Linear classification

LEARN

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Linear Regression

Data:

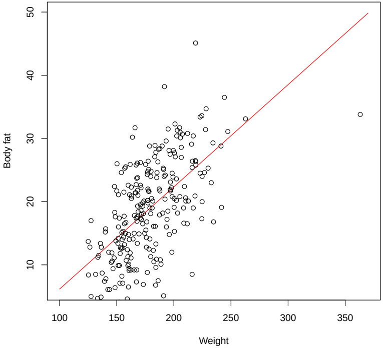
- $\mathbf{x}_i$ is a data point.
- y_i is a target value.
- each $\mathbf{x}_i$ has m features.

$$\mathbf{x}_i = (x_{i1}, \ldots, x_{im})^\top$$

- there are n such data points

→ Data matrix $\mathbf{X}$ (size $n \times m$)

→ Target vector $\mathbf{y}$ (size $n \times 1$)



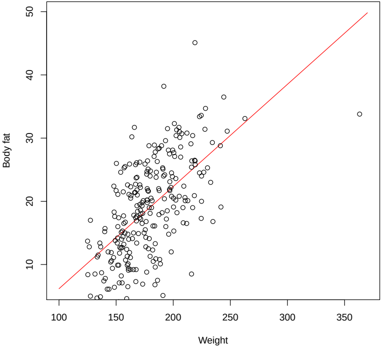
Linear Regression

Definition (Linear Regression)

$$y_i = w_0 + w_1 x_{i1} + \ldots + w_m x_{im}$$

$$y_i = w_0 + \mathbf{x}_i^\top \mathbf{w}$$

- w_i are **coefficients** or weights of each features.
- w_0 denotes the **intercept**.



Linear Regression

Ordinary Least Squares Estimation

Definition (Residual Sum of Squares; RSS)

$$\mathrm{RSS}(w_0, \ldots, w_m) = \sum_{i=1}^{n} (y_i - \hat{f}(\mathbf{x}_i))^2$$

- RSS gives the total loss over the whole training set
- Choose the coefficients $w_0, \ldots, w_m$ such that the total loss according to RSS is **minimized**.

Linear Regression

Ordinary Least Squares Estimation

- Set the partial derivative of RSS to zero
- In matrix form:

$$\mathrm{RSS}(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) \tag{1}$$

$$\frac{\partial \mathrm{RSS}(\mathbf{w})}{\partial \mathbf{w}} = -2\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}). \tag{2}$$

- **Note**: where $\mathbf{w} = (w_0, \ldots, w_m)^\top$ and the first column of $\mathbf{X}$ contains only 1 to accommodate the intercept w_0, i.e. $\mathbf{X}$ is a $n \times m + 1$ matrix.

Linear Models – Ordinary Least Squares Estimation

Definition (Ordinary Least Squares Estimate)

$$\hat{\mathbf{w}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{y}$$

- The minimum of the loss function is **unique**.
- Estimates of the coefficients can be obtained in **closed form** solution and therefore no optimization is required.
- $\mathbf{X}$ must have full column rank $\Rightarrow$ $\mathbf{X}^\top \mathbf{X}$ is positive definite.
- Prediction (regression) is performed by

$$\hat{f}(x_1, \dots, x_m) = \hat{w}_0 + \hat{w}_1 x_1 + \dots + \hat{w}_m x_m$$

Classification

Background: Linear Models

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The geometric margin

Classification– Definitions

- **Training sample** $\mathbf{x}_i$ consists of m **features** $(x_{i1}, \ldots, x_{im})^\top$
- To each training sample $\mathbf{x}_i$ is associated a training **output** y_i.
- **Training set** $\mathcal{T} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$.
- Data matrix $\mathbf{X}$ with the i-th sample in the i-th row
- $\mathbf{y} = (y_1, \ldots, y_n)^\top$ the vector of all outputs.

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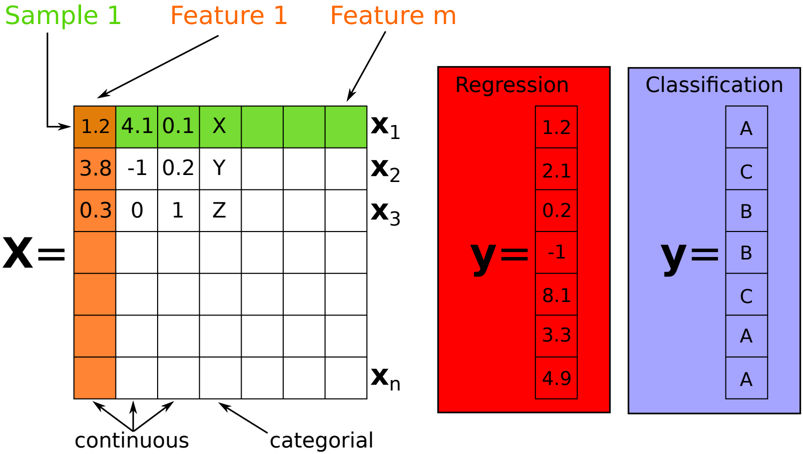
Question:

What is the difference with regression?

Classification – Definitions



Sample 1

Feature 1

Feature m

$\mathbf{X}=$

1.2	4.1	0.1	X				$\mathbf{x}_1$
3.8	-1	0.2	Y				$\mathbf{x}_2$
0.3	0	1	Z				$\mathbf{x}_3$
							$\mathbf{x}_n$

continuous

categorial

Regression

$\mathbf{y}=$

1.2
2.1
0.2
-1
8.1
3.3
4.9

Classification

$\mathbf{y}=$

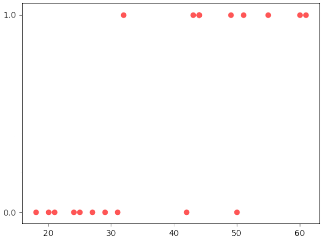
A
C
B
B
C
A
A

Classification – Definitions

- Each **feature** can be:
  - **continuous** (a number).
  - **discrete** (from a predefined set of values).

- The **output** can be:
  - continuous, we perform regression.
  - discrete, we perform classification.

Linear Classification – Definitions

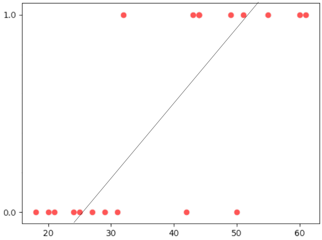


Classification Goal

Find a **decision function** f such that: $f(\mathbf{x}_i) = y_i$

- Assume a **linear model** for f.

Linear Classification – Definitions



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- We solved linear **regression** with least squares ...

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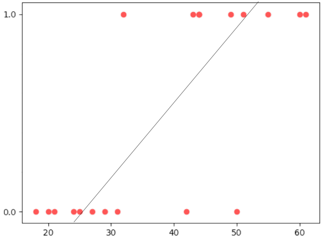

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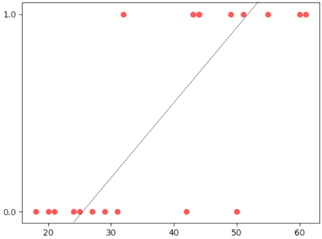
- We solved linear **regression** with least squares ...
- Problem?

Linear Classification – Definitions



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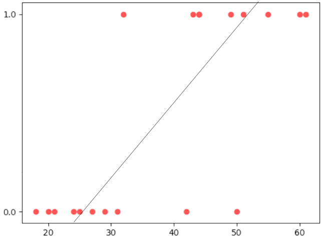
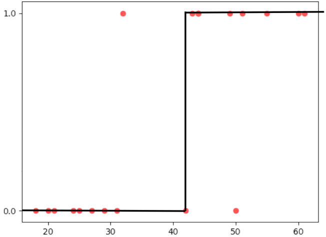


Classification Goal

Find a **decision function** f such that: $f(\mathbf{x}_i) = y_i$

- Assume a **linear model** for f.
- We solved linear **regression** with least squares ...
- Problem? in **classification** the outcome y_i is **categorical**.
- Naive solution: use a **threshold**.

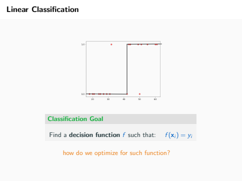
Linear Classification



Classification Goal

Find a **decision function** f such that: $f(\mathbf{x}_i) = y_i$

how do we optimize for such function?



Linear Classification

Classification Goal

Find a **decision function** f such that: $f(\mathbf{x}_i) = y_i$

how do we optimize for such function?

The straightforward way to approximate this ideal function is to use two line segments to fit the dots, which are also referred to as training data points. However, to be learnable, we want to use a differentiable function to do the fitting instead of the two line segments.

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Logistic Regression

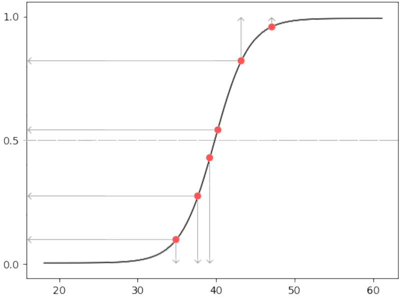
Pass the initial line through a **sigmoid function** ensuring that $0 \leq f(\mathbf{x}) \leq 1$

$$f(\mathbf{x}_i) = \mathrm{sigm}(\mathbf{w}^\top \mathbf{x}_i) \quad \text{where} \quad \mathrm{sigm}(\eta) = \frac{1}{1+e^{-\eta}} = \frac{e^\eta}{1+e^\eta}$$

The sigmoid function is also known as logistic function.

Prediction model:

$$f(\mathbf{x}_i) = \frac{1}{1 + e^{-(\mathbf{w}^\top \mathbf{x}_i)}}$$



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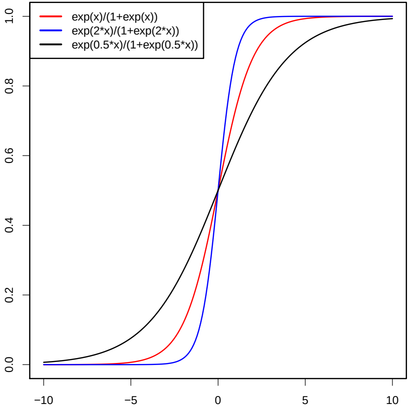

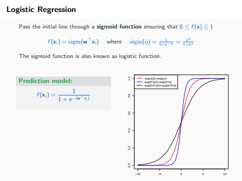

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The Logistic function, which is also referred to as sigmoid function, can be employed here. Logistic function is a monotonic, continuous function between 0 and 1

Logistic Regression

Pass the initial line through a **sigmoid function** ensuring that $0 \leq f(\mathbf{x}) \leq 1$

$$f(\mathbf{x}_i) = \mathrm{sigm}(\mathbf{w}^\top \mathbf{x}_i) \quad \text{where} \quad \mathrm{sigm}(\eta) = \frac{1}{1+e^{-\eta}} = \frac{e^\eta}{1+e^\eta}$$

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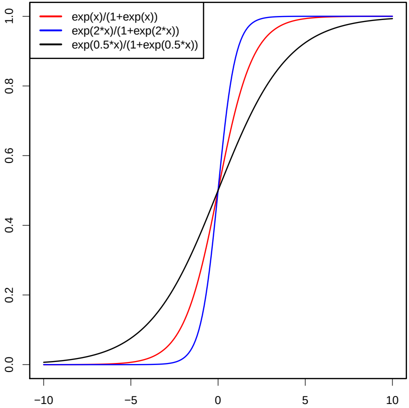
Logistic regression is a form of **probabilistic classification**!



Logistic Regression – Formally

- In the case of a **binary** classification problem $y_i \in \{0, 1\}$:
  - $y_i = 1$ is the **positive** class,
  - $y_i = 0$ is the **negative** class.
- The probability of variables taking one of two possible outcomes can be modelled with the discrete **Bernoulli** distribution:

$$P(y = 1) = q^y (1 - q)^{(1-y)}.$$

  with q the probability of the class 1 and $(1 - p)$ that of class 0

- The prediction function represents the **posterior probability** π_i of belonging to the positive class, given sample $\mathbf{x}_i$

$$\pi_i = P(y_i = 1 | x_{i1}, \ldots, x_{im})$$

Logistic Regression – Maximum Likelihood Estimation

The likelihood of the training set is modeled as the product of Bernoulli events:

Definition (Likelihood function)

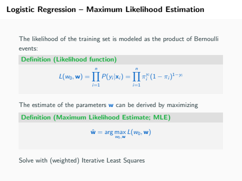
$$L(w_0, \mathbf{w}) = \prod_{i=1}^{n} P(y_i|\mathbf{x}_i) = \prod_{i=1}^{n} \pi_i^{y_i}(1-\pi_i)^{1-y_i}$$

The estimate of the parameters $\mathbf{w}$ can be derived by maximizing

Definition (Maximum Likelihood Estimate; MLE)

$$\hat{\mathbf{w}} = \arg\max_{w_0, \mathbf{w}} L(w_0, \mathbf{w})$$

Solve with (weighted) Iterative Least Squares



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Solve with (weighted) Iterative Least Squares

This formulation can be extended to multiple categorical output cases.

Homework: Derive the update rule for the iterative least squares problem.

Logistic regression optimization in action

logistic regression optimization video

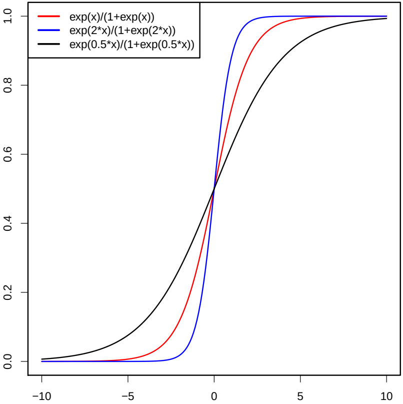
Logistic Regression – Response and link function

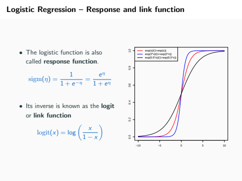
- The logistic function is also called **response function**.

$$\mathrm{sigm}(\eta) = \frac{1}{1+e^{-\eta}} = \frac{e^{\eta}}{1+e^{\eta}}$$

- Its inverse is known as the **logit** or **link function**

$$\mathrm{logit}(x) = \log\left(\frac{x}{1-x}\right)$$





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$$\mathrm{logit}(x) = \log\left(\frac{x}{1-x}\right)$$

Verify the inverse by replacing the logit function inside the sigmoid.

$$\mathrm{sigm}(\mathrm{logit}(x))\frac{\exp\left(\ln\left(\frac{x}{1-x}\right)\right)}{1+\exp\left(\ln\left(\frac{x}{1-x}\right)\right)}$$

Logistic Regression – Log odds

The logit or link function $\mathrm{logit}(x) = \ln\left(\frac{x}{1-x}\right)$ can be used to define the **Log odds**, which are an alternate way of expressing probabilities.

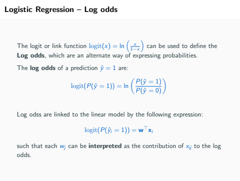
The **log odds** of a prediction $\hat{y} = 1$ are:

$$\mathrm{logit}(P(\hat{y} = 1)) = \ln\left(\frac{P(\hat{y} = 1)}{P(\hat{y} = 0)}\right)$$

Log odss are linked to the linear model by the following expression:

$$\mathrm{logit}(P(\hat{y}_i = 1)) = \mathbf{w}^\top \mathbf{x}_i$$

such that each w_j can be **interpreted** as the contribution of x_{ij} to the log odds.



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$$\begin{aligned}
P(y = 1) =& \frac{e^{\mathbf{w}^T\mathbf{x}}}{1 + e^{\mathbf{w}^T\mathbf{x}}} \\
P(y = 1)(1 + e^{\mathbf{w}^T\mathbf{x}}) =& e^{\mathbf{w}^T\mathbf{x}} \\
P(y = 1) + P(y = 1)e^{\mathbf{w}^T\mathbf{x}} =& e^{\mathbf{w}^T\mathbf{x}} \\
P(y = 1) =& e^{\mathbf{w}^T\mathbf{x}}(1 - P(y = 1)) \\
\frac{P(y = 1)}{(1 - P(y = 1))} =& e^{\mathbf{w}^T\mathbf{x}} \\
\ln\left(\frac{P(y = 1)}{P(y = 0)}\right) =& \mathbf{w}^T\mathbf{x}
\end{aligned}$$

Logistic Regression – Log-Odds Ratio

Definition (Log-Odds ratio)

The coefficient w_i represents the **log-odds ratio** of the i-th feature

- $w_i > 0 \Leftrightarrow$ Odds increase
- $w_i < 0 \Leftrightarrow$ Odds decrease
- $w_i = 0 \Leftrightarrow$ Odds remain unchanged
- This becomes very handy to assess which feature has the largest influence, especially if the goal is to predict which patients are diseased based on clinical features.

Logistic Regression – Example

Birth weight data contains data from 189 births to determine which of these factors were risk factors for low birth weight ($< 2.5\,$kg)

Feature	w / log-odds ratio	Chance
(Intercept)	0.924910	
Age	-0.042784	decreased
Mother's weight (pounds)	-0.015436	decreased
Race = White	0	
Race = Black	1.168452	increased
Race = Other	0.814620	increased
Previous premature labour	1.333970	increased
History of hypertension	1.740511	increased
Smoking during pregnancy	0.858332	increased

Logistic Regression – Log odds

Advantages

- low computational demand.
- highly interpretable.
- does not require features to be scaled.
- probabilistic output.
- easy to implement and fast training.
- good baseline model.

Disadvantages

- Works better with when removing unrelated and correlated attributes, so it is dependend on feature engineering.
- the decision surface is linear.
- its low complexity may lead to overfitting.

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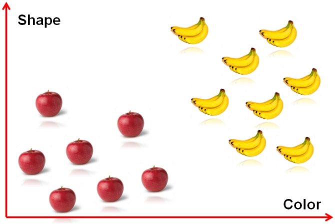
Binary classification problem

Input: Objects from 2 classes: 🍎 = -1, 🍌 = 1

Goal: Find a **decision function** f such that :

$$f(\mathbf{x}_i) = y_i,$$
$$\text{for all } i \in \{1, \cdots, n\}$$



$f($🍎$) =$ `'apple'` $= -1$

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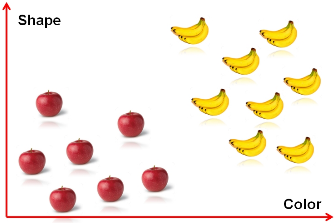
Question:

how?



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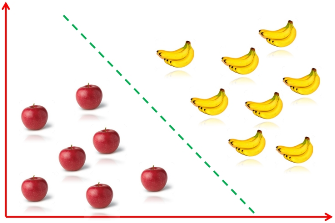
Binary classification problem – Generalized Linear Classifier

- Given training data $\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$
- Find a **hyperplane** h that separates the data points in 2 classes:

$$h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}_i + w_0$$

- The line of interest is created when the hyperplane cuts the feature space $(h = 0)$



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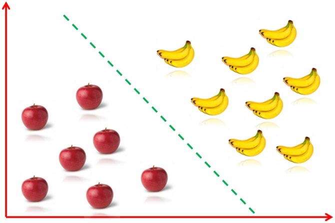
- The line of interest is created when the hyperplane cuts the feature space $(h = 0)$
- $w_0 = 0$
  $\mathbf{w} = [2, -1]$
  $\{\mathbf{x}_i\} = \{[2, 0], [0, 2], [2, 4]\}$
  $h(\mathbf{x}_i) = ?$



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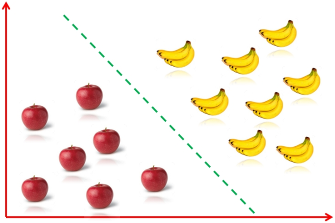
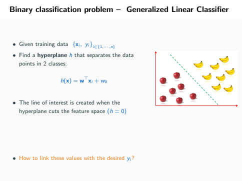


- How to link these values with the desired y_i?



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- The line of interest is created when the hyperplane cuts the feature space $(h = 0)$
- How to link these values with the desired y_i?

Use the signs of the hyperplane equation to make predictions.

$$\{h(x_i)\} = \{4, -2, 0\}$$

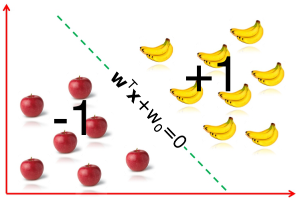
Binary classification problem – Generalized Linear Classifier

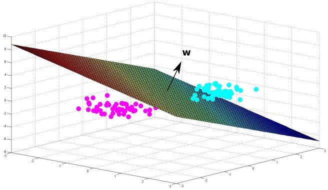
- Given training data $\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$
- Find hyperplane:

$$h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$$

Subject to constraints for all i:

$$\mathbf{w}^\top \mathbf{x}_i + w_0 > 0 \text{ if } y_i = +1$$
$$\mathbf{w}^\top \mathbf{x}_i + w_0 < 0 \text{ if } y_i = -1$$





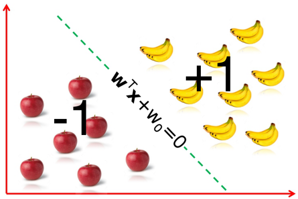
Binary classification problem – Generalized Linear Classifier

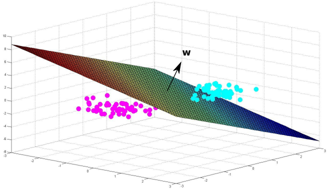
- Given training data $\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$
- Find hyperplane:

$$h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$$

Subject to constraints for all i:

$$\mathbf{w}^\top \mathbf{x}_i + w_0 > 0 \text{ if } y_i = +1$$
$$\mathbf{w}^\top \mathbf{x}_i + w_0 < 0 \text{ if } y_i = -1$$





- Another way to write it?

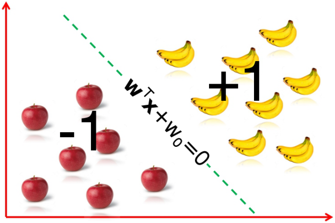
Binary classification problem – Generalized Linear Classifier

- Given training data $\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$
- Find hyperplane:

$$h = \mathbf{w}^\top \mathbf{x} + w_0 = 0$$

Subject to constraints for all i:

$$\mathbf{w}^\top \mathbf{x}_i + w_0 > 0 \text{ if } y_i = +1$$
$$\mathbf{w}^\top \mathbf{x}_i + w_0 < 0 \text{ if } y_i = -1$$



Decision function $f(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + w_0)$

Binary classification problem – Generalized Linear Classifier

Given training data

$$\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$$

Decision function

$$f(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + w_0)$$

And then?

Binary classification problem – Generalized Linear Classifier

Given training data

$$\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$$

Decision function

$$f(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + w_0)$$

And then?

Find the optimal parameters $\hat{\mathbf{w}}^*$ and $\hat{w}_0^*$ which minimize the classification errors by using a loss function.

Binary classification problem – Generalized Linear Classifier

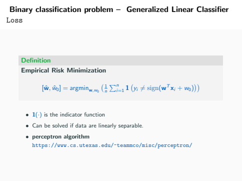
Loss

Definition

Empirical Risk Minimization

$$[\hat{\mathbf{w}}, \hat{w}_0] = \operatorname{argmin}_{\mathbf{w}, w_0} \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \left(y_i \neq \mathrm{sign}(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right)$$

- $\mathbf{1}(\cdot)$ is the indicator function
- Can be solved if data are linearly separable.
- **perceptron algorithm** https://www.cs.utexas.edu/~teammco/misc/perceptron/



Binary classification problem – Generalized Linear Classifier Loss

Definition

Empirical Risk Minimization

$$[\hat{\mathbf{w}}, \hat{w}_0] = \mathrm{argmin}_{\mathbf{w}, w_0} \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \left(y_i \neq \mathrm{sign}(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right)$$

- $\mathbf{1}(\cdot)$ is the indicator function
- Can be solved if data are linearly separable.
- **perceptron algorithm** https://www.cs.utexas.edu/~teammco/misc/perceptron/

The Perceptron algorithm is a simple **mistake-driven online algorithm**.

1. Start with a zero weight vector and process each training example in turn.
2. If the current weight vector classifies the current example incorrectly, move the weight vector in the right direction.
3. If weights stop changing, stop.

Homework: How is the perceptron algorithm implemented in practice?

Binary classification problem – Generalized Linear Classifier

Given training data

$$\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$$

Decision function:

$$f(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + w_0)$$

Optimal parameters $\hat{\mathbf{w}}^*$ and $\hat{w}_0^*$.

And then?

Binary classification problem – Generalized Linear Classifier

Given training data

$$\{\mathbf{x}_i,\ y_i\}_{i\in\{1,\cdots,n\}}$$

Decision function:

$$f(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + w_0)$$

Optimal parameters $\hat{\mathbf{w}}^*$ and $\hat{w}_0^*$.

Prediction:

$$\hat{f}(\mathbf{x}) = \mathrm{sign}(\hat{\mathbf{w}}^{*\top} \mathbf{x} + \hat{w}_0^*)$$

Binary classification problem – Generalized Linear Classifier

Loss

Definition

Empirical Risk Minimization 0-1 Loss

$$[\hat{\mathbf{w}}, \hat{w}_0] = \text{argmin}_{\mathbf{w}, w_0} \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \left(y_i \neq \text{sign}(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right)$$

- Can be solved if data are linearly separable. E.g. perceptron algorithm
- Problem?

Binary classification problem – Generalized Linear Classifier

Loss

Definition

Empirical Risk Minimization 0-1 Loss

$$[\hat{\mathbf{w}}, \hat{w}_0] = \mathrm{argmin}_{\mathbf{w}, w_0} \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \left(y_i \neq \mathrm{sign}(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right)$$

- Can be solved if data are linearly separable. E.g. perceptron algorithm
- Problem?
  - if data is not linearly separable → NP-hard!
  - Loss 0-1 is not convex and its gradient is either 0 or undefined.
  - Different $\mathbf{w}$ solutions may have the same loss.

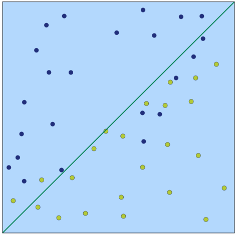
Binary classification problem – Generalized Linear Classifier

Loss

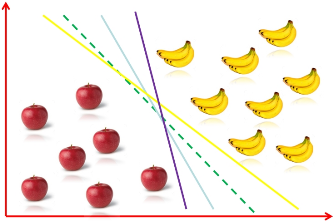
Definition

Empirical Risk Minimization

$$[\hat{\mathbf{w}}, \hat{w}_0] = \text{argmin}_{\mathbf{w}, w_0} \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \left(y_i \neq \mathrm{sign}(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right)$$



NP-hard



trop de solutions?

Background: Linear Models

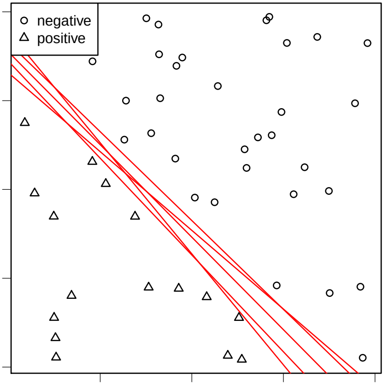
- Ordinary Least Squares

Classification

- Logistic Regression
- Linear Classifiers
- Optimal Separating Hyperplanes
- The geometric margin

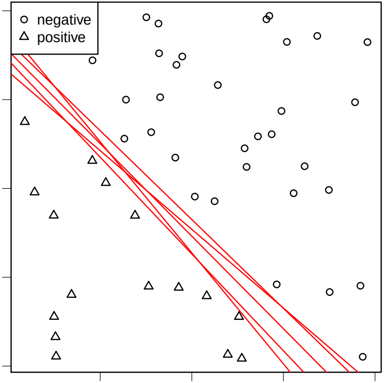
Optimal Separating Hyperplanes

- Consider a binary classification problem where two classes are optimally separable.
- A lot of hyperplanes solve this problem but which one is the best?
- Solution?



Optimal Separating Hyperplanes

- Consider a binary classification problem where two classes are optimally separable.
- A lot of hyperplanes solve this problem but which one is the best?
- **Intuition:** the **margin** separating both classes has to be **maximized**.



Background: Linear Models

- Ordinary Least Squares

Classification

- Logistic Regression
- Linear Classifiers
- Optimal Separating Hyperplanes
- The geometric margin

The geometric margin

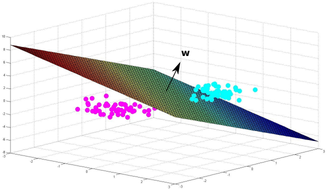
- Hyperplane equation:

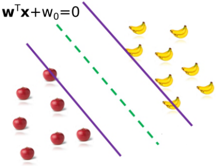
  $h(\mathbf{x}) = w_0 + \mathbf{x}^\top \mathbf{w}$

- To find the decision boundary:

  $h(\mathbf{x}) = 0$

- $\mathbf{w}$ is orthogonal to the hyperplane.
  - $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^m$ two points on the hyperplane,
  - $(\mathbf{x}_1 - \mathbf{x}_2)^\top \mathbf{w} = 0$





The geometric margin

- Hyperplane equation:

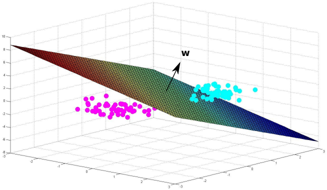
  $h(\mathbf{x}) = w_0 + \mathbf{x}^\top \mathbf{w}$

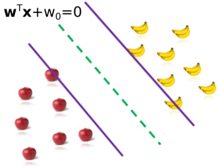
- To find the decision boundary:

  $h(\mathbf{x}) = 0$

- $\mathbf{w}$ is orthogonal to the hyperplane.
  - $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^m$ two points on the hyperplane,
  - $(\mathbf{x}_1 - \mathbf{x}_2)^\top \mathbf{w} = 0$

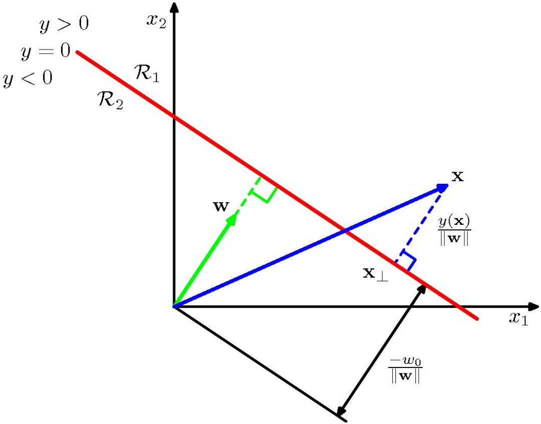
- Signed distance of a point to a hyperplane?





The geometric margin

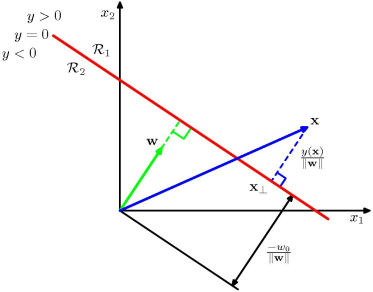
Signed distance of a point to a hyperplane?



The geometric margin

- $\mathbf{x}_{i\perp}$ is the projection of $\mathbf{x}_i$ onto the hyperplane
- $\tilde{\mathbf{x}}_i = (\mathbf{x}_i - \mathbf{x}_{i\perp})$ a vector from the hyperplane to point $\mathbf{x}_i$
- Project $\tilde{\mathbf{x}}_i$ onto $\mathbf{w}$

$$\mathrm{proj}_{\mathbf{w}}\tilde{\mathbf{x}}_i = \frac{\tilde{\mathbf{x}}_i \cdot \mathbf{w}}{\|\mathbf{w}\|} = \frac{(\mathbf{x}_i - \mathbf{x}_{i\perp})^\top \mathbf{w}}{\|\mathbf{w}\|}$$



Bishop, 2006

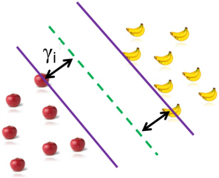
Since $\mathbf{x}_{i\perp}$ on the plane $w_0 + \mathbf{x}_{i\perp}^\top \mathbf{w} = 0$

$$\mathrm{proj}_{\mathbf{w}}\tilde{\mathbf{x}}_i = \frac{\mathbf{x}_i^\top \mathbf{w} - \cancel{\mathbf{x}_{i\perp}^\top \mathbf{w}}}{\|\mathbf{w}\|} = \frac{\mathbf{x}_i^\top \mathbf{w} + w_0}{\|\mathbf{w}\|}$$

The geometric margin

Margin: Signed distance of a point to the hyperplane:

$$\gamma_i = \frac{y_i \left(\mathbf{w}^\top \mathbf{x}_i + w_0\right)}{\|\mathbf{w}\|}$$

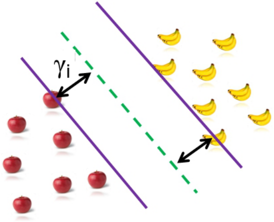


The geometric margin

Definition

Margin: smallest distance over all points

$$\gamma = \min_i (\gamma_i) = \min_i \left(\frac{y_i \left(\mathbf{w}^\top \mathbf{x}_i + w_0 \right)}{\|\mathbf{w}\|} \right)$$



Optimal Separating Hyperplanes

Question

How to define the classification problem in terms of the margin?

Optimal Separating Hyperplanes

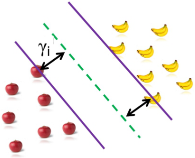
Goal

$$\mathbf{max}_{w_0,\mathbf{w}}\ \gamma$$

$$\textbf{s.t.}\ \ \frac{1}{\|\mathbf{w}\|} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq \gamma, \quad i = 1, \ldots, n$$

Find a hyperplane that

- separates the two classes
- maximizes the distance to the closest point from either class

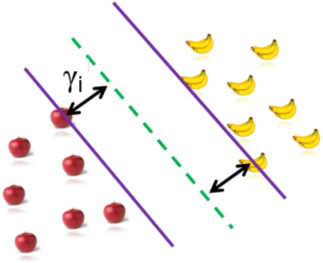


Optimal Separating Hyperplanes

Goal

$$\max_{w_0,\mathbf{w}} \gamma$$

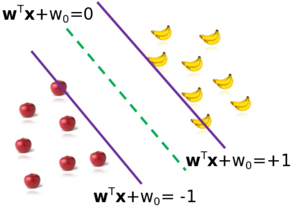
$$\textbf{s.t.} \quad \frac{1}{\|\mathbf{w}\|} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq \gamma, \quad i = 1, \ldots, n$$



Ex:bananas and apples

Optimal Separating Hyperplanes

$$\textbf{s.t. } \frac{1}{\|\mathbf{w}\|} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq \gamma, \quad i = 1, \ldots, n$$


$\mathbf{w}^T\mathbf{x}+w_0=0$
$\mathbf{w}^T\mathbf{x}+w_0=+1$
$\mathbf{w}^T\mathbf{x}+w_0=$ -1

Since changing the scaling of $\mathbf{w}$ and w_0 does not change the margin, we can arbitrarily set: $y_i\left(\mathbf{w}^\top \mathbf{x}_i + w_0\right) \geq 1$

Margin

$$\gamma = \frac{1}{\|\mathbf{w}\|}$$

which leads to an easier equivalent problem.

Optimal Separating Hyperplanes

$\max \frac{1}{\|\mathbf{w}\|}$ is equivalent to $\min \|\mathbf{w}\|^2$

Maximum margin problem

- **Minimize** $\frac{1}{2}\|\mathbf{w}\|^2$
- **subject to**: $y_i\left(\mathbf{w}^\top \mathbf{x}_i + w_0\right) \geq 1$ for all $i = 1, \ldots, n$

Optimal Separating Hyperplanes – Optimization

Maximum margin problem

- **Minimize** $\frac{1}{2}\left\|\mathbf{w}\right\|^2$
- **subject to**: $y_i\left(\mathbf{w}^\top\mathbf{x}_i + w_0\right) \geq 1$ for all $i = 1, \ldots, n$

- The functional to miminize $f(\mathbf{w}) = \frac{1}{2}\left\|\mathbf{w}\right\|^2$ is convex,
- The **constraints** $1 - y_i\left(\mathbf{w}^\top\mathbf{x}_i + w_0\right) \leq 0$ are **linear**.

Can be solved with convex optimization, e.g. using **quadratic programming**! (`quadprog` in both python and matlab)

Optimal Separating Hyperplanes – Optimization

Maximum margin problem

- **Minimize** $\frac{1}{2}\left\|\mathbf{w}\right\|^2$
- **subject to**: $y_i\left(\mathbf{w}^\top\mathbf{x}_i + w_0\right) \geq 1$ for all $i = 1, \ldots, n$

Construct the **Lagrangian** :

Lagrangian

$$\mathcal{L}(\mathbf{w}, w_0, \alpha) = \frac{1}{2}\left\|\mathbf{w}\right\|^2 + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\mathbf{w}^\top\mathbf{x}_i + w_0)\right)$$

Optimal Separating Hyperplanes – Optimization

It is a Constrained Optimization with an inequality constraints.

With g_i the constraint $g_i(\mathbf{w}) = 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)$.

the solution $\hat{\mathbf{w}}^*, w_0^*, \alpha_i^* \forall i$ has to verify the **KKT Conditions:**

1. Lagrangian Stationarity: $\frac{\partial \mathcal{L}(\hat{\mathbf{w}}^*, \hat{w}_0^*, \alpha^*)}{\partial \mathbf{w}} = 0$ & $\frac{\partial \mathcal{L}(\hat{\mathbf{w}}^*, \hat{w}_0^*, \alpha^*)}{\partial w_0} = 0$
2. Primal Feasibility:$g_i(\mathbf{w}^*) \leq 0$
3. Dual Feasibility: $\alpha_i^* \geq 0$
4. Complementary Slackness:$\alpha_i^* g_i(\mathbf{w}^*) = 0$

KKT conditions establish a generalization of Lagrange multipliers, for inequality constraints.