Linear Models for Regression and Classification, Learning

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Notes

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.

Notes

There are more kinds od machine learning:

- Self-supervised
- Unsupervised
- Weakly supervised
- . . .

but this lecture will be about fully supervised learning

Learning by 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} error on training (multi)set $\mathcal{T} = \{(x^{(i)}, s^{(i)})\}_{i=1}^{N}$, $x \in \mathcal{X}$, $s \in \mathcal{S}$:

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

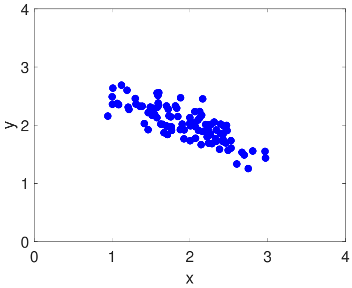
- Optimal strategy $\delta^* = \operatorname{argmin}_\delta R_{\mathrm{emp}}(\delta)$.
- We expect the data are from the right distribution.

Notes

Examples of some method: Perceptron, neural networks, classification trees, ...
It is essentially about statistic, out-of distribution data are always problematic. We can help somewhat to make the methods a bit more robust - to generalize more. Remember regularization trick we learned last week (Laplacian smoothing)?

Quiz: Line fitting

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

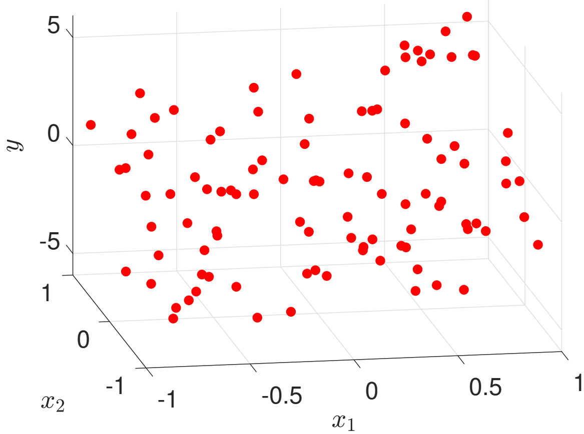


The parameters of a line with a good fit will likely be

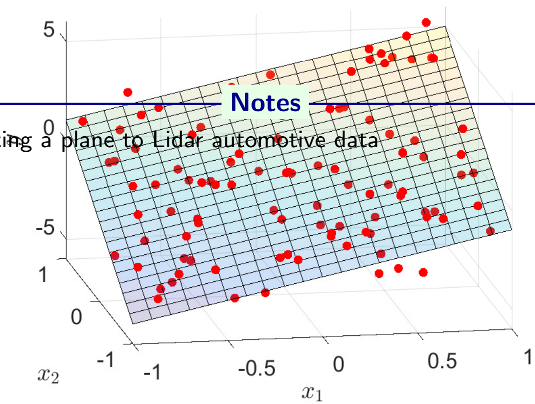
- A $w_0 = -1,\ w_1 = -2$
- B $w_0 = -\frac{1}{2},\ w_1 = 1$
- C $w_0 = 3,\ w_1 = -\frac{1}{2}$
- D $w_0 = 2,\ w_1 = \frac{1}{3}$

Notes

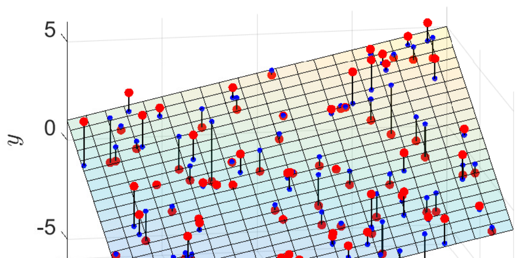
Linear regression: Illustration



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



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



Notes

For instance, think about fitting a plane to Lidar automotive data

Regression

Reformulating Linear algebra in a machine learning language.

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

- a training (multi)set $\mathcal{T} = \{(\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(N)}, y^{(N)})\}$ 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) $\boldsymbol{x} = (x_1, \ldots, x_D)$ and the dependent variable (output) y.

Notes

Linear Regression

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

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

where

- $\widehat{y}$ is the model *prediction* (*estimate* of the true value y),
- $\delta(\boldsymbol{x})$ 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*,
- $\langle \boldsymbol{w}, \boldsymbol{x} \rangle$ is a *dot product* of vectors $\boldsymbol{w}$ and $\boldsymbol{x}$ (scalar product),
- which can be also computed as a matrix product $\boldsymbol{w}^\top \boldsymbol{x}$ if $\boldsymbol{w}$ and $\boldsymbol{x}$ are *column vectors*, i.e. matrices of size $[D \times 1]$.

Notes

Notation remarks

Homogeneous coordinates :

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

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

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

$$\boldsymbol{X} = \begin{pmatrix} 1 & \dots & 1 \\ \boldsymbol{x}^{(1)} & \dots & \boldsymbol{x}^{(N)} \end{pmatrix} \quad \text{and} \quad \boldsymbol{y} = \left(y^{(1)}, \dots, y^{(N)} \right),$$

and similarly with $\widehat{\boldsymbol{y}}$, then we can write a batch computation of predictions for all data in $\boldsymbol{X}$ as

$$\widehat{\boldsymbol{y}} = \left(\delta(\boldsymbol{x}^{(1)}), \dots, \delta(\boldsymbol{x}^{(N)}) \right) = \left(\boldsymbol{w}^\top \boldsymbol{x}^{(1)}, \dots, \boldsymbol{w}^\top \boldsymbol{x}^{(N)} \right) = \boldsymbol{w}^\top \boldsymbol{X}.$$

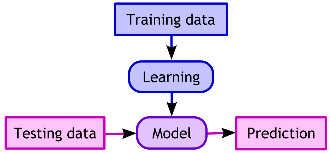
Notes

What are dimensions of $\widehat{\boldsymbol{y}}, \boldsymbol{w}, \boldsymbol{X}$?

Two operation modes

Any ML model has 2 operation modes:

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



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

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

$$\widehat{y} = \delta(\boldsymbol{x}, \boldsymbol{w}) = \delta_{\boldsymbol{w}}(\boldsymbol{x}).$$

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

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} R_{\mathrm{emp}}(\delta_{\boldsymbol{w}}) = \operatorname*{argmin}_{\boldsymbol{w}} J(\boldsymbol{w}, \mathcal{T})$$

$J(\boldsymbol{w}, \mathcal{T})$ and $\ell(\boldsymbol{w}, \mathcal{T})$ are closely related. Optimization criterium $J()$ is a broader term. $\ell()$ essentially measures discrepancy between true data and the predictions. How to train the model?

Notes

All $\ell()$ can be used as $J()$ but not the other way round.

- $\delta(\boldsymbol{x}, \boldsymbol{w})$ represents a whole family of strategies if $\boldsymbol{w}$ is not fixed.
- By fixing $\boldsymbol{w}$ we chose a particular strategy from this family.
- Empirical risk evalautes prediction error on all data points.

Simple (univariate) linear regression

Simple regression

- $\boldsymbol{x}^{(i)} = x^{(i)}$, 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 to fit a line depending on the number of training examples N:

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

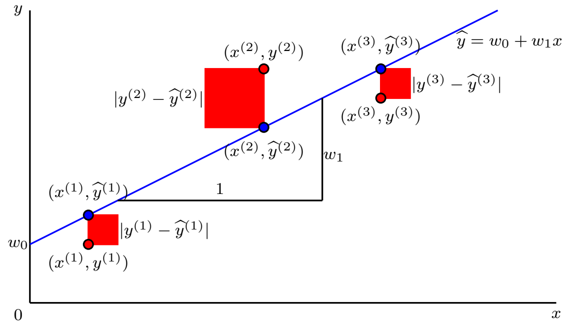
$$\boldsymbol{w}^* = (w_0^*, w_1^*) = \operatorname*{argmin}_{w_0, w_1} R_{\mathrm{emp}}(w_0, w_1) = \operatorname*{argmin}_{w_0, w_1} J(w_0, w_1, \mathcal{T}).$$

Notes

The least squares method

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

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



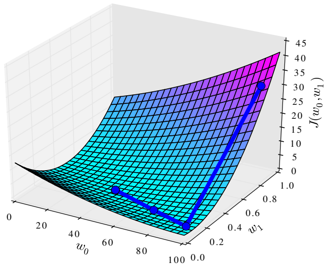
Is there a (closed-form) solution? Explicit solution:

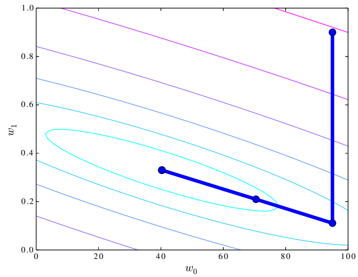
$$w_1 = \frac{\sum_{i=1}^{N}(x^{(i)} - \bar{x})(y^{(i)} - \bar{y})}{\sum_{i=1}^{N}(x^{(i)} - \bar{x})^2} = \frac{s_{xy}}{s_x^2} = \frac{\text{covariance of } X \text{ and } Y}{\text{variance of } X} \qquad w_0 = \bar{y} - w_1\bar{x}$$

Notes

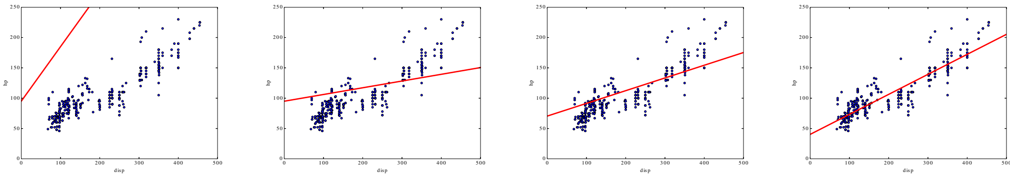
Universal fitting method: minimization of cost function J

The landscape of J in the space of parameters w_0 and w_1:





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



Notes

Bottom images from left to right correspond to points on the polyline above.

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:

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

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

Notes

Gradient descent for MSE minimization

For the cost function

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

the gradient can be computed as

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

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

Notes

Multivariate linear regression

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

Training: foreach (i): $y^{(i)} = \boldsymbol{w}^\top \boldsymbol{x}^{(i)}$.
In the matrix form:

$$\boldsymbol{y} = \boldsymbol{w}^\top \boldsymbol{X}$$

What is the dimension of $\boldsymbol{X}$?

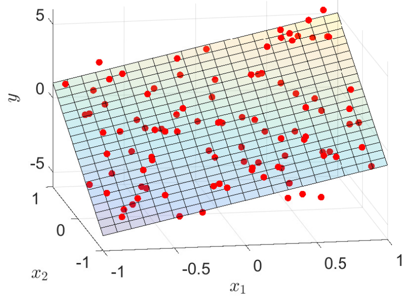
A $(D+1) \times (D+1)$

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.



Notes

Re-write set of (i) equations in to a matrix form:

$$\boldsymbol{y} = \boldsymbol{w}^\top \boldsymbol{X}$$

Inspect dimensions, how are the elements contructed? Quiz

Multivariate linear regression: learning

1. Numeric optimization of $J(\boldsymbol{w}, T)$:
   - 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:

$$\boldsymbol{w}^* = (\boldsymbol{X}\boldsymbol{X}^\top)^{-1}\boldsymbol{X}\boldsymbol{y}^\top$$

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

Notes

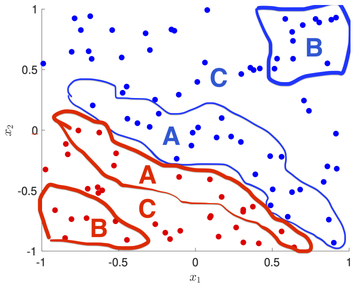
D could by quite big! Think about pixel values in images! We, humans are used to low dimensions - world is 3D, not the machine.

Classification

- 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

Notes

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.

Notes

TS note: A,B,C can be visualized as areas in the figure

Binary classification task

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

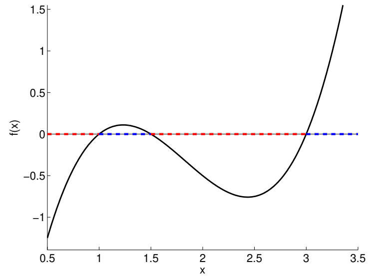
- each example described by a vector $\boldsymbol{x} = (x_1, \ldots, x_D)$,
- labeled with the correct class $y \in \{+1, -1\}$.

The goal:

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

Notes

Discriminant function



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

- It assigns a real number to each observation $\boldsymbol{x}$, 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):

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

  i.e. $\widehat{y} = \delta(\boldsymbol{x}) = \mathrm{sign}(f(\boldsymbol{x}))$.
- Decision boundary: $\{\boldsymbol{x} | f(\boldsymbol{x}) = 0\}$
- Linear classification: the decision boundaries must be linear.
- *Learning* then amounts to finding (suitable parameters of) function f.

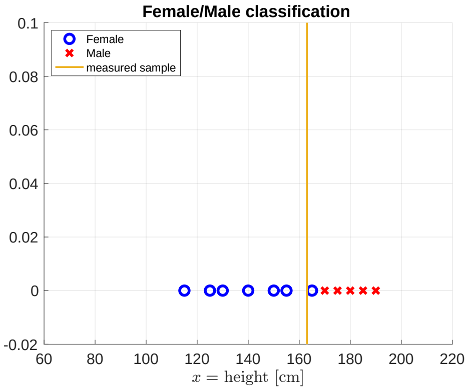
Notes

Linearity is required for the decision boundary not for the discriminant function itself!

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



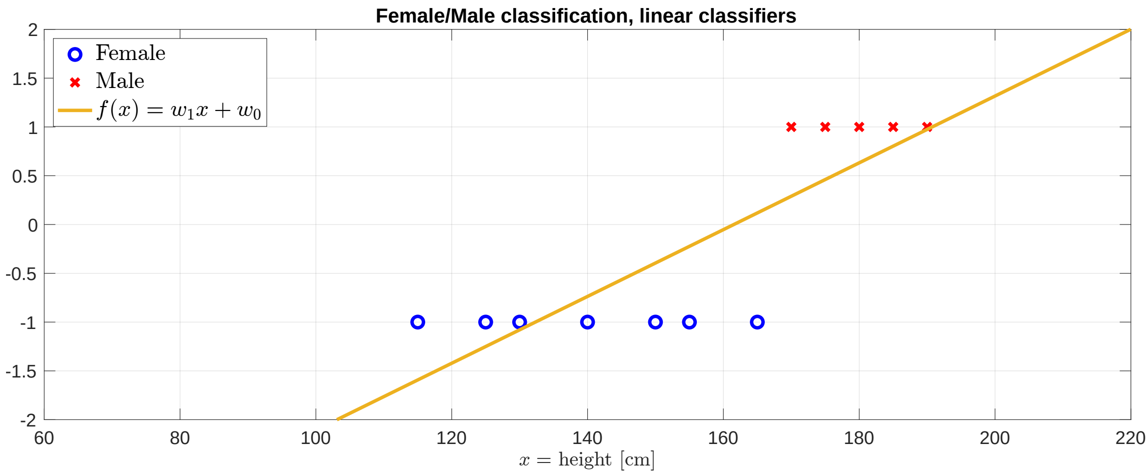
A new point to clasify: $x^Q = 163$

Which class does x^Q belong to? $d^Q = ?$

Notes

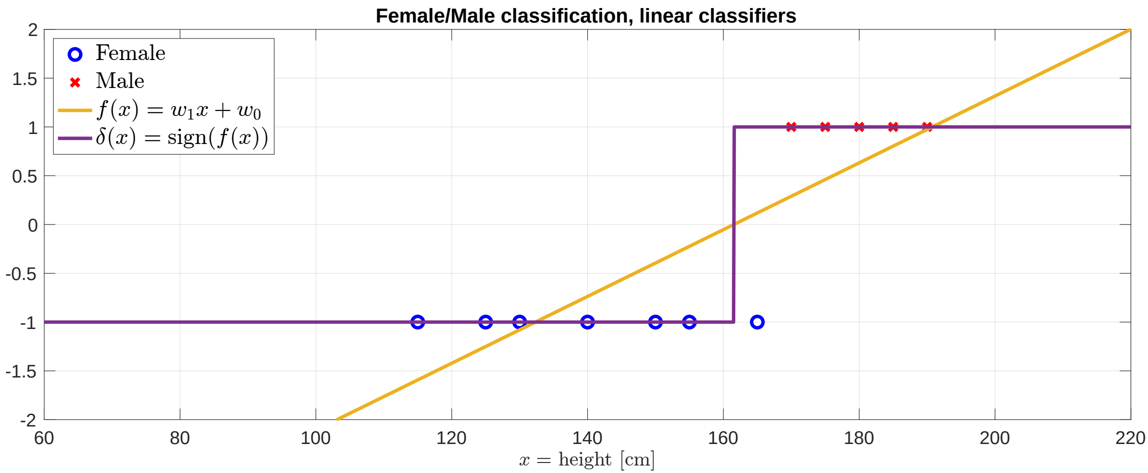
Run `onedim_linclass_learning`

Linear function LSQ fit



Notes

Linear function LSQ fit, discriminant function



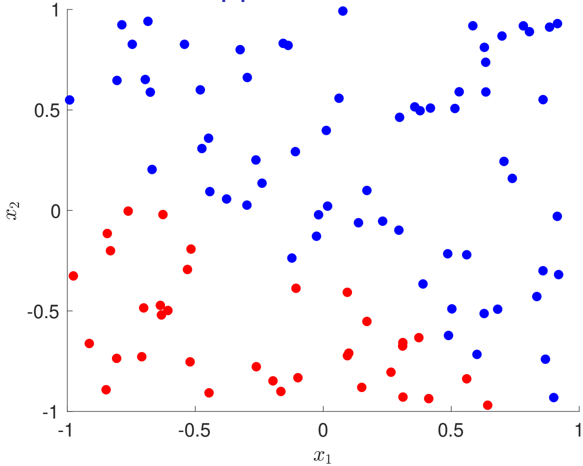
Notes

Can we do better than fitting a linear function?

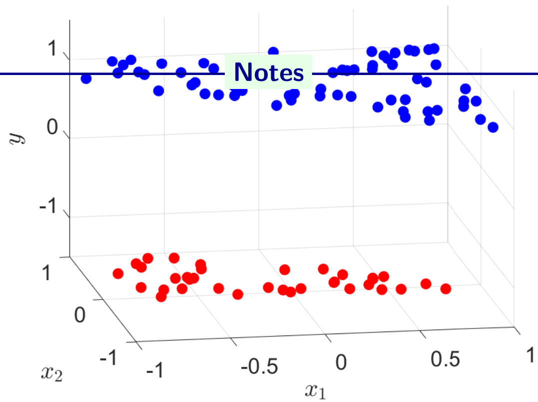
Recap the naive linear approach first.

Notes

Learning linear classifier: naive approach, illustration

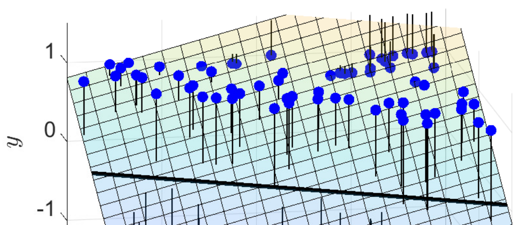


Given a dataset of input vectors $\boldsymbol{x}^{(i)}$ and their classes $y^{(i)}$ ...

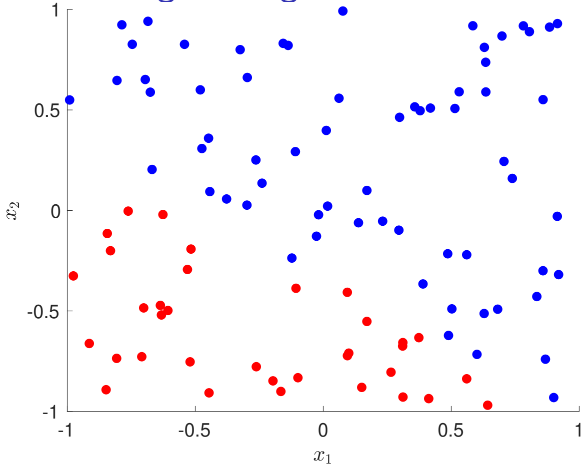


Notes

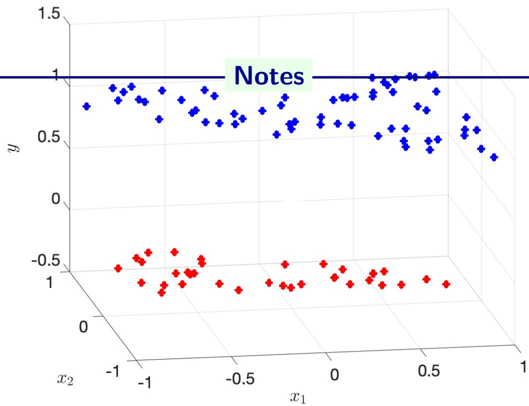
... we shall encode the class label as $y = -1$ and $y = 1$ ...



Fitting a better function: Logistic regression

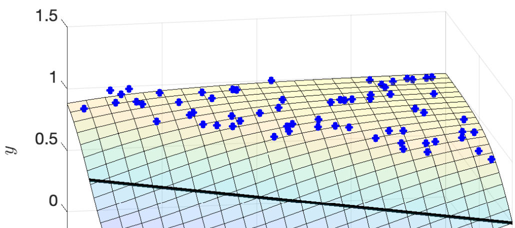


Given a dataset of input vectors $\boldsymbol{x}^{(i)}$ and their classes $y^{(i)}$ ...



Notes

...we shall encode the class label as $y = 0$ and $y = 1$ ...



Logistic regression model

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

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

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

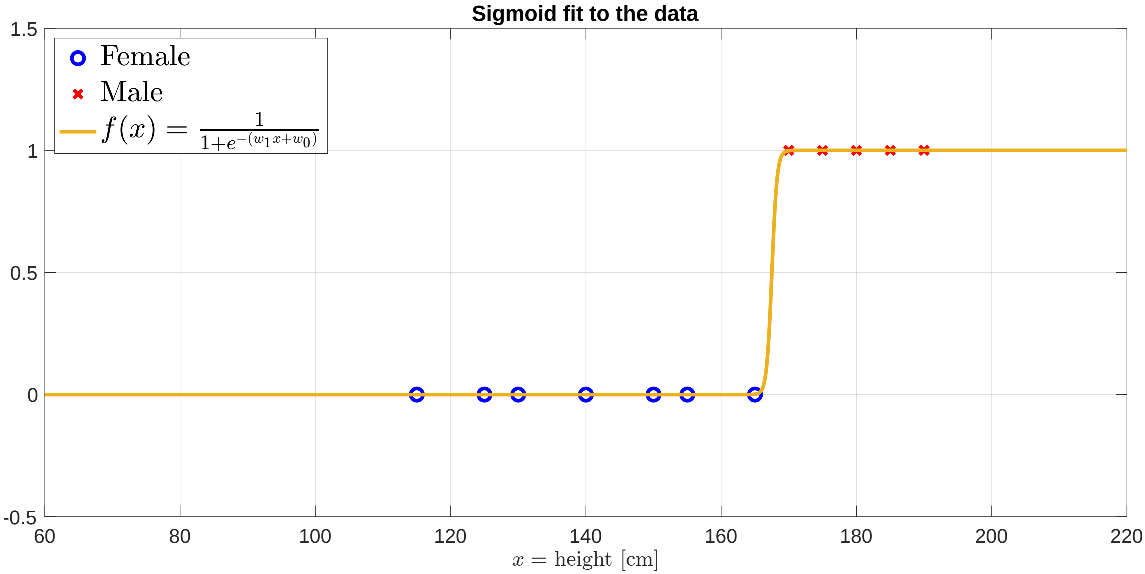
Interpretation of the model:

- $f_{\boldsymbol{w}}(\boldsymbol{x})$ is interpretted as an estimate of the probability that $\boldsymbol{x}$ belongs to class 1.
- The decision boundary is defined using a different level-set: $\{\boldsymbol{x} : f_{\boldsymbol{w}}(\boldsymbol{x}) = 0.5\}$.
- Logistic *regression* is a *classification model!*
- The discriminant function $f_{\boldsymbol{w}}(\boldsymbol{x})$ 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 far from the decision boundary!

Notes

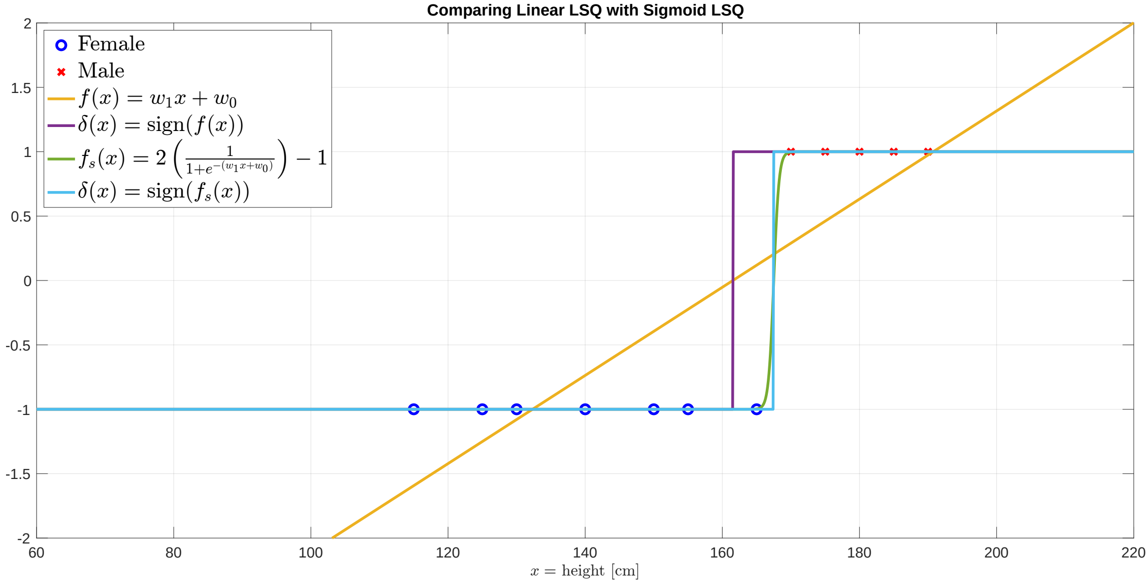
Try to draw the course of the function by hand.

Sigmoid LSQ fit



Notes

Comparing Linear and Sigmoid LSQ fit



Notes

What is the proper loss function ℓ?

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

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

Log. reg. uses a loss function called cross-entropy :

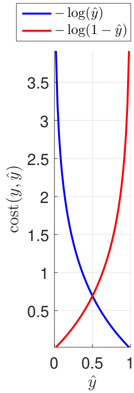
$$J(\boldsymbol{w}, \mathcal{T}) = \frac{1}{N} \sum_{i=1}^{N} \ell(y^{(i)}, f_{\boldsymbol{w}}(\boldsymbol{x}^{(i)})), \text{ where}$$

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

which can be rewritten in a single expression as

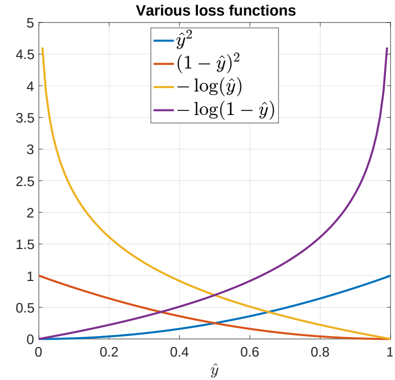
$$\ell(y, \widehat{y}) = -y \cdot \log(\widehat{y}) - (1-y) \cdot \log(1-\widehat{y}).$$

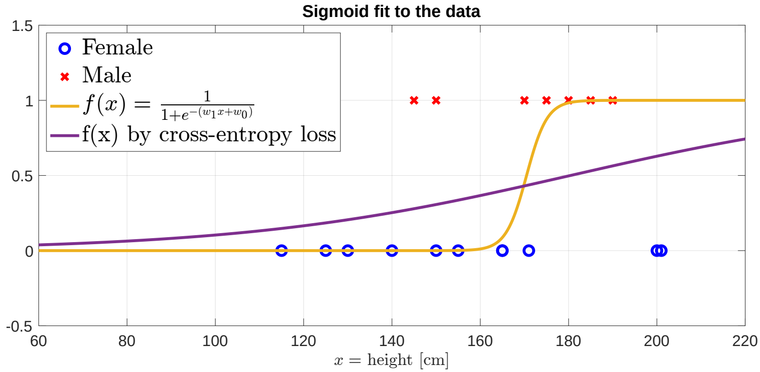
- simpler to optimize for numerical solvers.



Notes

MSE vs cross entropy loss





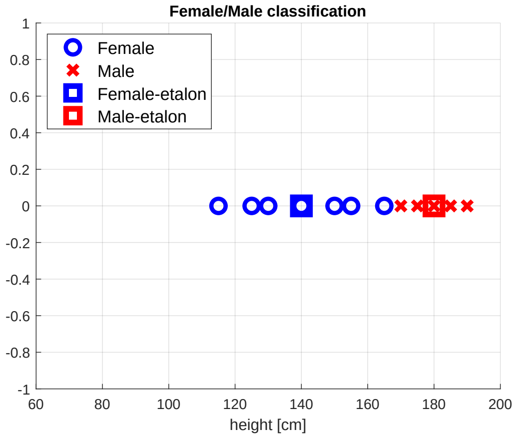
Sigmoidal $f(x)$ can be also interpreted as $p(s = \text{Male} \mid x)$ – Learning **Dicriminative model** directly.

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

Notes

Alternative idea: F/M classification – Etalons

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



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

Based on etalons: $d_Q = ?$

- **A** $d^Q = F$
- **B** $d_Q = M$
- **C** Both classes equally likely
- **D** Cannot provide any decision

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

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

Notes

Based on etalons: $d^Q = M$

Etalon classifier is a Linear classifier

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

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

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

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

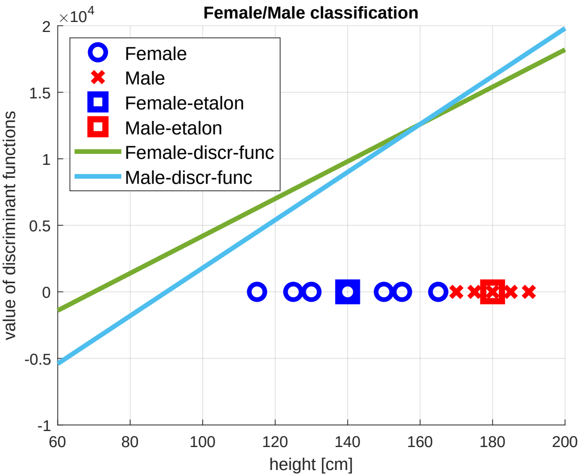
$$\delta(x) = \operatorname*{argmax}_{s \in S} f_s(x)$$

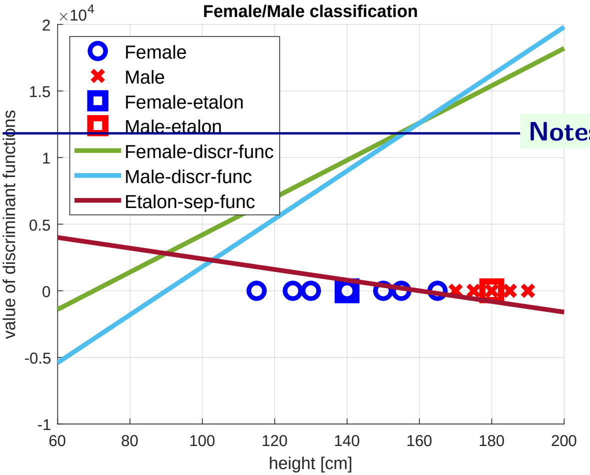
Binary classification: a single linear discriminant function $g(x)$ is sufficient and

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

Notes

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





Discriminant functions for 2 classes:

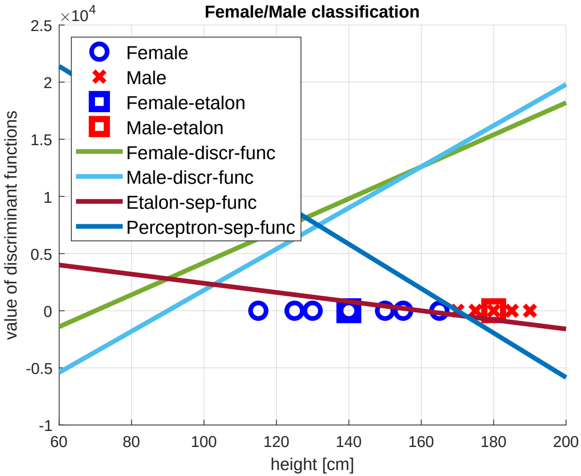
$$f_F(x) = a_F x + b_F = $$
$$= e_F x - \frac{1}{2} e_F^2 = 140x - 9800$$
$$f_M(x) = a_M x + b_M = $$
$$= e_M x - \frac{1}{2} e_M^2 = 180x - 16200$$

A single discriminant function separating 2 classes:

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

Notes

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

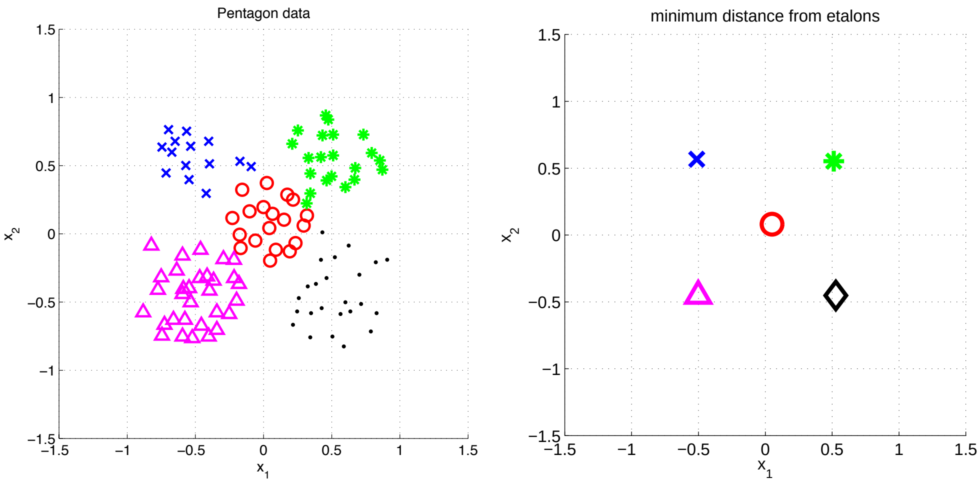


Etalon-based linear classifier makes some errors.

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

Notes

Etalon based classification

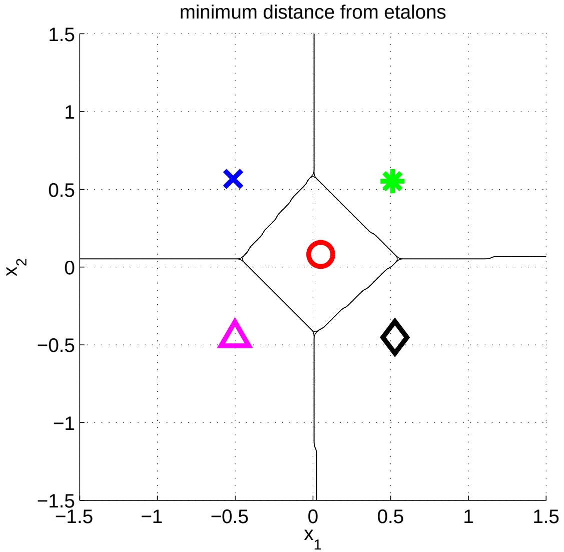


Represent $\vec{x}$ by etalon, $\vec{e}_s$ per each class $s \in S$.

Notes

Separate etalons

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



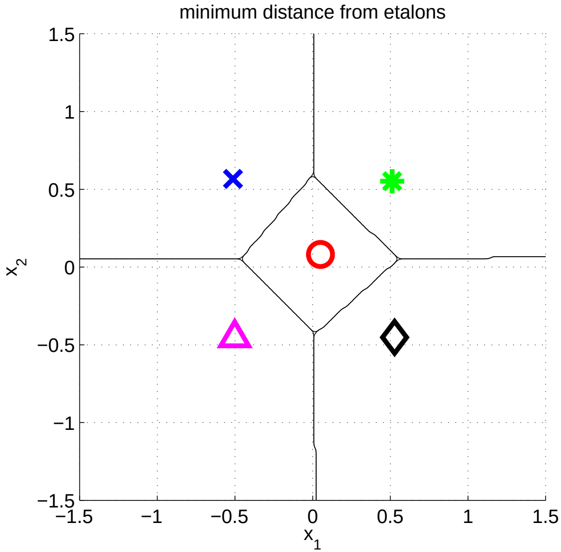
Notes

What etalons?

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

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

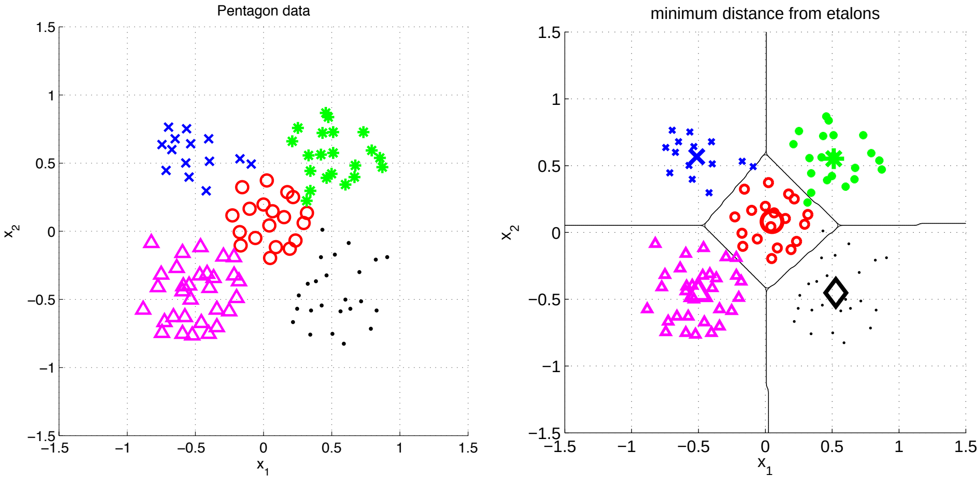
and separating hyperplanes halve distances between pairs.



Notes

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

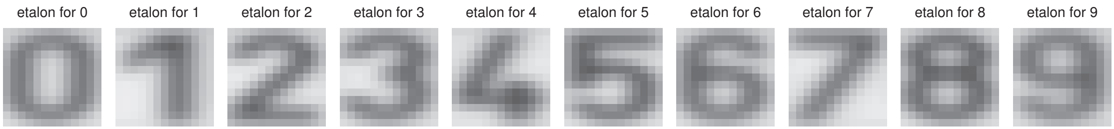
Etalon based classification, $\vec{e}_s = \vec{\mu}_s$



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 [7].

Notes

Keep in mind, that etalon – mean value is a kind of handcrafted heuristics. In general, it does not optimize (minimize) any loss function.

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

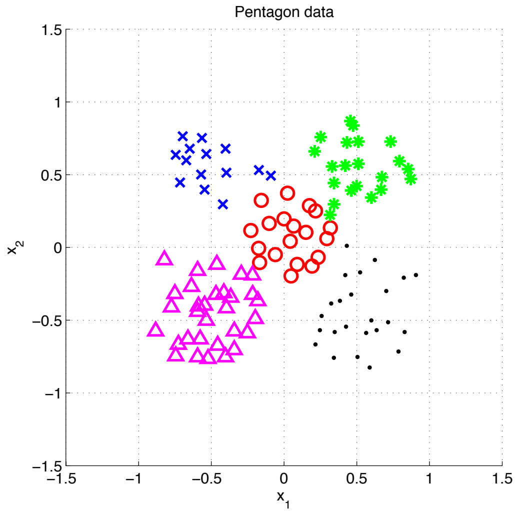
$$s^* = \operatorname*{argmax}_{s \in \mathcal{S}} f(\vec{x}, s)$$

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:

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

Discriminant function:

$$s^* = \operatorname*{argmax}_{s \in \mathcal{S}} f(\vec{x}, s) = P(s)\mathcal{N}(\vec{x}|\vec{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\{-\frac{1}{2}(\vec{x} - \vec{\mu})^\top \Sigma^{-1}(\vec{x} - \vec{\mu})\}$$

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, generalization to higher dimensions

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

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 $\vec{x}$.

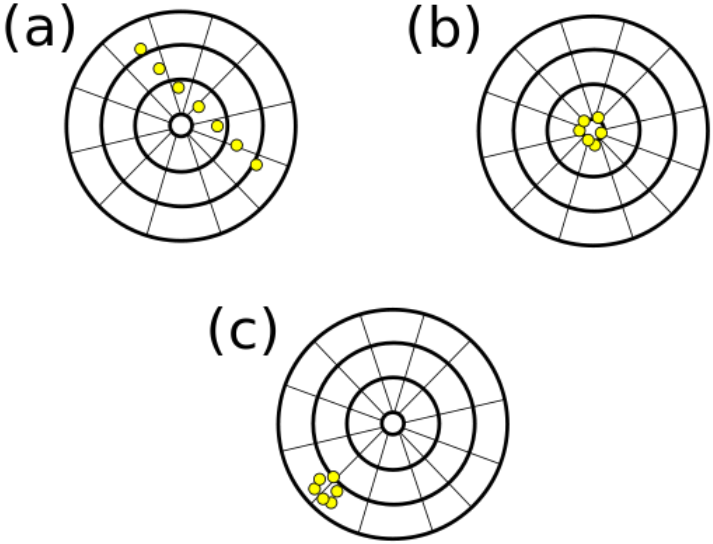
What to learn?

- 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 $\vec{x}$.

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

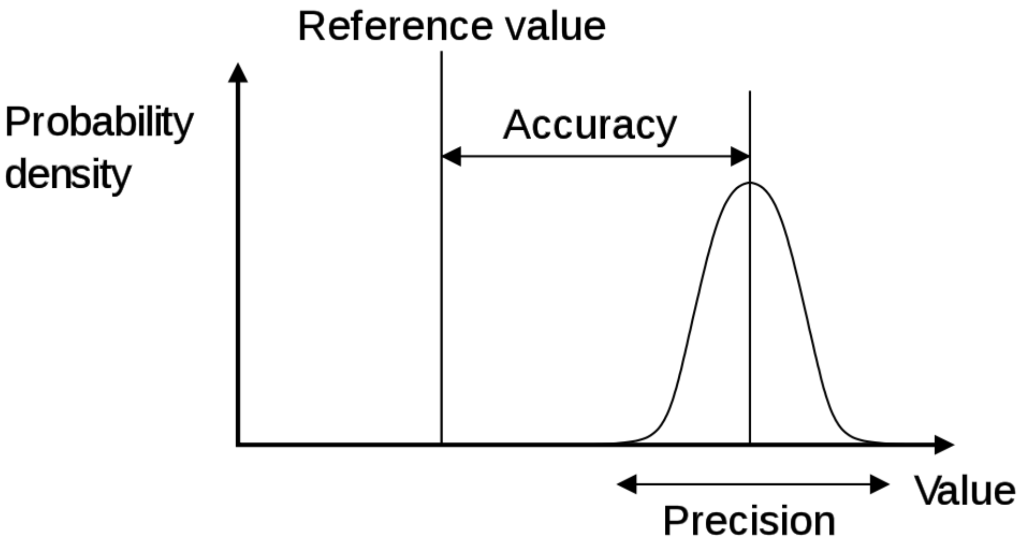
In German:

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

In Czech:

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

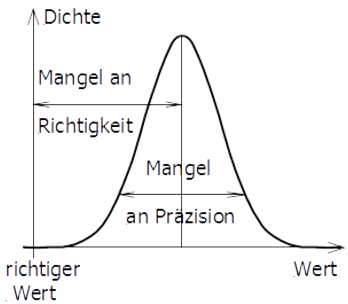
Accuracy vs precision



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 [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])

[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.

Notes

References II

[4] D. Kahneman, O. Sibony, and C.R. Sunstein.
Noise: A Flaw in Human Judgment.
Little Brown Spark, 2021.

[5] D. Kahneman, O. Sibony, and C.R. Sunstein.
Šum, O chybách v lidském úsudku.
Jan Melvil Publishing, 2021.

[6] Stuart Russell and Peter Norvig.
Artificial Intelligence: A Modern Approach.
Prentice Hall, 3rd edition, 2010.
http://aima.cs.berkeley.edu/.

[7] 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/.

Notes