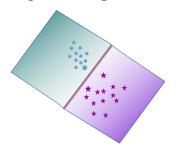
Introduction to Al Logistic Regression



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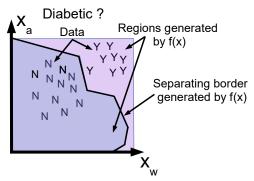
Outline

- 1. Classification: binary, multi-class and linear classifiers
- 2. Logistic regression for binary classification
- 3. Nonlinear feature transformations
- Model adequacy
- 5. Regularized logistic regression
- 6. Conclusions

- 1. Classification: binary, multi-class and linear classifiers
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Classification

- Supervised learning
- y can take only a finite number of predefined values (quantitative) or labels/classes (qualitative)



It is assumed that there is an underlying unknown function

$$f(\mathbf{x}): \mathbb{R}^2 \Rightarrow \{Y, N\}$$

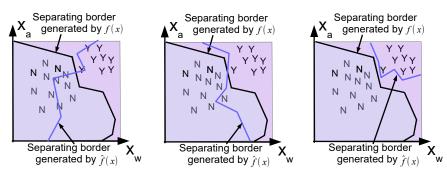
that separates the two classes (even unseen data) in the best possible manner.

Function $f(\mathbf{x})$ separates the input space into regions.

Classification

Objective:

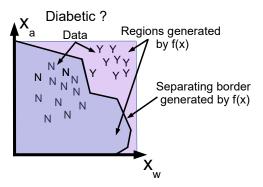
Adjust a function $\hat{f}(\mathbf{x})$ to data, such that $\hat{f}(\mathbf{x})$ is close in some sense to the unknown $f(\mathbf{x})$.



In practice, we are going to define a class of candidate functions for $\hat{f}(\mathbf{x})$ and then choose a function from that class such that $\hat{\mathbf{y}}$ are mostly close to \mathbf{y} from the available dataset.

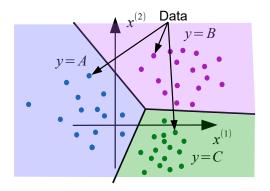
Binary classification

When we have only 2 possible labels, as in the example below, we say that we want to solve a binary classification problem.



Multi-class classification

When we have more than 2 possible labels, as in the example below, we say that we want to solve a multi-class classification problem.



▶ The class of candidate functions is often a parametric class, that is, the prediction function depends on the values of a parameter vector $\beta \in \mathbb{R}^M$.

Choosing a good candidate within a class of parametric functions $\hat{f}(\mathbf{x}; \beta)$ means choosing the parameter vector β that leads to good fit to data.

One such class of parametrized classifiers are linear classifiers.

In the binary classification case, a linear classifier decides on the predicted value based on a linear combination of the input features:

$$\hat{y} = g(\mathbf{x}\boldsymbol{\beta}) = g\left(\beta_0 + \sum_{i=1}^{M} \beta_i x^{(i)}\right)$$

where $g(\cdot)$ is a decision function.

Note that the weights of the combination are the parameters of the classifier.

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In the binary classification case, a linear classifier decides on the predicted value based on a linear combination of the input features:

$$\hat{y} = g(\mathbf{x}\beta)$$

▶ Often $g(\cdot)$ is simply a threshold function, for example, for two classes y = 0 or y = 1

$$\hat{y} = \begin{cases} 1, & \text{if } \mathbf{x}\boldsymbol{\beta} \ge \tau, \\ 0, & \text{if } \mathbf{x}\boldsymbol{\beta} < \tau, \end{cases}$$

for some previously defined threshold value τ .

For 1 feature plus an implicit feature of 1, we have

$$\hat{\mathbf{y}} = \begin{cases} 1, & \text{if } \beta_0 + \beta_1 \mathbf{x} \ge \tau, \\ 0, & \text{if } \beta_0 + \beta_1 \mathbf{x} < \tau, \end{cases}$$

which can be rewritten as (supposing $\beta_1 > 0$)

$$\hat{y} = \begin{cases} 1, & \text{if } x \ge \frac{\tau - \beta_0}{\beta_1}, \\ 0, & \text{if } x < \frac{\tau - \beta_0}{\beta_1}, \end{cases}$$

thus the predicted classes regions correspond to 2 complementary halfspaces of \mathbb{R} .

For 2 features plus an implicit feature of 1, we have

$$\hat{\mathbf{y}} = \begin{cases} 1, & \text{if } \beta_0 + \beta_1 \mathbf{x}^{(1)} + \beta_2 \mathbf{x}^{(2)} \ge \tau, \\ 0, & \text{if } \beta_0 + \beta_1 \mathbf{x}^{(1)} + \beta_2 \mathbf{x}^{(2)} < \tau, \end{cases}$$

which can be rewritten as (supposing $\beta_2 > 0$)

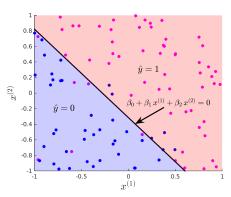
$$\hat{y} = \begin{cases} 1, & \text{if } x^{(2)} \ge \left(\frac{\beta_1}{\beta_2}\right) x^{(1)} + \left(\frac{\tau - \beta_0}{\beta_2}\right), \\ 0, & \text{if } x^{(2)} < \left(\frac{\beta_1}{\beta_2}\right) x^{(1)} + \left(\frac{\tau - \beta_0}{\beta_2}\right), \end{cases}$$

thus the predicted classes regions correspond to 2 complementary halfspaces of \mathbb{R}^2 .

The border between the 2 classes is a line

$$X^{(2)} = \left(\frac{\beta_1}{\beta_2}\right) X^{(1)} + \left(\frac{\tau - \beta_0}{\beta_2}\right).$$





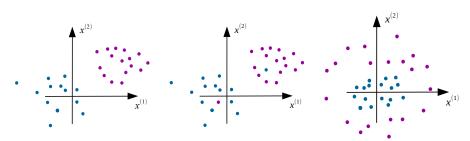
- For 3 features the predicted classes regions correspond to 2 complementary halfspaces of \mathbb{R}^3 .
- ► The border between the 2 classes is a plane.
- For N features the predicted classes regions correspond to 2 complementary halfspaces of \mathbb{R}^N .
- The border between the 2 classes is a hyperplane.
- Adjusting a linear classifier is equivalent to choosing a hyperplane that separates adequately available data.

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- For N features the predicted classes regions correspond to 2 complementary halfspaces of \mathbb{R}^N .
- ► The border between the 2 classes is a hyperplane.
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We say that the classes of a dataset are linearly separable when a linear classifier can be found such that there are no prediction errors.

Which of these datasets are linearly separable?

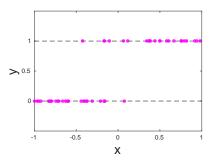


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Binary classification

Scatter plot for binary classification with 1 feature

- Assume one input feature x with N observations, one output feature y with two possible labels.
- ▶ Without loss of generality we can assume $y_i \in \{0, 1\}$.
- Scatter plot looks like this



Can we use a linear regression prediction model?

Binary classification: approximation with regression

Can we use linear regression to approximate the labels?

$$\hat{y} = \beta_0 + \beta_1 x$$

- Large errors for large absolute values of x.
- Can we transform the linear regression output to have more adapted predictions?

Answer: use an increasing smooth function
$$f(z)$$
 such that $\lim_{\substack{z \to -\infty \\ \text{lim } f(z) = 1}} f(z) = 0$

Binary classification: approximation with regression

Sigmoidal functions

• Use an increasing smooth function f(z) such that

$$\lim_{z \to -\infty} f(z) = 0$$
$$\lim_{z \to +\infty} f(z) = 1$$

- ► Sigmoidal functions, *i.e.* S-shaped functions, can be used.

 ⇒ Smooth versions of the *sign* function.
- Examples:
 - Gompertz: $f(z) = \exp[-\exp(-z)]$
 - ► Hyperbolic tangent with offset: $f(z) = \frac{1}{2} + \frac{1}{2} \tanh(\frac{z}{2})$
 - Gaussian cumulative distribution: $f(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} \exp\left(-\frac{1}{2}t^2\right) dt$
 - ▶ Logistic function: $f(z) = \frac{1}{1 + \exp(-z)}$

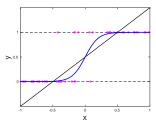
Logistic function

- In practice, the most used function is the logistic function.
- Applying it to the output of the linear regression model we have

$$f_{\beta}(x) = \frac{1}{1 + \exp\left[-\left(\beta_0 + \beta_1 x\right)\right]} \tag{1}$$

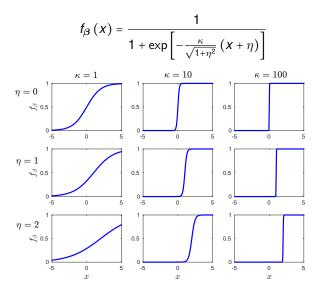
- This gives a smooth transition from 0 to 1, without large errors for large absolute values of x.
- ▶ Interpretation as a probability $\mathbb{P}(y = 1|x) = f_{\beta}(x)$

Logistic regression model in blue below.



Logistic function - effect of the parameters

▶ Rewriting the function with a slightly different parametrization



Binary classification

How do we learn the model parameters?

- Can we use the least squares approach?
- For N observations, we would solve the following optimization problem to retrieve β:

minimize
$$J(\beta) = \sum_{i=1}^{N} j(y_i, f_{\beta}(x_i))$$

with respect to

$$\boldsymbol{\beta}$$

where
$$j(y_i, f_{\beta}(x_i)) = \varepsilon_i^2 = (y_i - f_{\beta}(x_i))^2$$

Binary classification

How do we learn the model parameters?

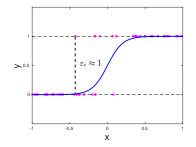
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- ▶ Issue: $j(y_i, f_{\beta}(x_i)) \le 1$
- The cost term should grow unbounded when prediction is completely false.

How do we learn the model parameters?

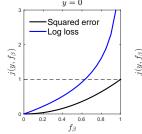
- Which cost function should be used?
- Cost function should grow unbounded when prediction is completely false.

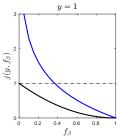
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- Which cost function should be used?
- Cost function should grow unbounded when prediction is completely false.
- Commonly used cost function is the following:

$$j(y, f_{\beta}(x)) = -y \log(f_{\beta}(x)) - (1 - y) \log(1 - f_{\beta}(x))$$
 (2)

which is called the log-loss function.





How do we learn the model parameters?

Optimization problem corresponding to logistic regression parameter learning:

minimize
$$J(\beta) = \sum_{i=1}^{N} j(y_i, f_{\beta}(x_i))$$
 with respect to
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 where
$$j(y_i, f_{\beta}(x_i)) = -y_i \log(f_{\beta}(x_i)) - (1 - y_i) \log(1 - f_{\beta}(x_i))$$
 with
$$f_{\beta}(x_i) = \frac{1}{1 + \exp\left[-(\beta_0 + \beta_1 x_i)\right]}$$

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- Unfortunately, there is no closed-form solution for this problem.
- However, it is a smooth convex optimization problem.
 Efficient optimization algorithms can be used to solve it, e.g. gradient descent method or Newton's method.

Prediction - 1D example

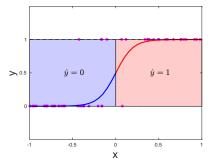
Prediction can be done as follows

$$\hat{y} = \begin{cases} 1, & \text{if } f_{\hat{\beta}}(x_i) \ge 0.5 \\ 0, & \text{if } f_{\hat{\beta}}(x_i) < 0.5 \end{cases}$$

This can be rewritten in a simpler equivalent form

$$\hat{y} = \begin{cases} 1, & \text{if } \hat{\beta}_0 + \hat{\beta}_1 x \ge 0 \\ 0, & \text{if } \hat{\beta}_0 + \hat{\beta}_1 x < 0 \end{cases}$$

Feature space is partitioned in half-axis as in the example below:



Generalization to *p* feature vectors

 If you have p features corresponding to different explanatory variables and/or transformations of them

$$\mathbf{x} = \begin{bmatrix} 1 & x^{(1)} & \cdots & x^{(p)} \end{bmatrix}$$

simply change
$$f_{\beta}(x)$$
 to $f_{\beta}(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{x}\beta)}$ with $\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$

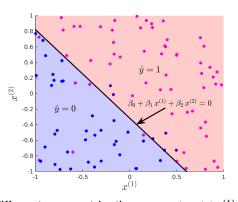
The prediction is given by

$$\hat{y} = \begin{cases} 1, & \text{if } \mathbf{x}\boldsymbol{\beta} \ge 0 \\ 0, & \text{if } \mathbf{x}\boldsymbol{\beta} < 0 \end{cases}$$

This is a linear classifier.

Prediction - 2D example

The previously shown example of a 2D linear classifier was obtained through logistic regression:

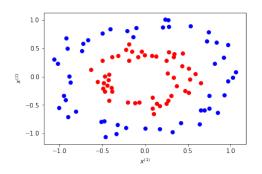


Slightly different parametrization: $\frac{\kappa}{\sqrt{1+\eta^2}}(\cos(\theta)x^{(1)} + \sin(\theta)x^{(2)} + \eta)$ $\Longrightarrow (\theta, \eta)$ describe the separation line and κ the steepness of the transition from one class to the other.

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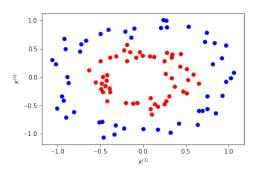
Classes not linearly separable

What do we do if the classes are not close to linearly separability?



Classes not linearly separable

What do we do if the classes are not close to linearly separability?



Separating border is close to an ellipse. General equation:

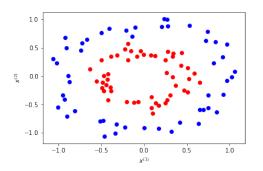
$$\frac{\left[(x^{(1)}-a)\cos(\theta)+(x^{(2)}-b)\sin(\theta)\right]^2}{c^2}+\frac{\left[(x^{(1)}-a)\sin(\theta)+(x^{(2)}-b)\cos(\theta)\right]^2}{d^2}=1$$

Developing, we can rewrite it in the following form

$$\beta_5 \left(X^{(2)} \right)^2 + \beta_4 \left(X^{(1)} \right)^2 + \beta_3 X^{(1)} X^{(2)} + \beta_2 X^{(2)} + \beta_1 X^{(1)} + \beta_0 = 0$$

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Polynomial equation for the separating border:

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We apply the same trick as for fitting polynomials with linear regression.

We need to add the transformed features

$$(x^{(2)})^2, (x^{(1)})^2 \text{ and } x^{(1)}x^{(2)}$$

to the dataset

Polynomial equation for the separating border:

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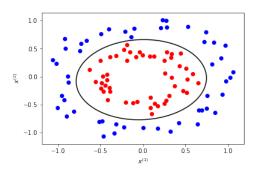
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Separating border obtained with logistic regression and transformed features



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How do we evaluate the performance of a classifier?

 A natural measure of performance is the fraction of corrected predictions on a test dataset. This is called the accuracy of the classifier on the test dataset.

For a dataset $(\mathbf{X}_{test}, \mathbf{y}_{test})$ with N_{test} observations, the accuracy $Acc_{\hat{\mathbf{y}}(\mathbf{x})}(\mathbf{X}_{test}, \mathbf{y}_{test})$ of a classifier is

$$\mathsf{Acc}_{\hat{\mathbf{y}}(\mathbf{x})}(\mathbf{X}_{\mathsf{test}}, \mathbf{y}_{\mathsf{test}}) = \frac{1}{N_{\mathsf{test}}} \sum_{i=1}^{N_{\mathsf{test}}} \mathbb{1} \left[\hat{y}(\mathbf{x}_{\mathsf{test}}^i) = y_{\mathsf{test}}^i \right]$$

where $(\mathbf{x}_{\text{test}}^i, y_{\text{test}}^i)$ is the *i*-th observation of the dataset and $\mathbb{1}[\hat{y} = y_{\text{test}}]$ is an indicator function:

$$\mathbb{1}\left[\hat{y} = y_{\text{test}}\right] = \begin{cases} 1, & \text{if } \hat{y} = y_{\text{test}}, \\ 0, & \text{otherwise.} \end{cases}$$

$$\mathsf{Acc}_{\hat{\boldsymbol{y}}(\boldsymbol{x})}(\boldsymbol{X}_{\mathsf{test}},\boldsymbol{y}_{\mathsf{test}}) = 1 - \left\{ \frac{1}{N_{\mathsf{test}}} \sum_{i=1}^{N_{\mathsf{test}}} \mathbb{1}\left[\hat{\boldsymbol{y}}(\boldsymbol{x}_{\mathsf{test}}^i) \neq \boldsymbol{y}_{\mathsf{test}}^i\right] \right\}$$

- $\quad \bullet \ \ 0 \leq Acc_{\hat{y}(x)}(X_{test},y_{test}) \leq 1.$
- $\label{eq:condition} \begin{array}{l} \bullet \mbox{ Good classifiers should have } Acc_{\hat{y}(x)}(\boldsymbol{X}_{test},\boldsymbol{y}_{test}) \mbox{ close to 1.} \\ \mbox{ When } Acc_{\hat{y}(x)}(\boldsymbol{X}_{test},\boldsymbol{y}_{test}) = 1, \mbox{ there are no errors.} \end{array}$
- ▶ When $Acc_{\hat{y}(x)}(X_{test}, y_{test}) = 0$, the labels are all flipped.
- In binary classification the worst case is $Acc_{\hat{y}(x)}(X_{test}, y_{test}) = 0.5$, why?

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• Why not use accuracy as a criterion $J(\beta)$ for learning the parameters of a classifier?

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Due to the presence of the indicator function, accuracy is a non smooth, non convex criterion. Very difficult to be maximized directly by numerical optimization algorithms.

Interpretation of accuracy in the binary case

▶ Denote \mathcal{I}_0 the set of indexes of the observations in the test dataset for which y = 0 and N_{test}^0 the corresponding number of observations.

Denote \mathcal{I}_1 the set of indexes of the observations in the test dataset for which y = 1 and N_{test}^1 the corresponding number of observations.

Then we can write

$$\begin{split} & \mathsf{Acc}_{\hat{\mathbf{y}}(\mathbf{x})}(\mathbf{X}_{\mathsf{test}}, \mathbf{y}_{\mathsf{test}}) = \frac{1}{N_{\mathsf{test}}} \sum_{i=1}^{N_{\mathsf{test}}} \mathbb{1} \left[\hat{\mathbf{y}}(\mathbf{x}_{\mathsf{test}}^i) = \mathbf{y}_{\mathsf{test}}^i \right] \\ &= \frac{1}{N_{\mathsf{test}}^0 + N_{\mathsf{test}}^1} \left\{ \sum_{i \in \mathcal{I}_0} \mathbb{1} \left[\hat{\mathbf{y}}(\mathbf{x}_{\mathsf{test}}^i) = 0 \right] + \sum_{j \in \mathcal{I}_1} \mathbb{1} \left[\hat{\mathbf{y}}(\mathbf{x}_{\mathsf{test}}^j) = 1 \right] \right\} \\ &= \left(\frac{N_{\mathsf{test}}^0}{N_{\mathsf{test}}^0 + N_{\mathsf{test}}^1} \right) \frac{\sum_{i \in \mathcal{I}_0} \mathbb{1} \left[\hat{\mathbf{y}}(\mathbf{x}_{\mathsf{test}}^i) = 0 \right]}{N_{\mathsf{test}}^0} + \left(\frac{N_{\mathsf{test}}^1}{N_{\mathsf{test}}^0 + N_{\mathsf{test}}^1} \right) \frac{\sum_{j \in \mathcal{I}_1} \mathbb{1} \left[\hat{\mathbf{y}}(\mathbf{x}_{\mathsf{test}}^j) = 1 \right]}{N_{\mathsf{test}}^1} \end{split}$$

Interpretation of accuracy in the binary case

$$\begin{aligned} &\mathsf{Acc}_{\hat{\mathbf{y}}(\mathbf{x})}(\mathbf{X}_{\text{test}}, y_{\text{test}}) = \frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} \mathbb{1}\left[\hat{y}(\mathbf{x}_{\text{test}}^i) = y_{\text{test}}^i\right] \\ &= \left(\frac{N_{\text{test}}^0}{N_{\text{test}}^0 + N_{\text{test}}^1}\right) \frac{\sum\limits_{i \in \mathcal{I}_0} \mathbb{1}\left[\hat{y}(\mathbf{x}_{\text{test}}^i) = 0\right]}{N_{\text{test}}^0} + \left(\frac{N_{\text{test}}^1}{N_{\text{test}}^0 + N_{\text{test}}^1}\right) \frac{\sum\limits_{j \in \mathcal{I}_1} \mathbb{1}\left[\hat{y}(\mathbf{x}_{\text{test}}^j) = 1\right]}{N_{\text{test}}^1} \end{aligned}$$

- Accuracy is a weighted combination of the fractions of correct predictions for each class.
- ▶ The weights are the fraction of observations for each class.
- Consequence: accuracy is not sensitive to the prediction errors in rare classes.

Confusion matrix

A more complete picture of the classifier performance can be obtained by gathering in a **table** the **number of occurences of each possible couple** (y,\hat{y}) .

Example for binary classification:

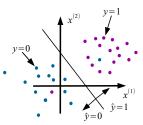
Predicted \hat{y} True y	0	1
0	$\sum_{i \in \mathcal{I}_0} \mathbb{1} \left[\hat{y}(\mathbf{x}_{test}^i) = 0 \right]$ True Negatives	$\sum_{i \in \mathcal{I}_0} \mathbb{1} \left[\hat{y}(\mathbf{x}_{test}^i) = 1 \right]$ False Positives
1	$\sum_{i \in \mathcal{I}_1} \mathbb{1} \left[\hat{y}(\mathbf{x}_{test}^i) = 0 \right]$ False Negatives	$\sum_{i \in \mathcal{I}_1} \mathbb{1} \left[\hat{y}(\mathbf{x}_{test}^i) = 1 \right]$ True Positives

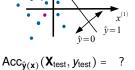
This table is called the **confusion matrix**.

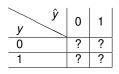
Simple examples

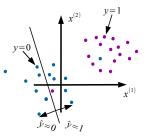
Give the accuracy and the confusion matrix for the classifiers below

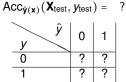
$$N_{\text{test}} = ?$$
 $N_{\text{test}}^0 = ?$ $N_{\text{test}}^1 = ?$

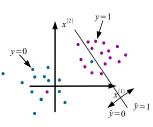












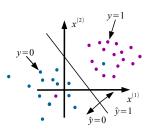
$Acc_{\hat{\mathbf{y}}(\mathbf{x})}$	$(\mathbf{X}_{test}, \mathbf{y}_{test})$	est) =	?
	î/	1	ı

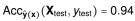
ŷ	0	1
0	?	?
1	?	?

Simple examples

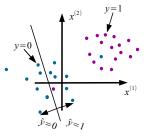
Give the accuracy and the confusion matrix for the classifiers below

$$N_{test} = 31$$
 $N_{test}^{0} = 14$ $N_{test}^{1} = 17$



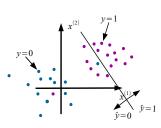


ŷ	0	1
0	13	1
1	1	16



$Acc_{\hat{\mathbf{v}}(\mathbf{x})}$	$(\mathbf{X}_{test},$	V _{test})	= ().77

ŷ	0	1
0	7	7
1	0	17



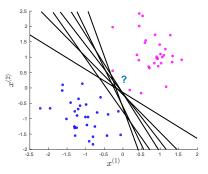
ŷ	0	1
0	14	0
1	6	11

- 1. Classification: binary, multi-class and linear classifiers
- Logistic regression for binary classification
- 3. Nonlinear feature transformations
- 4. Model adequacy
- 5. Regularized logistic regression
- Conclusions

Logistic regression

What happens if the classes are linearly separable?

Which line do you choose?



- Logistic regression suffers from two major issues in this case:
 - 1. $\kappa \to +\infty$ to have $J \to 0$: optimization algorithms become unstable.
 - 2. The solution of the problem is not unique.

Regularized logistic regression

Solution

• Add a regularization term $\|\beta\|_2^2$ to $J(\beta)$:

minimize
$$J'(\beta) = \left[\sum_{i=1}^{N} j(y_i, f_{\beta}(\mathbf{x}_i))\right] + \lambda \|\beta\|_2^2$$
 with respect to
$$\beta$$
 where
$$j(y_i, f_{\beta}(\mathbf{x}_i)) = -y_i \log(f_{\beta}(\mathbf{x}_i)) - (1 - y_i) \log(1 - f_{\beta}(\mathbf{x}_i))$$

some fixed
$$\lambda > 0$$
.

 $f_{\beta}(\mathbf{x}_i) = \frac{1}{1 + \exp[-\mathbf{x}_i \cdot \beta]}$

- ightharpoonup eta is not allowed to grow unbounded. This stabilizes numerical optimizers.
- We get a unique solution.

with

▶ When $\lambda \rightarrow 0$, we get standard logistic regression.

- 1. Classification: binary, multi-class and linear classifiers
- Logistic regression for binary classification
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- 5. Regularized logistic regression
- 6. Conclusions

Conclusions

Logistic regression

- Logistic regression can be seen as a simple adaptation of linear regression to do classification. Learning is equivalent to solve a smooth optimization problem.
- Logistic regression is a linear classifier. If the classifier needs nonlinear separation boundaries, we can include nonlinear transformations of the features to the feature matrix (but we need to know what to add).
- Parameter vector $\hat{\boldsymbol{\beta}}$ allows for interpretation of results.
- Complexity of underlying optimization problem depends on the dimension of feature space.
- It is sensible to outliers (it is designed for this).
- Its standard form cannot be used for classifying linear separable classes. Its regularized version should be used in this case.