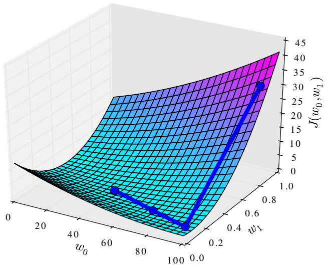
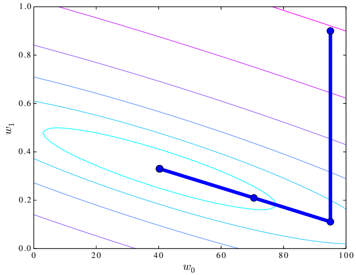
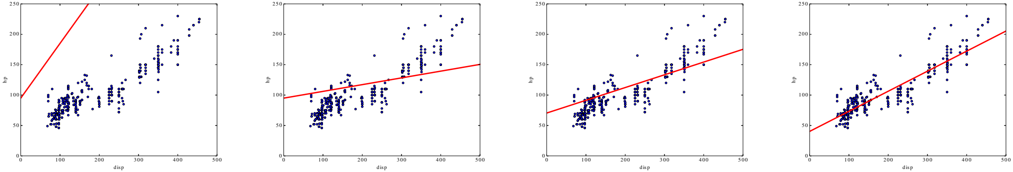
Universal fitting method: minimization of cost function J

The landscape of J in the space of parameters w_0 and w_1 (for the data below):





Gradually better linear models found by an optimization method (BFGS):



Gradient descent algorithm

Given a function $J(w_0, w_1)$ that should be minimized,

- start with a guess of w_0 and w_1 and
- change it, so that $J(w_0, w_1)$ decreases, i.e.
- update our current guess of w_0 and w_1 by taking a step in the direction opposite to the gradient:

$$\vec{w} \leftarrow \vec{w} - \alpha \nabla J(w_0, w_1), \text{ i.e.}$$
$$w_i \leftarrow w_i - \alpha \frac{\partial}{\partial w_i} J(w_0, w_1),$$

where all w_is are updated simultaneously and α is a learning rate (step size).

Gradient descent for MSE minimization

For the cost function

$$J(w_0, w_1) = \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - \delta_{\vec{w}}(x^{(i)}) \right)^2 = \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - (w_0 + w_1 x^{(i)}) \right)^2 ,$$

the gradient can be computed as

$$\frac{\partial}{\partial w_0} J(w_0, w_1) = -\frac{2}{N} \sum_{i=1}^{N} \left(y^{(i)} - \delta_{\vec{w}}(x^{(i)}) \right)$$

$$\frac{\partial}{\partial w_1} J(w_0, w_1) = -\frac{2}{N} \sum_{i=1}^{N} \left(y^{(i)} - \delta_{\vec{w}}(x^{(i)}) \right) x^{(i)}$$

Multivariate linear regression

- $\vec{x}^{(i)} = (x_1^{(i)}, \dots, x_D^{(i)})^\top$, i.e. the examples are described by more than 1 feature (they are D-dimensional).
- Find the parameters $\vec{w} = (w_0, \dots, w_D)^\top$ of a linear model $\widehat{y} = \vec{w}^\top \vec{x}$ given the training (multi)set $\mathcal{T} = \{(\vec{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$.

Training: we would like
for each (i): $y^{(i)} = \vec{w}^\top \vec{x}^{(i)}$.
Or, in the matrix form: $\mathbf{Y} = \vec{w}^\top \mathbf{X}$

What is the shape of $\mathbf{X}$?

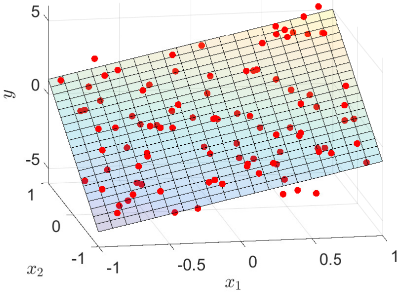
A $(D+1) \times (D+1)$

B $(D+1) \times N$

C $N \times (D+1)$

D $N \times N$

The model is a *hyperplane* in the $(D+1)$-dimensional space.



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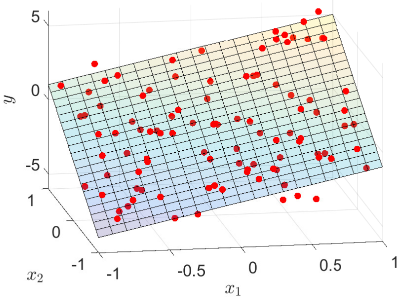

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Multivariate linear regression: learning

1. Numeric optimization of $J(\vec{w}, T)$:
   - Works as for simple regression, it only searches a space with more dimensions.
   - Sometimes one needs to tune some parameters of the optimization algorithm to work properly (learning rate in gradient descent, etc.).
   - May be slow (many iterations needed), but works even for very large D.

2. Normal equation :

$$\vec{w}^* = (\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{X}\mathbf{Y}^\top$$

   - Method to solve for the optimal $\vec{w}^*$ analytically!
   - No need to choose optimization algorithm parameters. No iterations.
   - Needs to compute $(\mathbf{X}\mathbf{X}^\top)^{-1}$, which is $O((D+1)^3)$. Becomes intractable for large D.

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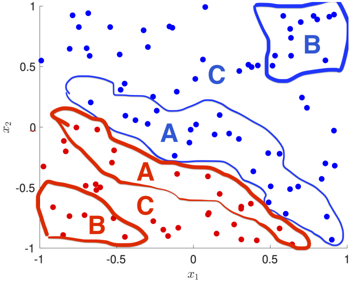
- Binary classification
- Discriminant function
- Classification as a regression problem (linear, logistic regression)
- What is the right loss function?
- Etalon classifier (meeting nearest neighbour and linear classifier)
- Acuracy vs precision

Quiz: Importance of training examples



Intuitively, which of the training data points should have the biggest influence on the decision whether a new, unlabeled data point shall be red or blue?

- **A** Those which are closest to data points with the opposite color.
- **B** Those which are farthest from the data points of the opposite color.
- **C** Those which are near the middle of the points with the same color.
- **D** None. All of the data points have the same importance.

Binary classification task

Let's have a training dataset $\mathcal{T} = \{(\vec{x}^{(1)}, y^{(1)}), \ldots, (\vec{x}^{(N)}, y^{(N)})$:

- each example described by a vector $\vec{x} = (x_1, \ldots, x_D)$,
- labeled with the correct class $y \in \{+1, -1\}$.

The goal:

- Find the classifier (decision strategy/rule) δ that minimizes the empirical risk $R_{\mathrm{emp}}(\delta)$.

Discriminant function

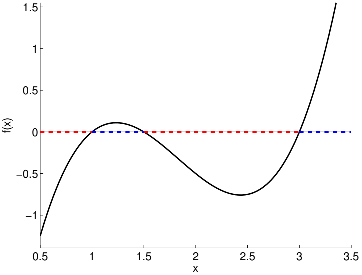
Discriminant function $f(\vec{x})$:

- It assigns a real number to each observation $\vec{x}$. It may be linear or non-linear.
- For 2 classes, 1 discriminant function is enough.
- It is used to create a **decision rule** (which then assigns a class to an observation):

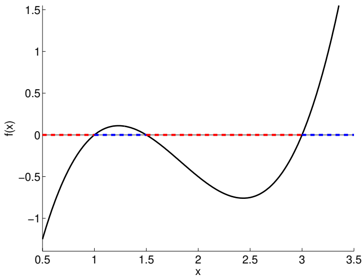
$$\widehat{y} = \delta(\vec{x}) = \begin{cases} +1 & \text{iff} \quad f(\vec{x}) > 0, \text{ and} \\ -1 & \text{iff} \quad f(\vec{x}) < 0, \end{cases}$$

i.e., $\widehat{y} = \delta(\vec{x}) = \operatorname{sign}(f(\vec{x}))$.

- Decision boundary: $\{\vec{x} | f(\vec{x}) = 0\}$
- Linear classification: **the decision boundaries must be linear.**
- *Learning* then amounts to finding a suitable function f (or its parameters).



Discriminant function



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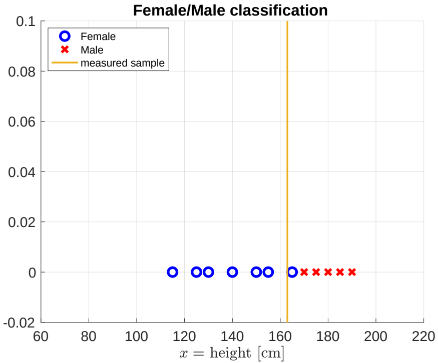
Example: Female/Male classification based on height

Training (multi)set $\mathcal{T} = \{(x^{(i)}, s^{(i)})\}_{i=1}^{N}$, $x^{(i)} \in \mathcal{X}$, $s^{(i)} \in \mathcal{S} = \{F, M\}$

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
Gender $y^{(i)}$ (+1/-1)	-1	-1	-1	-1	-1	-1	-1	+1	+1	+1	+1	+1



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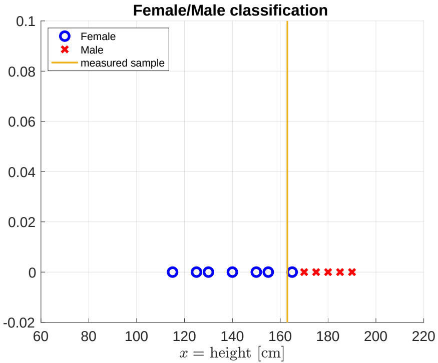
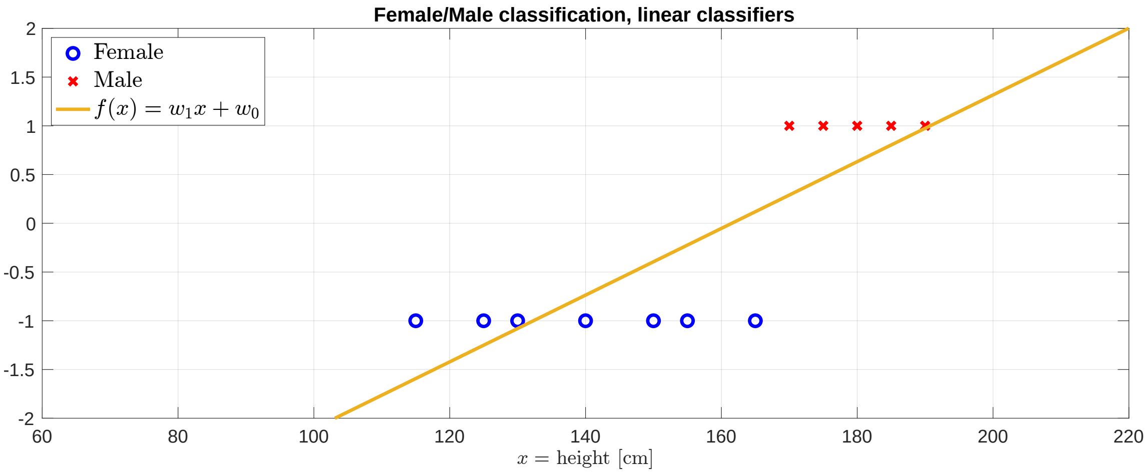


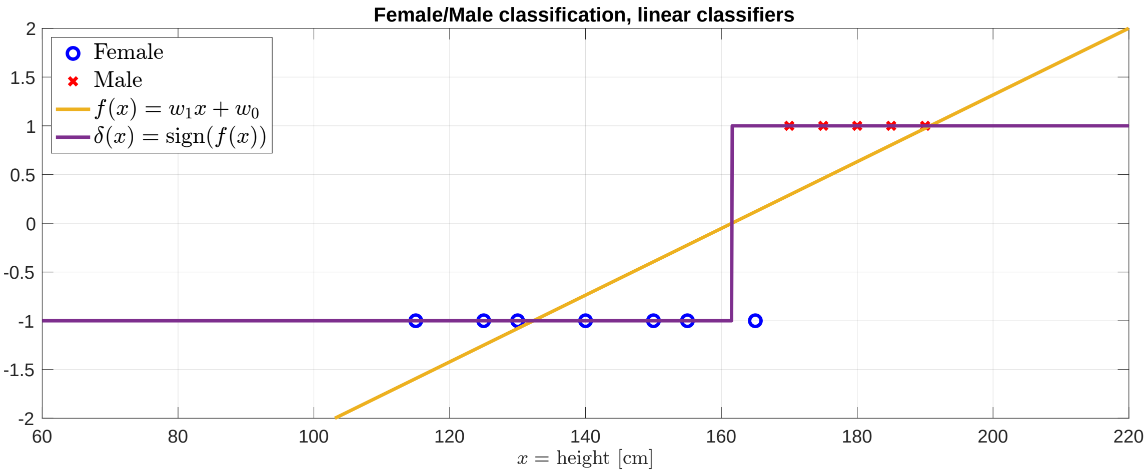
A new point to clasify: $x^Q = 163$

Which class does x^Q belong to? $\delta(x^Q) = ?$

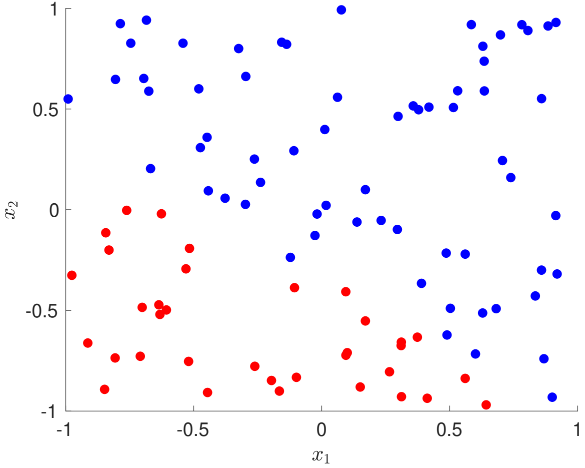
Example: Linear discr. function, LSQ fit



Example: Corresponding decision strategy

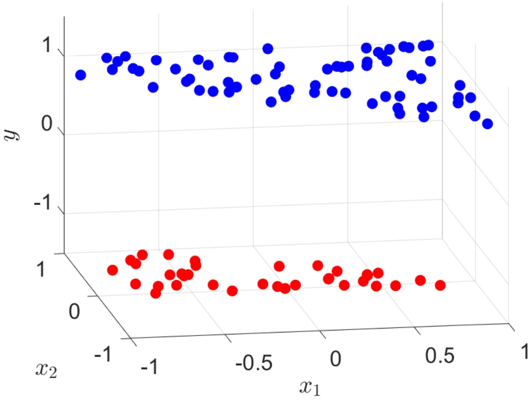


Learning linear classifier: naive approach



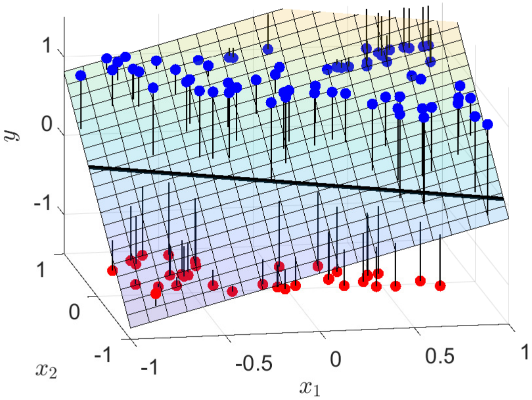
Let's have a dataset of input vectors $\vec{x}^{(i)}$ and their classes $s^{(i)}$.

Learning linear classifier: naive approach



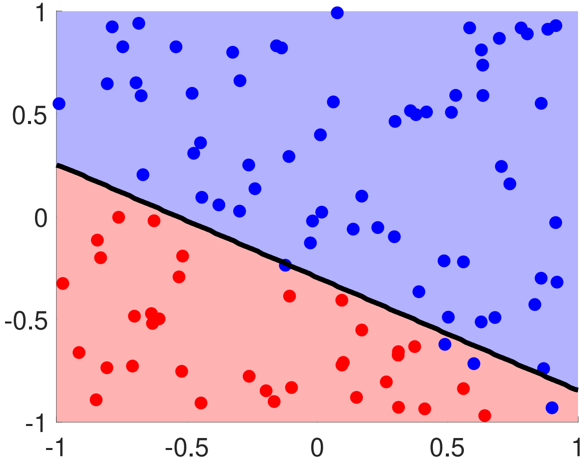
Let's encode the classes corresponding $y^{(i)} = -1$ or $y^{(i)} = 1$.

Learning linear classifier: naive approach



Let's fit a linear discriminant function by minimizing MSE as in regression.
The contour line $y = 0$ ...

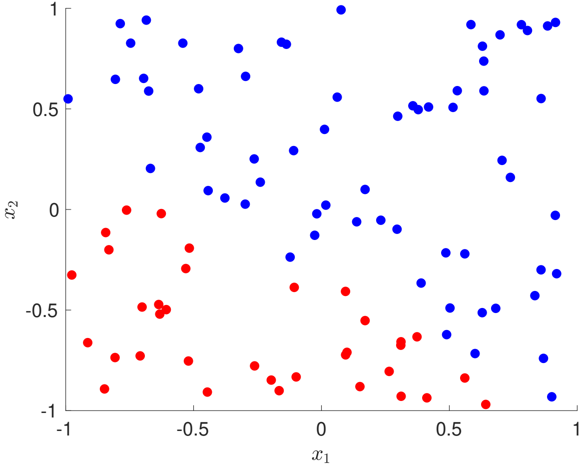
Learning linear classifier: naive approach



. . . then forms a linear decision boundary in the original 2D space.
But is such a classifier good in general?

Can we do better than fitting a linear function?

Fitting a better function: Logistic regression



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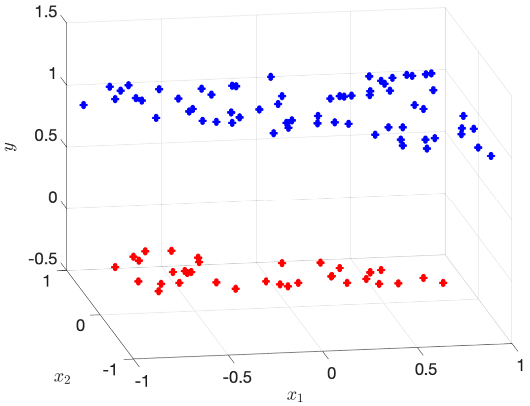
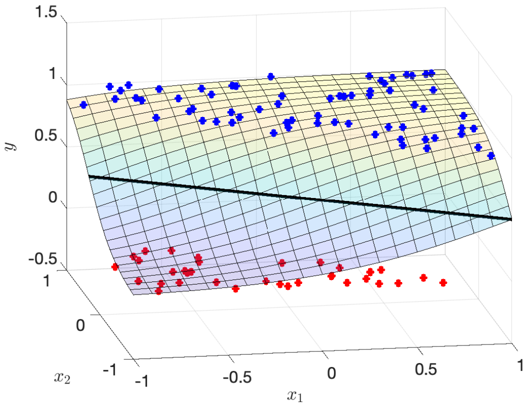


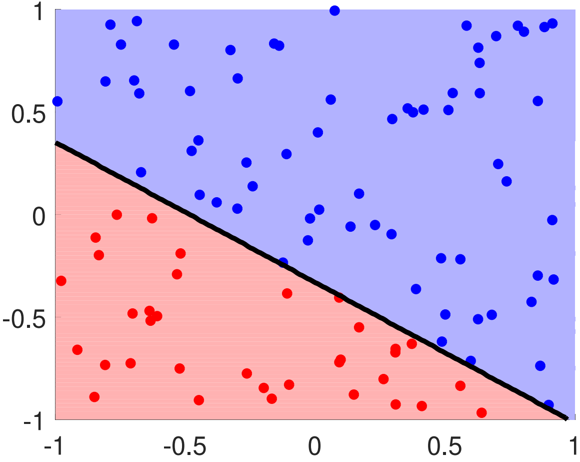
Let's encode the classes corresponding $y^{(i)} = 0$ or $y^{(i)} = 1$.

Fitting a better function: Logistic regression



Let's fit a **sigmoidal** discriminant function by minimizing MSE as in regression.
The contour line $y = 0.5$ ...

Fitting a better function: Logistic regression



. . . then forms a linear decision boundary in the original 2D space.

Logistic regression model

Logistic regression uses a discriminant function which is a nonlinear transformation of the values of a linear function

$$f_{\vec{w}}(\vec{x}) = g(\vec{w}^\top \vec{x}) = \frac{1}{1 + e^{-\vec{w}^\top \vec{x}}},$$

where $g(z) = \dfrac{1}{1 + e^{-z}}$ is the sigmoid function (a.k.a logistic function).

Interpretation of the model:

- $f_{\vec{w}}(\vec{x})$ can be interpretted as an estimate of the probability that $\vec{x}$ belongs to class 1.
- The decision boundary is defined using a level-set/countour $\{\vec{x} : f_{\vec{w}}(\vec{x}) = 0.5\}$.
- Logistic *regression* is a *classification* model!
- The discriminant function $f_{\vec{w}}(\vec{x})$ itself is not linear anymore; but the *decision boundary is still linear!*
- Thanks to the sigmoidal transformation, logistic regression is much less influenced by examples that are far from the decision boundary!

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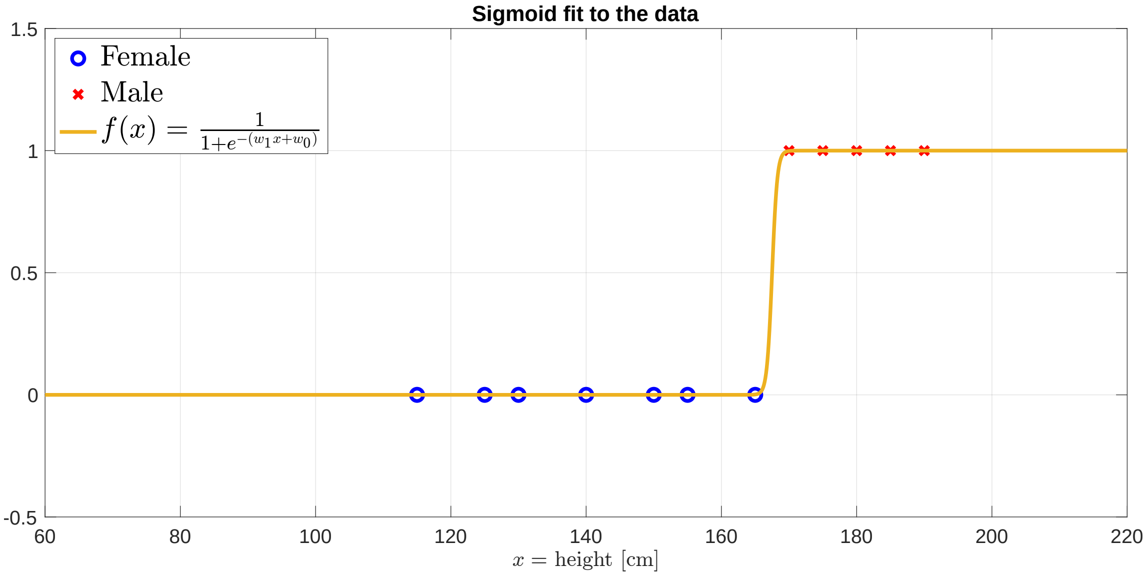
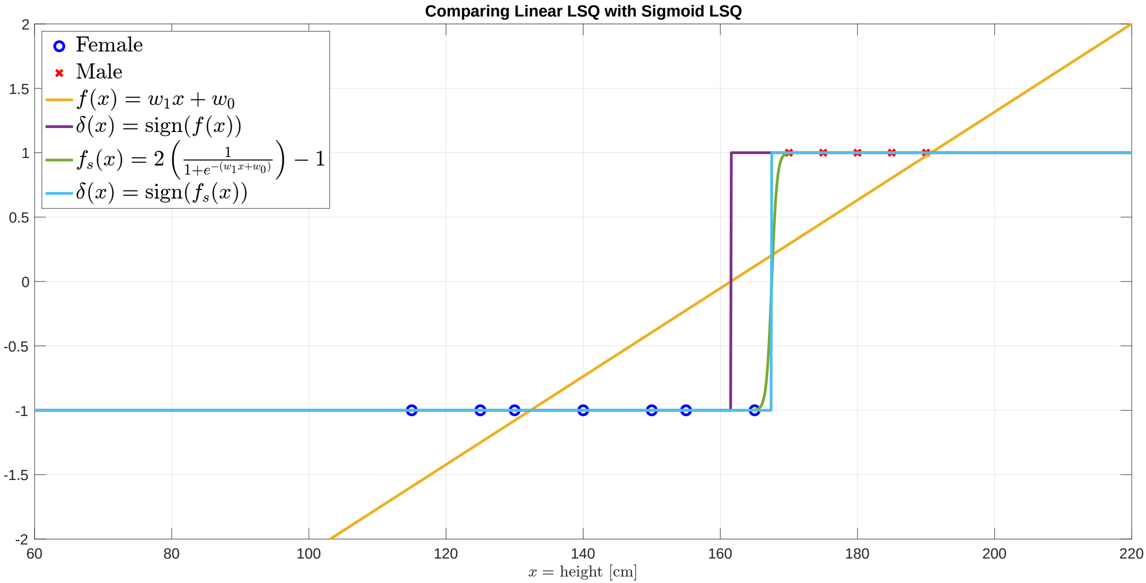
LSQ fit of a sigmoid



Comparing Linear and Sigmoid LSQ fit



What loss function ℓ is suitable?

To train the logistic regression model, one can minimize the J_{MSE} criterion:

- a non-convex, multimodal landscape which is hard to optimize.

Logistic regression uses a loss function called "cross-entropy":

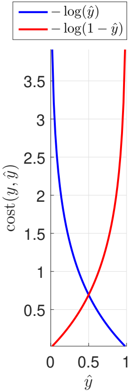
$$J(\vec{w}, \mathcal{T}) = \frac{1}{N}\sum_{i=1}^{N} \ell(y^{(i)}, f_{\vec{w}}(\vec{x}^{(i)})), \text{ where}$$

$$\ell(y, \widehat{y}) = \begin{cases} -\log(\widehat{y}) & \text{if } y = 1 \\ -\log(1-\widehat{y}) & \text{if } y = 0 \end{cases},$$

which can be rewritten in a single expression as

$$\ell(y, \widehat{y}) = -y \cdot \log(\widehat{y}) - (1-y) \cdot \log(1-\widehat{y}).$$

- Easier to optimize for numerical solvers.



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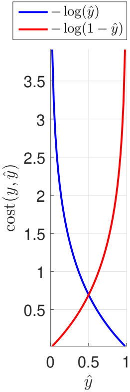
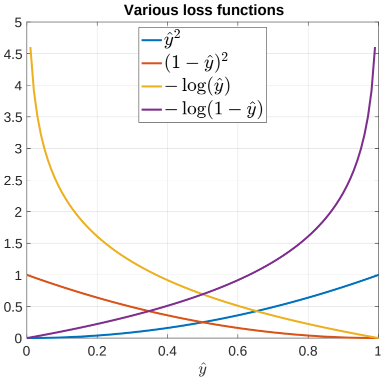
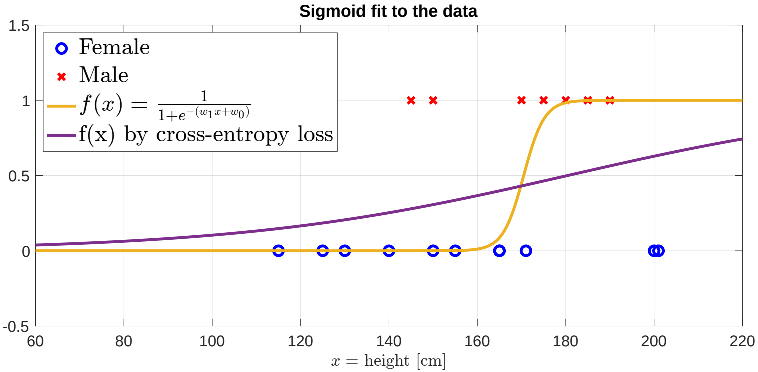


MSE vs cross entropy loss



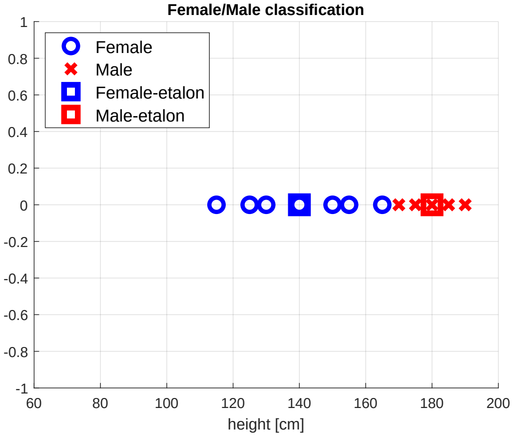


Sigmoidal $f(x)$ can be also interpreted as $P(s = \text{Male} \mid x)$: direct learning of a discriminative model .

Cross-entropy loss strongly penalizes hard errors, complete mismatches.

Alternative idea: Etalons

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



$$e_F = \mathrm{ave}(\{x^{(i)} : s^{(i)} = F\}) = 140$$
$$e_M = \mathrm{ave}(\{x^{(i)} : s^{(i)} = M\}) = 180$$

$x^Q = 163$

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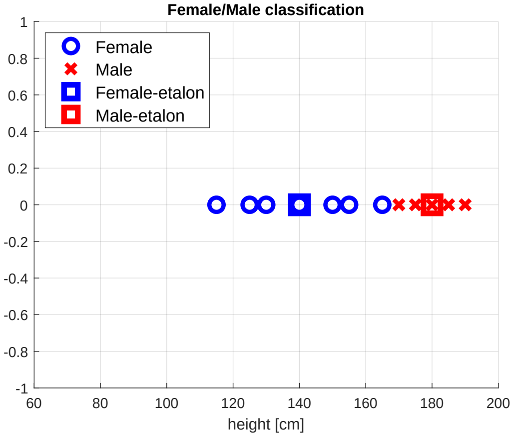

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A $d^Q = F$

B $d^Q = M$

C Both classes equally likely

D Cannot provide any decision

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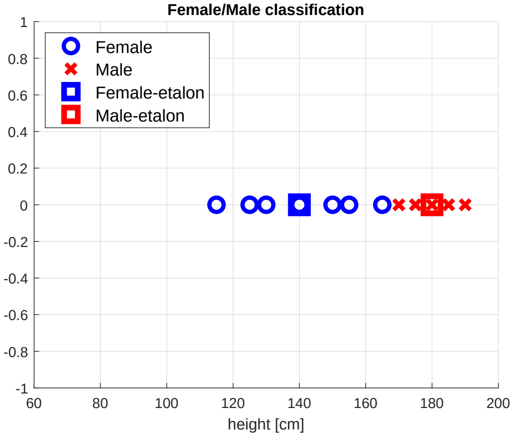

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Classify as $d^Q = \text{argmin}_{s \in \mathcal{S}} \text{dist}(x^Q, e_s)$

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

Etalon classifier is a Linear classifier!

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

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

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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

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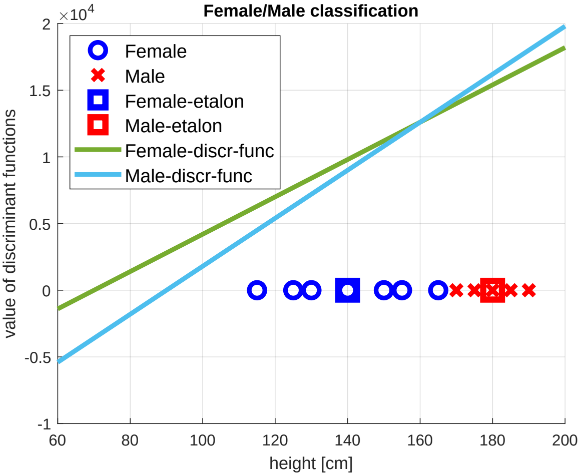
Example: F/M – Linear discriminant functions based on etalons



Discriminant functions for 2 classes:

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

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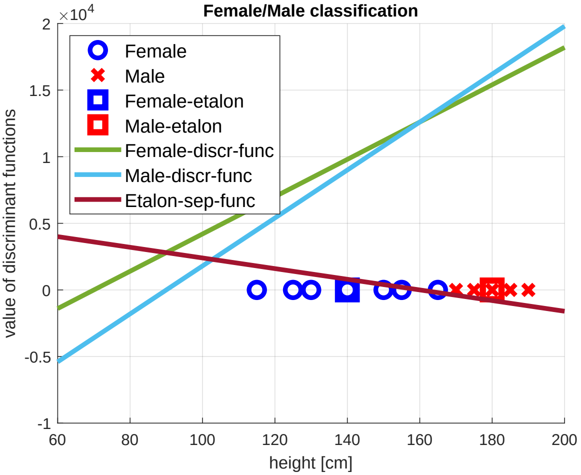

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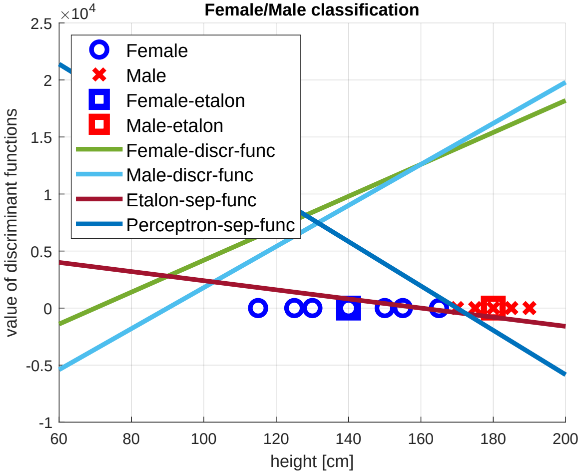
$$= e_M x - \frac{1}{2} e_M^2 = 180x - 16200$$

A single discr. func. separating 2 classes:

$$g(x) = f_F(x) - f_M(x) = $$
$$= -40x + 6400$$

Example: F/M – Can we do better etalons?

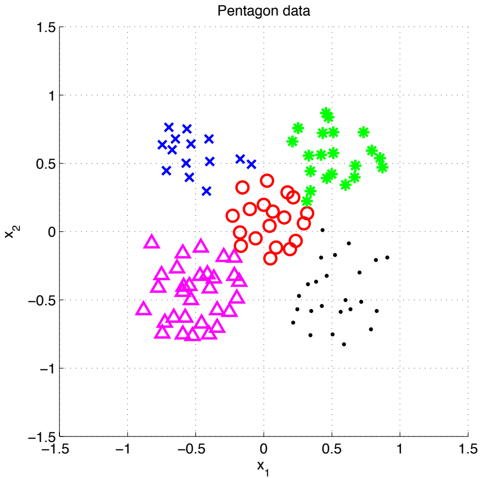


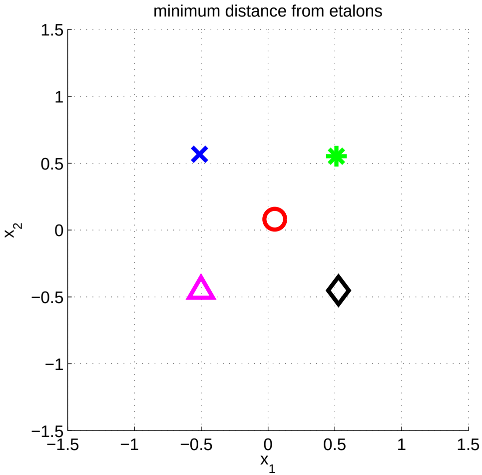
Linear classifiers based on average etalons make some errors.

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

Contents

Etalons in multidimensional spaces





From $\mathcal{T} = \{(\vec{x}^{(i)}, s^{(i)})\}$, extract one etalon $\vec{e}_s$ for each class $s \in \mathcal{S}$.

Etalons in multidimensional spaces (cont.)

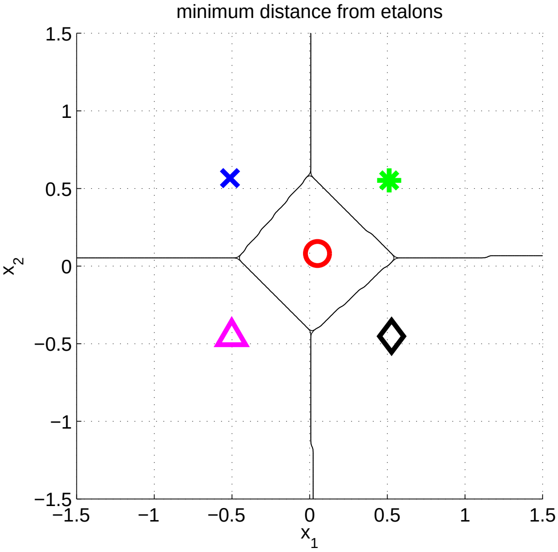
Extract etalon for each class s:

$$\vec{e}_s = \text{ave}(\{\vec{x}^{(i)} : s^{(i)} = s\})$$

Decision strategy

$$\delta(\vec{x}) = \underset{s \in S}{\text{argmin}} \|\vec{x} - \vec{e}_s\|^2$$

The corresponding decision boundaries halve the distances between pairs of etalons.



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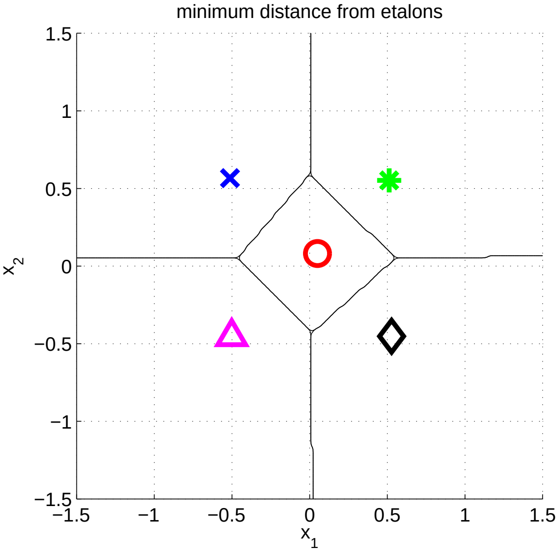

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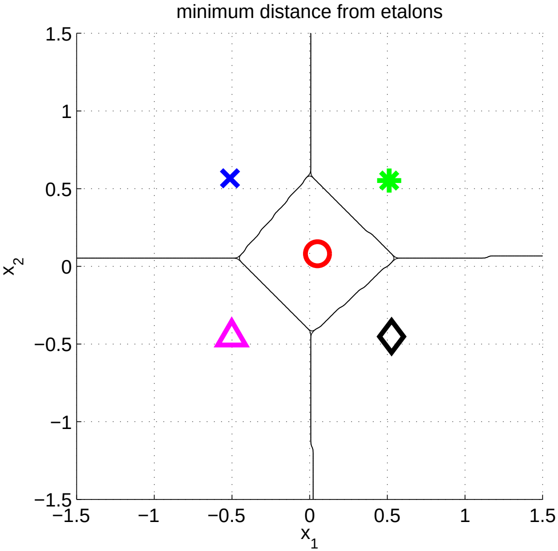
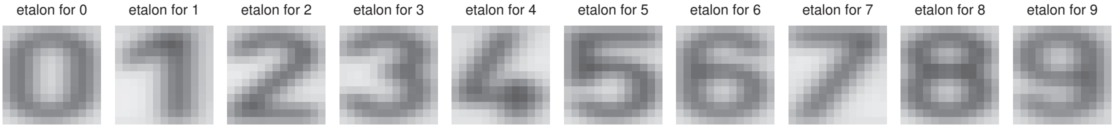


Digit recognition – average-based etalons



Figures from [7].

Contents

Bayesian classification vs Discriminant functions

Decision based on discriminant function:

$$\delta(\vec{x}) = \underset{s \in \mathcal{S}}{\operatorname{argmax}}\, f(\vec{x}, s)$$

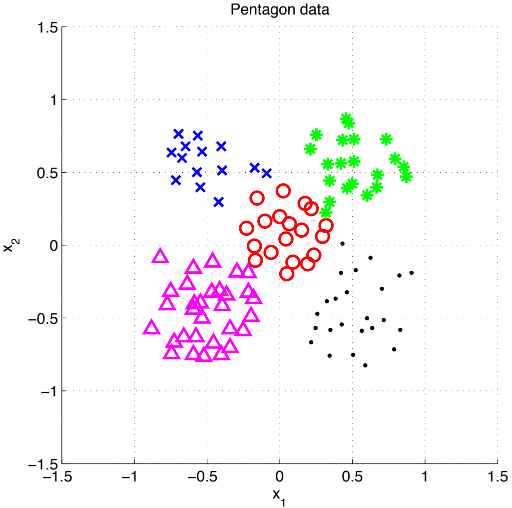
Decision based on posterior prob. (Bayes):

$$\delta(\vec{x}) = \underset{s \in \mathcal{S}}{\operatorname{argmax}}\, P(s|\vec{x}) = \underset{s \in \mathcal{S}}{\operatorname{argmax}}\, \frac{P(\vec{x} \mid s)P(s)}{P(\vec{x})}$$

If we choose

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

the two methods coincide.



Etalon classifier: generalization to higher dimensions

$$
\begin{aligned}
\delta(\vec{x}) &= \operatorname*{argmin}_{s\in S} \|\vec{x} - \vec{e}_s\|^2 = \operatorname*{argmin}_{s\in S}(\vec{x}^\top\vec{x} - 2\,\vec{e}_s^\top\vec{x} + \vec{e}_s^\top\vec{e}_s) = \\
&= \operatorname*{argmin}_{s\in S}\left(\vec{x}^\top\vec{x} - 2\left(\vec{e}_s^\top\vec{x} - \frac{1}{2}(\vec{e}_s^\top\vec{e}_s)\right)\right) = \\
&= \operatorname*{argmax}_{s\in S}\left(\vec{e}_s^\top\vec{x} - \frac{1}{2}(\vec{e}_s^\top\vec{e}_s)\right) = \\
&= \operatorname*{argmax}_{s\in S}(\vec{w}_s^\top\vec{x} + w_{s0}) = \operatorname*{argmax}_{s\in S} g_s(\vec{x}).
\end{aligned}
$$

Linear function (plus offset)

$$
g_s(\vec{x}) = \vec{w}_s^\top\vec{x} + w_{s0}, \quad \text{where} \quad \vec{w}_s = \vec{e}_s \quad \text{and} \quad w_{s0} = -\frac{1}{2}\vec{e}_s^\top\vec{e}_s.
$$

Learning and decision

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

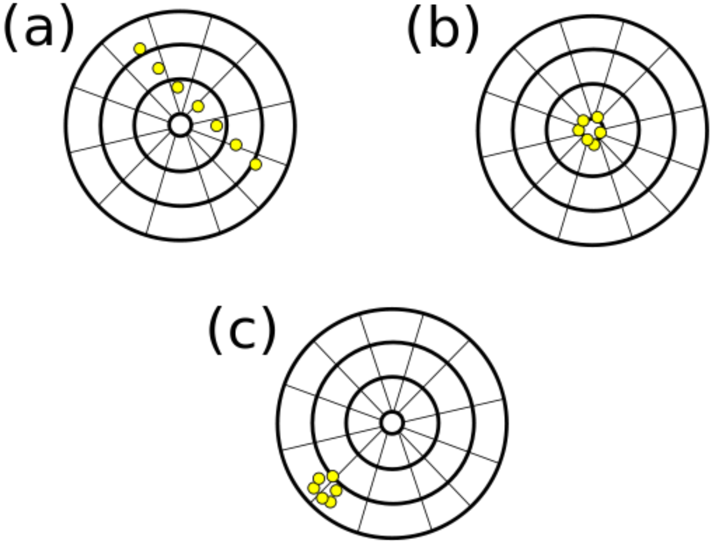
Decision stage - decide about a query $\vec{x}$.

What to learn?

- **Generative model** : Learn $P(\vec{x}, s)$. Decide according to $\mathrm{argmax}_s\, P(s|\vec{x})$.
- **Discriminative model** : Learn directly $P(s|\vec{x})$ and use it for decisions.
- **Discriminant functions** : Learn $f_s(\vec{x})$ and decide according to $\mathrm{argmax}_s\, f_s(\vec{x})$.

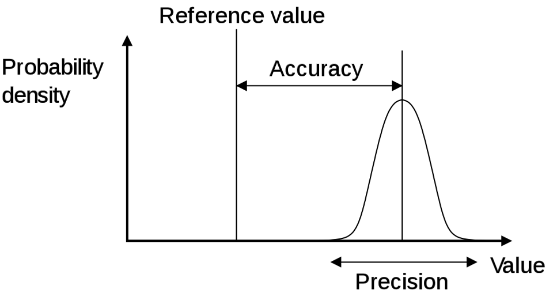
Contents

Accuracy vs precision



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

Accuracy, trueness, precision



- Trueness : closeness of the average to the correct value (systematic error, bias)
- Precision : closeness of individual measurements (variance, repeatability, reproducibility)
- Accuracy : contains both trueness and precision

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

Contents

References I

Further reading: Chapter 18 of [6], 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 [7].
Human deciding and predicting under noise, [4] (in Czech [5])

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