Big Data Computing

Master's Degree in Computer Science

2019-2020

Gabriele Tolomei

Department of Computer Science

Sapienza Università di Roma

tolomei@di.uniroma1.it

SAPIENZA UNIVERSITÀ DI ROMA

Recap from Last Lectures

- We described linear regression as a powerful technique to predict real-valued function
- Linear regression tries to fit a straight hyperplane between features (i.e., independent variables) and the target (i.e., dependent variable)
- OLS method to easily estimate the parameters of the model
- More advanced techniques may be applied if the relationship between features and the target is not linear (e.g., polynomial regression)

Classification vs. Regression

- Very often, the response variable to predict is **qualitative** (categorical)

Classification vs. Regression

- Very often, the response variable to predict is **qualitative** (categorical)
- **Classification** (as opposed to regression) deals with predicting categorical responses

Classification vs. Regression

- Very often, the response variable to predict is **qualitative** (categorical)
- **Classification** (as opposed to regression) deals with predicting categorical responses
- Examples:
  - spam vs. non-spam emails
  - click vs. non-click on a web page or an advertisement

Classification vs. Regression

- Very often, the response variable to predict is **qualitative** (categorical)
- **Classification** (as opposed to regression) deals with predicting categorical responses
- Examples:
  - spam vs. non-spam emails
  - click vs. non-click on a web page or an advertisement
- Classification methods may first predict the probability of each category of a qualitative response to make in turn a decision

Why Not Linear Regression, Then?

- Suppose we want to predict the health condition of a patient arriving in the ER on the basis of her symptoms

Why Not Linear Regression, Then?

- Suppose we want to predict the health condition of a patient arriving in the ER on the basis of her symptoms
- Imagine there are only the following 3 possible diagnoses: stroke, drug overdose, and epileptic seizure

Why Not Linear Regression, Then?

- Suppose we want to predict the health condition of a patient arriving in the ER on the basis of her symptoms
- Imagine there are only the following 3 possible diagnoses: stroke, drug overdose, and epileptic seizure
- We may encode the above values as a categorical response variable Y

$$Y = \begin{cases} 1 & \text{if } \texttt{stroke}; \\ 2 & \text{if } \texttt{drug overdose}; \\ 3 & \text{if } \texttt{epileptic seizure}. \end{cases}$$

source: http://faculty.marshall.usc.edu/gareth-james/ISL/ISLR%20Seventh%20Printing.pdf

Why Not Linear Regression, Then?

- With the previous encoding we can fit a linear regression model using OLS from a set of n features $x_1, \ldots, x_n$

Why Not Linear Regression, Then?

- With the previous encoding we can fit a linear regression model using OLS from a set of n features $x_1, \ldots, x_n$
- Unfortunately, this coding implies an **ordering** on the outcomes
  - drug overdose is in between stroke and epileptic seizure
  - the difference between stroke and drug overdose is the same as the difference between drug overdose and epileptic seizure

Why Not Linear Regression, Then?

- With the previous encoding we can fit a linear regression model using OLS from a set of n features $x_1, \ldots, x_n$
- Unfortunately, this coding implies an **ordering** on the outcomes
    - drug overdose is in between stroke and epileptic seizure
    - the difference between stroke and drug overdose is the same as the difference between drug overdose and epileptic seizure
- In practice, there is no particular reason to choose the encoding above!

Why Not Linear Regression, Then?

- With the previous encoding we can fit a linear regression model using OLS from a set of n features $x_1, \ldots, x_n$
- Unfortunately, this coding implies an **ordering** on the outcomes
  - drug overdose is in between stroke and epileptic seizure
  - the difference between stroke and drug overdose is the same as the difference between drug overdose and epileptic seizure
- In practice, there is no particular reason to choose the encoding above!
- Different (and still legitimate) encodings will produce different models

Why Not Linear Regression, Then?

- The encoding above would work if the response variable values take on an **equally-spaced natural ordering** (e.g., mild, moderate, and severe)

Why Not Linear Regression, Then?

- The encoding above would work if the response variable values take on an **equally-spaced natural ordering** (e.g., mild, moderate, and severe)
- In general, there is no natural way to convert a K-ary (K > 2) response into a quantitative response that is ready for linear regression

Why Not Linear Regression, Then?

- The encoding above would work if the response variable values take on an **equally-spaced natural ordering** (e.g., mild, moderate, and severe)
- In general, there is no natural way to convert a K-ary (K > 2) response into a quantitative response that is ready for linear regression
- For a binary response with a 0/1 encoding, linear regression by OLS does anyway make sense
  - Predict 1 if the outcome is > 0.5, 0 otherwise

Why Not Linear Regression, Then?

- The encoding above would work if the response variable values take on an **equally-spaced natural ordering** (e.g., mild, moderate, and severe)
- In general, there is no natural way to convert a K-ary (K > 2) response into a quantitative response that is ready for linear regression
- For a binary response with a 0/1 encoding, linear regression by OLS does anyway make sense
  - Predict 1 if the outcome is > 0.5, 0 otherwise
- Still, it is preferable to use a classification method which works by design

LOGISTIC REGRESSION

Example: Default(Y) vs. Balance(X)

Consider a binary response Default(Y) taking on two values: Yes or No

Example: Default(Y) vs. Balance(X)

Consider a binary response Default(Y) taking on two values: Yes or No

Suppose we want to predict the value of Y from the value of Balance(X)

Example: Default(Y) vs. Balance(X)

Consider a binary response Default(Y) taking on two values: Yes or No

Suppose we want to predict the value of Y from the value of Balance(X)

We can model it **directly** via linear regression (i.e., predicting its value)

Example: Default(Y) vs. Balance(X)

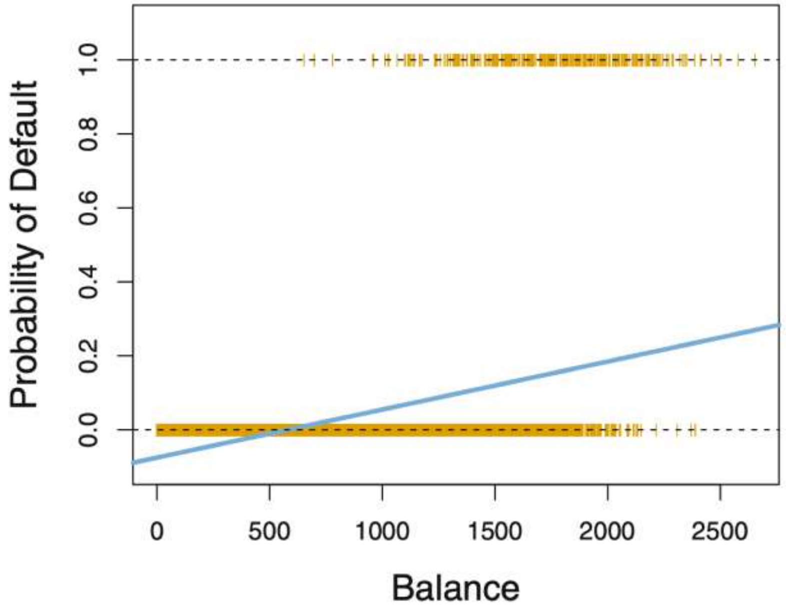
Consider a binary response Default(Y) taking on two values: Yes or No

Suppose we want to predict the value of Y from the value of Balance(X)

We can model it **directly** via linear regression (i.e., predicting its value)

Logistic Regression instead models the **probability** that Y belongs to one of the two possible outcome values

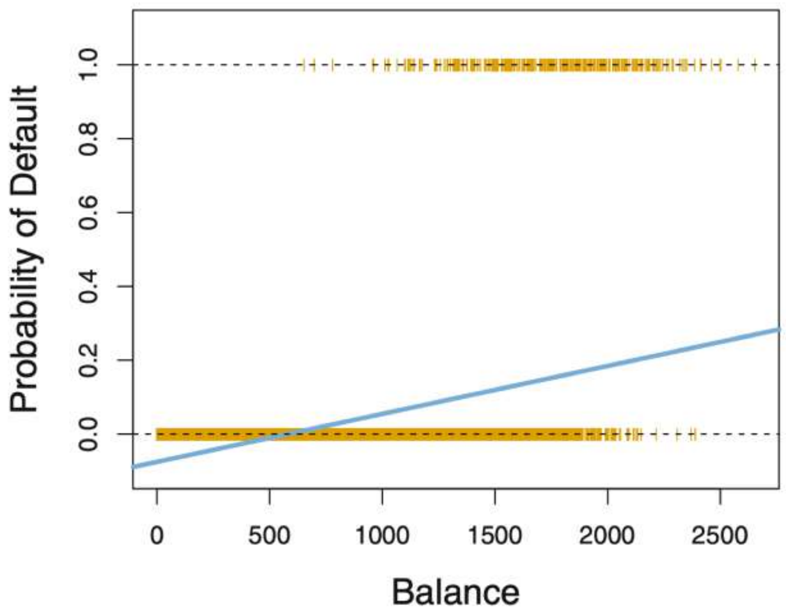
Example: Default(Y) vs. Balance(X)



Predicted probability using linear regression
(some estimated probabilities are negative!)

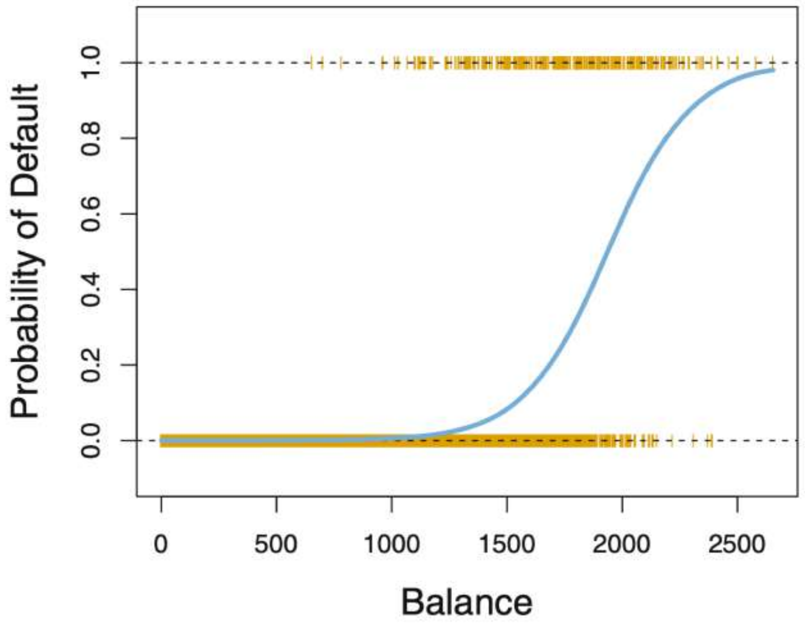
Linear Regression

Example: Default(Y) vs. Balance(X)



Predicted probability using linear regression (some estimated probabilities are negative!)

Linear Regression



Predicted probability using logistic regression (all probabilities lie between 0 and 1)

Logistic Regression

General Concepts

$\boxed{\textbf{3} \text{ components need to be specified}}$

General Concepts

3 components need to be specified

Model

Defines the space of representable hypotheses

General Concepts

3 components need to be specified

Model

Defines the space of representable hypotheses

Error Measure
(Cost Function)

Measures the price of misclassification errors

General Concepts

3 components need to be specified

Model

Defines the space of representable hypotheses

Error Measure
(Cost Function)

Measures the price of misclassification errors

Learning Algorithm

Picks the *best* hypothesis exploring search space

MODEL

Linear Signal

- Let $\mathbf{x} = (x_0, x_1, \ldots, x_d)$ be the (d+1)-dimensional input

Linear Signal

- Let $\mathbf{x} = (x_0, x_1, \ldots, x_d)$ be the (d+1)-dimensional input
- Let *F* be the family of real-valued functions parametrized by $\boldsymbol{\theta}$ so that $\boldsymbol{\theta}^T = (\theta_0, \theta_1, \ldots, \theta_d)$

$$\mathcal{F} = \{f_{\boldsymbol{\theta}} : \mathbb{R}^{d+1} \longmapsto \mathbb{R} \mid f_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x} = \sum_{i=0}^{d} \theta_i x_i\}$$

Linear Signal

- Let $\mathbf{x} = (x_0, x_1, \ldots, x_d)$ be the (d+1)-dimensional input
- Let *F* be the family of real-valued functions parametrized by $\boldsymbol{\theta}$ so that $\boldsymbol{\theta}^T = (\theta_0, \theta_1, \ldots, \theta_d)$

$$\mathcal{F} = \{f_{\boldsymbol{\theta}} : \mathbb{R}^{d+1} \longmapsto \mathbb{R} \mid f_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x} = \sum_{i=0}^{d} \theta_i x_i\}$$

- Each function in *F* outputs a real number (i.e., a scalar) as a linear combination of the input $\mathbf{x}$ with the parameters $\boldsymbol{\theta}$

Linear Signal

- Let $\mathbf{x} = (x_0, x_1, \ldots, x_d)$ be the (d+1)-dimensional input
- Let *F* be the family of real-valued functions parametrized by $\boldsymbol{\theta}$ so that $\boldsymbol{\theta}^T = (\theta_0, \theta_1, \ldots, \theta_d)$

$$\mathcal{F} = \{f_{\boldsymbol{\theta}} : \mathbb{R}^{d+1} \longmapsto \mathbb{R} \mid f_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x} = \sum_{i=0}^{d} \theta_i x_i\}$$

- Each function in *F* outputs a real number (i.e., a scalar) as a linear combination of the input $\mathbf{x}$ with the parameters $\boldsymbol{\theta}$
- $f_\theta(\mathbf{x})$ is referred to as (**linear**) **signal**

Hypothesis Space (Revisited)

- The signal alone is not enough to define the hypothesis space *H*

Hypothesis Space (Revisited)

- The signal alone is not enough to define the hypothesis space H
- Usually the signal is passed through a "filter", i.e. another real-valued function g

Hypothesis Space (Revisited)

- The signal alone is not enough to define the hypothesis space *H*
- Usually the signal is passed through a "filter", i.e. another real-valued function *g*
- $h_\theta(\mathbf{x}) = g(f_\theta(\mathbf{x}))$ defines the hypothesis space:

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : \mathbb{R}^{d+1} \longmapsto \mathbb{R} \mid h_{\boldsymbol{\theta}}(\mathbf{x}) = g(f_{\boldsymbol{\theta}}(\mathbf{x})) = g(\boldsymbol{\theta}^T\mathbf{x}) = g\big(\sum_{i=0}^{d} \theta_i x_i\big)\}$$

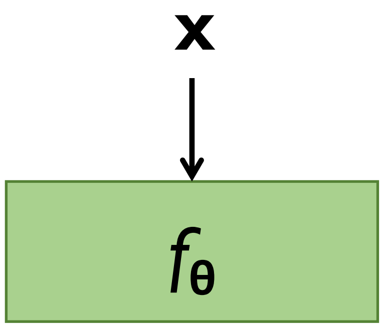
Hypothesis Space (Revisited)

- The signal alone is not enough to define the hypothesis space *H*
- Usually the signal is passed through a "filter", i.e. another real-valued function *g*
- $h_\theta(\mathbf{x}) = g(f_\theta(\mathbf{x}))$ defines the hypothesis space:

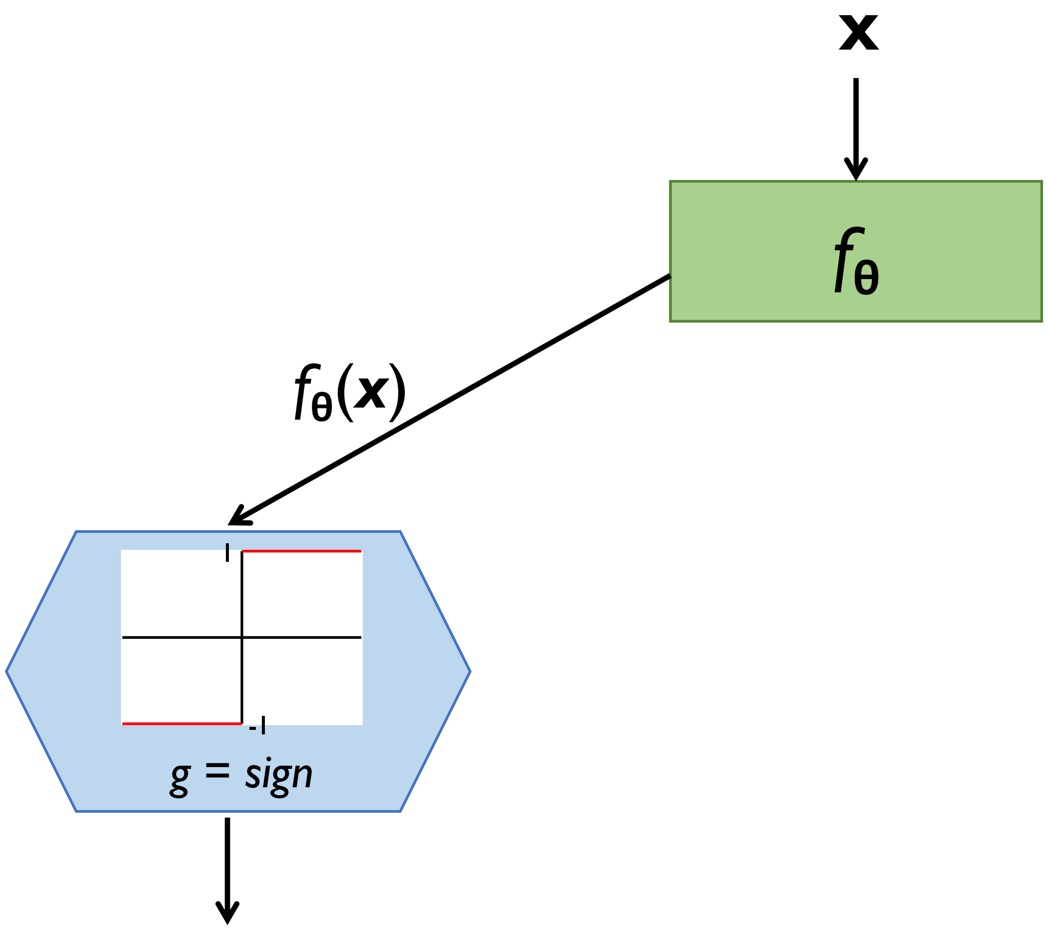
$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : \mathbb{R}^{d+1} \longmapsto \mathbb{R} \mid h_{\boldsymbol{\theta}}(\mathbf{x}) = g(f_{\boldsymbol{\theta}}(\mathbf{x})) = g(\boldsymbol{\theta}^T\mathbf{x}) = g\big(\sum_{i=0}^{d} \theta_i x_i\big)\}$$

The set of possible hypotheses *H* changes depending on the parametric model (f_θ) and on the **thresholding function** (*g*)

Filtering (Thresholding)

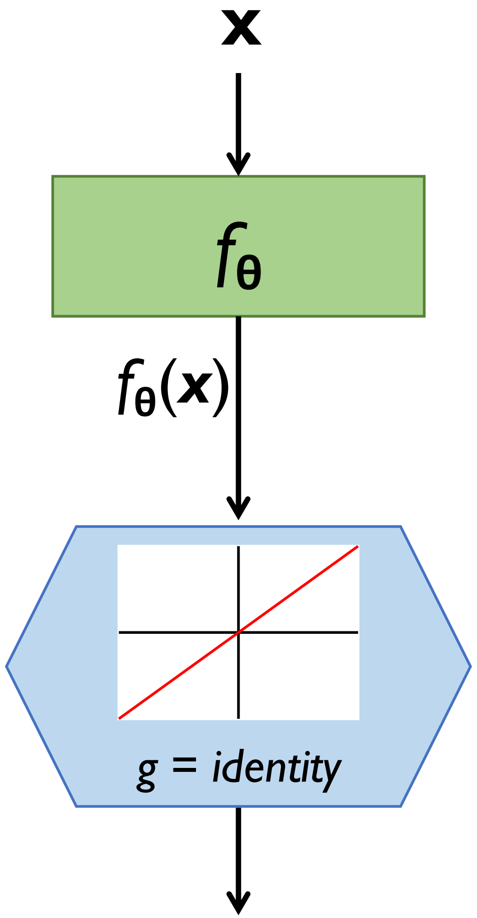


Filtering (Thresholding)



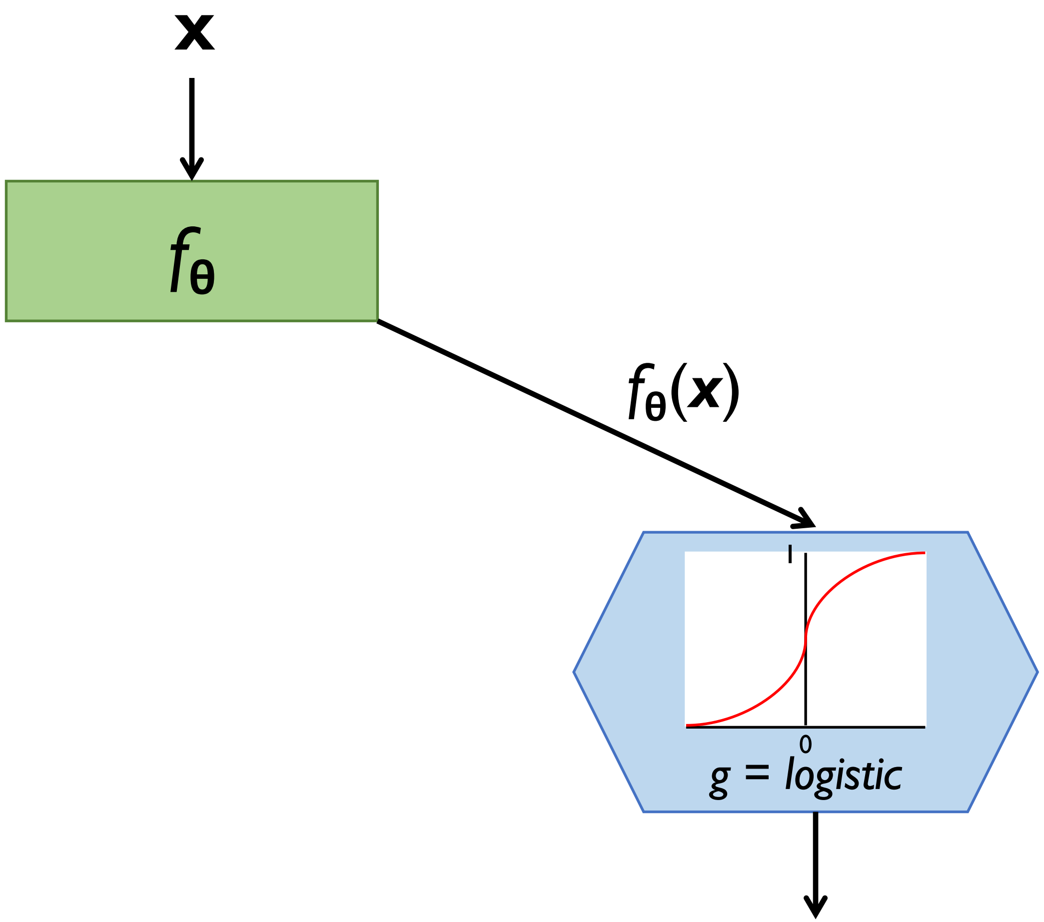
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \mathrm{sign}(f_{\boldsymbol{\theta}}(\mathbf{x})) = \mathrm{sign}(\boldsymbol{\theta}^T \mathbf{x})$$

Filtering (Thresholding)



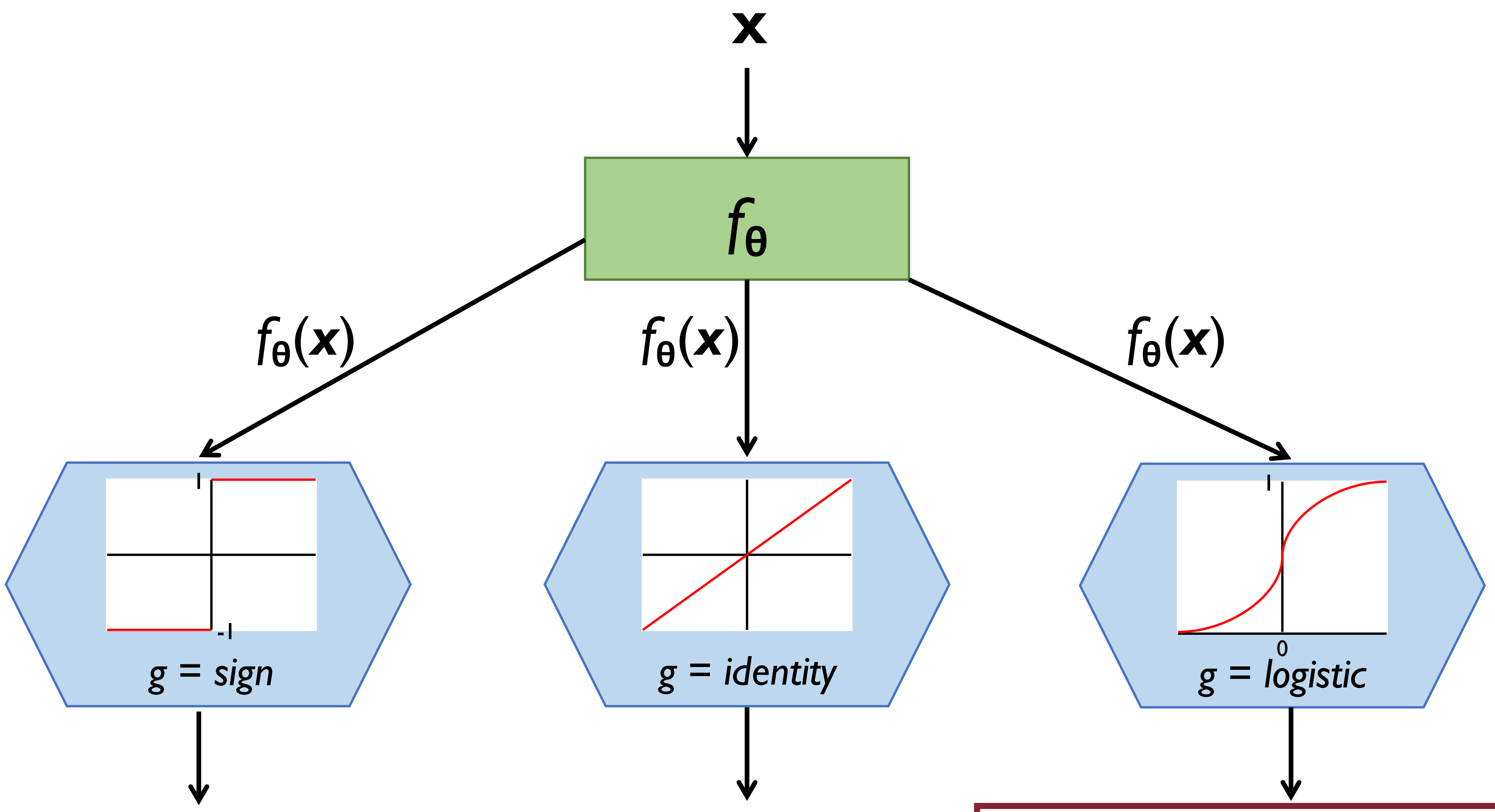
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = f_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T\mathbf{x}$$

Filtering (Thresholding)



$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

Filtering (Thresholding)

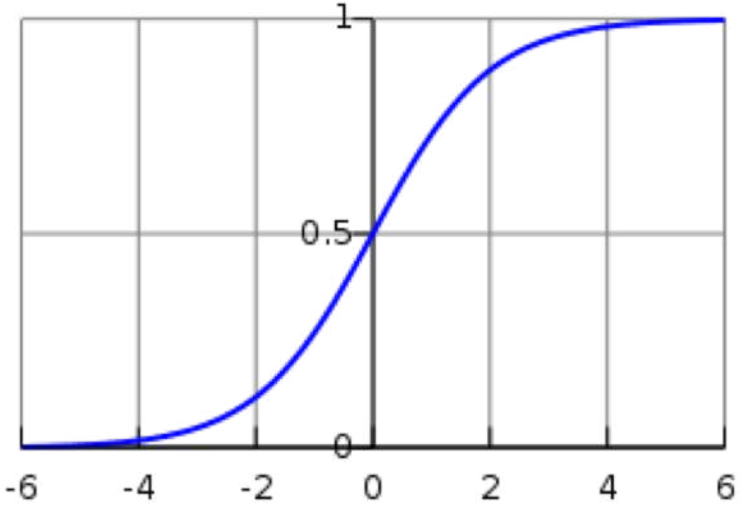


$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \mathrm{sign}(f_{\boldsymbol{\theta}}(\mathbf{x})) = \mathrm{sign}(\boldsymbol{\theta}^T\mathbf{x})$$

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = f_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T\mathbf{x}$$

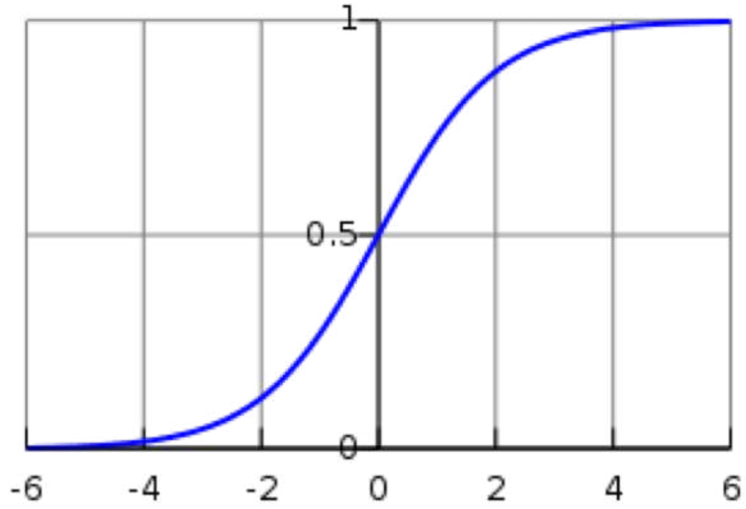
$$\boxed{h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}}$$

The Logistic Function



$$\ell(z) = \frac{e^z}{1+e^z}$$

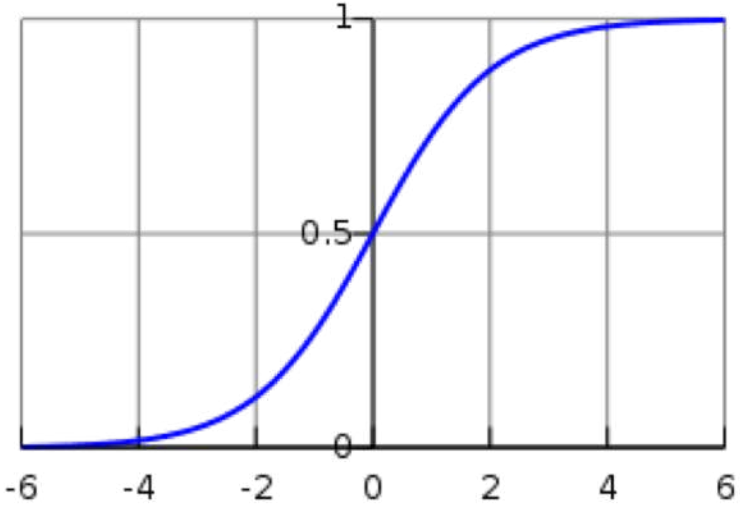
The Logistic Function



$$\ell(z) = \frac{e^z}{1+e^z}$$

- Also known as sigmoid function do to its "S" shape or soft threshold (compared to hard threshold imposed by *sign*)

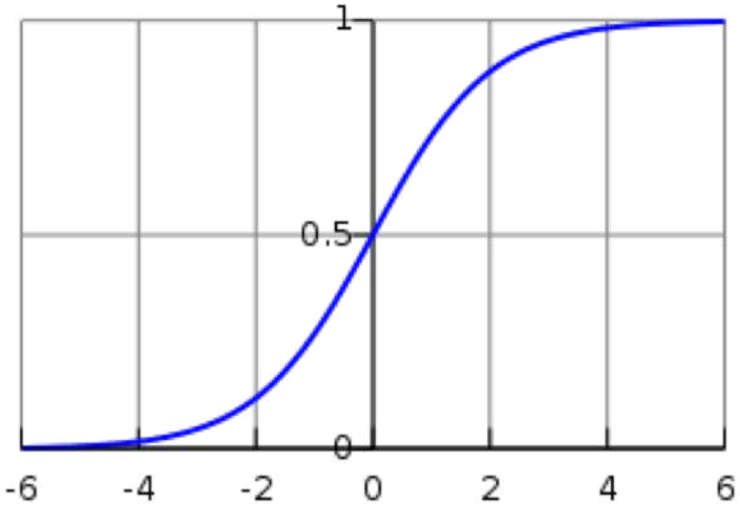
The Logistic Function



$$\ell(z) = \frac{e^z}{1+e^z}$$

- Also known as sigmoid function do to its "S" shape or soft threshold (compared to hard threshold imposed by *sign*)
- When $z = \boldsymbol{\theta}^T\mathbf{x}$ we are applying a *non-linear* transformation to our *linear* signal

The Logistic Function



$$\ell(z) = \frac{e^z}{1+e^z}$$

- Also known as sigmoid function do to its "S" shape or soft threshold (compared to hard threshold imposed by *sign*)
- When $z = \boldsymbol{\theta}^T\mathbf{x}$ we are applying a *non-linear* transformation to our *linear* signal
- Output can be *genuinely* interpreted as a probability value

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

- Describing the set of hypotheses using the **logistic function** is not enough to state that the output can be interpreted as a probability

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

- Describing the set of hypotheses using the **logistic function** is not enough to state that the output can be interpreted as a probability
- All we know is that the logistic function always produce a real value between 0 and 1

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

- Describing the set of hypotheses using the **logistic function** is not enough to state that the output can be interpreted as a probability
- All we know is that the logistic function always produce a real value between 0 and 1
- Other functions may have the same property [e.g., 1/π *arctan(x)* + *1/2*]

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

- The key points here are:

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

- The key points here are:
  - the output of the logistic function can be interpreted as a probability even during learning

Probabilistic Interpretation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}$$

- The key points here are:
  - the output of the logistic function can be interpreted as a probability even during learning
  - the logistic function is mathematically convenient!

Odds

- Let p (resp., $q = 1\text{-}p$) be the probability of success (resp., failure) of an event

Odds

- Let p (resp., $q = 1\text{-}p$) be the probability of success (resp., failure) of an event
- $odds(success) = p/q = p/(1\text{-}p)$

Odds

- Let p (resp., $q = 1\text{-}p$) be the probability of success (resp., failure) of an event
- $odds(success) = p/q = p/(1\text{-}p)$
- $odds(failure) = q/p = 1/p/q = 1/odds(success)$

Odds

- Let p (resp., $q = 1\text{-}p$) be the probability of success (resp., failure) of an event
- $odds(success) = p/q = p/(1\text{-}p)$
- $odds(failure) = q/p = 1/p/q = 1/odds(success)$
- $logit(p) = ln(odds(success)) = ln(p/q) = ln(p/1\text{-}p) = ln(p) - ln(1\text{-}p)$

Odds

Logistic Regression is in fact an ordinary linear regression where the logit is the response variable!

$$\boxed{\text{logit}(p) = \ln\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}}$$

The coefficients of logistic regression are expressed in terms of the natural logarithm of odds

Why Odds instead of Probability?

Odds are defined on the range [0, +inf]

Why Odds instead of Probability?

Odds are defined on the range [0, +inf]

Logit (i.e., natural log of odds) are defined on the range [-inf, +inf]

Why Odds instead of Probability?

Odds are defined on the range [0, +inf]

Logit (i.e., natural log of odds) are defined on the range [-inf, +inf]

Therefore we can use "standard" regression equation:

$$\boxed{\operatorname{logit}(p) = \ln\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}}$$

Why Odds instead of Probability?

Odds are defined on the range [0, +inf]

Logit (i.e., natural log of odds) are defined on the range [-inf, +inf]

Therefore we can use "standard" regression equation:

$$\boxed{\mathrm{logit}(p) = \ln\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}}$$

For any value of the regression coefficients and features a valid value for the odds are predicted

Why Odds instead of Probability?

Odds are defined on the range [0, +inf]

Logit (i.e., natural log of odds) are defined on the range [-inf, +inf]

Therefore we can use "standard" regression equation:

$$\boxed{\text{logit}(p) = \ln\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}}$$

For any value of the regression coefficients and features a valid value for the odds are predicted

Probabilities are only defined on the range [0, 1]

It would need very complicated constraints on the regression coefficients to work with probability

From Odds to Probability

$$\mathrm{logit}(p) = \ln\left(\tfrac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}$$

From Odds to Probability

$$\text{logit}(p) = \ln\left(\tfrac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}$$

$$e^{\text{logit}(p)} = e^{\ln\left(\frac{p}{1-p}\right)} = \frac{p}{1-p} = e^{(\boldsymbol{\theta}^T \mathbf{x})}$$

$$p = e^{(\boldsymbol{\theta}^T \mathbf{x})}(1-p) = e^{(\boldsymbol{\theta}^T \mathbf{x})} - e^{(\boldsymbol{\theta}^T \mathbf{x})}p$$

$$p + e^{(\boldsymbol{\theta}^T \mathbf{x})}p = e^{(\boldsymbol{\theta}^T \mathbf{x})}$$

$$p(1 + e^{(\boldsymbol{\theta}^T \mathbf{x})}) = e^{(\boldsymbol{\theta}^T \mathbf{x})}$$

$$\boxed{p = \frac{e^{(\boldsymbol{\theta}^T \mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T \mathbf{x})}} = \frac{1}{e^{-(\boldsymbol{\theta}^T \mathbf{x})}+1}}$$

Odds Ratio

Using (log) odds rather than actual probabilities provides an easier interpretation of the model's coefficients learned

$$\ln\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}$$

$$\left(\frac{p}{1-p}\right) = e^{\theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d} = e^{\boldsymbol{\theta}^T \mathbf{x}}$$

Odds Ratio

Using (log) odds rather than actual probabilities provides an easier interpretation of the model's coefficients learned

$$\ln\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d = \boldsymbol{\theta}^T \mathbf{x}$$

$$\left(\frac{p}{1-p}\right) = e^{\theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d} = e^{\boldsymbol{\theta}^T \mathbf{x}}$$

Suppose we want to measure the effect of a unit increase in one of the predictors to the output response

Odds Ratio

Let's measure the ratio between the odds computed at a certain input **x** and the odds computed at a different point **x**'

Odds Ratio

Let's measure the ratio between the odds computed at a certain input **x** and the odds computed at a different point **x**'

$$\mathbf{x} = x_1 + \ldots + x_i + \ldots + x_d$$
$$\mathbf{x}' = x_1 + \ldots + (x_i + 1) + \ldots + x_d$$

x' is just the same as **x** where the i-th predictor/feature is increased by 1 unit

Odds Ratio

Let's measure the ratio between the odds computed at a certain input **x** and the odds computed at a different point **x**'

$$\mathbf{x} = x_1 + \ldots + x_i + \ldots + x_d$$
$$\mathbf{x}' = x_1 + \ldots + (x_i + 1) + \ldots + x_d$$

x' is just the same as **x** where the i-th predictor/feature is increased by 1 unit

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}}$$

Odds Ratio

Odds Ratio

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}} =$$

Odds Ratio

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}} =$$

$$\frac{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i(x_i+1)+\ldots+\theta_d x_d}}{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}}$$

Odds Ratio

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}} =$$

$$\frac{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i(x_i+1)+\ldots+\theta_d x_d}}{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} = \frac{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d} * e^{\theta_i}}{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}}$$

Odds Ratio

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}} =$$

$$\frac{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i(x_i+1)+\ldots+\theta_d x_d}}{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} = \frac{\cancel{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} * e^{\theta_i}}{\cancel{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}}}$$

Odds Ratio

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}} =$$

$$\frac{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i(x_i+1)+\ldots+\theta_d x_d}}{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} = \frac{\cancel{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} * e^{\theta_i}}{\cancel{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}}}$$

$$= e^{\theta_i}$$

The ratio of the odds for 1-unit increase in x_i

Odds Ratio

$$\frac{e^{\boldsymbol{\theta}^T \mathbf{x}'}}{e^{\boldsymbol{\theta}^T \mathbf{x}}} =$$

$$\frac{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i(x_i+1)+\ldots+\theta_d x_d}}{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} = \frac{\cancel{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}} * e^{\theta_i}}{\cancel{e^{\theta_0+\theta_1 x_1+\ldots+\theta_i x_i+\ldots+\theta_d x_d}}}$$

$$= e^{\theta_i}$$

The ratio of the odds for 1-unit increase in x_i

or

θ_i is the ratio of the natural log(odds) for 1-unit increase in x_i

Why Odds Ratio?

This ratio is **constant**: it does not change according to the value of the other x_j because they cancel out in the calculation

Why Odds Ratio?

This ratio is **constant**: it does not change according to the value of the other x_j because they cancel out in the calculation

If we used probability rather than odds this wouldn't be constant!

Why Odds Ratio?

This ratio is **constant**: it does not change according to the value of the other x_j because they cancel out in the calculation

If we used probability rather than odds this wouldn't be constant!

The effect of x_i on the probability of success p is different depending on the value of x_i

Why Odds Ratio?

This ratio is **constant**: it does not change according to the value of the other x_j because they cancel out in the calculation

If we used probability rather than odds this wouldn't be constant!

The effect of x_i on the probability of success *p* is different depending on the value of x_i

Example

An odds ratio of 1.08 will give an 8% increase in the odds at *any* value of x_i

Probabilistically-Generated Data

As with any other supervised learning problem we are given a finite set *D* of *m* i.i.d. labelled examples which we can try to learn from

$$\mathcal{D} = \{(\mathbf{x_1}, y_1)\}, \ldots, (\mathbf{x_m}, y_m)\}$$

where each y_i is a binary variable taking on two values (e.g., {-1,+1})

Probabilistically-Generated Data

That means we **do not** have access to the individual probability associated with each training sample!

Probabilistically-Generated Data

That means we **do not** have access to the individual probability associated with each training sample!

The data we observe from *D* is actually generated by an *underlying and unknown probability function* (**noisy target**) which we want to estimate

$$P(y|\mathbf{x}) = \begin{cases} \phi(\mathbf{x}) & \text{if } y = +1 \\ 1 - \phi(\mathbf{x}) & \text{if } y = -1 \end{cases}$$

Deterministic vs. Noisy Target

- Deterministic function: given **x** as input it always outputs either $y = +1$ or $y = -1$ (mutually exclusive)

Deterministic vs. Noisy Target

- Deterministic function: given **x** as input it always outputs either $y = +1$ or $y = -1$ (mutually exclusive)
- Noisy target function: given **x** as input it always outputs both $y = +1$ and $y = -1$, each with a "degree of certainty" associated

Deterministic vs. Noisy Target

- Deterministic function: given **x** as input it always outputs either $y = +1$ or $y = -1$ (mutually exclusive)
- Noisy target function: given **x** as input it always outputs both $y = +1$ and $y = -1$, each with a "degree of certainty" associated

Goal

$\phi: R^{d+1} \rightarrow [0,1]$ is the unknown noisy target which generates our examples, our aim is to find an estimate ϕ^* which best approximates ϕ

Estimating Noisy Target

$$P(y|\mathbf{x}) = \begin{cases} \phi^*(\mathbf{x}) & \text{if } y = +1 \\ 1 - \phi^*(\mathbf{x}) & \text{if } y = -1 \end{cases}$$

Estimating Noisy Target

$$P(y|\mathbf{x}) = \begin{cases} \phi^*(\mathbf{x}) & \text{if } y = +1 \\ 1 - \phi^*(\mathbf{x}) & \text{if } y = -1 \end{cases}$$

We claim that the best estimate ϕ^* of ϕ is $h^*_{\boldsymbol{\theta}}(\mathbf{x})$ which in turn is picked from the set of hypotheses defined by logistic function

$$\boxed{\phi^*(\mathbf{x}) = h^*_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(\boldsymbol{\theta}^T \mathbf{x}) \approx \phi(\mathbf{x})}$$

Hypothesized Noisy Target

- How do we estimate $h^*_{\boldsymbol{\theta}}(\mathbf{x})$?

Hypothesized Noisy Target

- How do we estimate $h^*_{\boldsymbol{\theta}}(\mathbf{x})$?
- We will use the same general framework introduced for the supervised learning problem!

Hypothesized Noisy Target

- How do we estimate $h^*_{\boldsymbol{\theta}}(\mathbf{x})$?
- We will use the same general framework introduced for the supervised learning problem!
- We already fixed the set of hypothesis function to select from

Hypothesized Noisy Target

- How do we estimate $h^{*}_{\boldsymbol{\theta}}(\mathbf{x})$?
- We will use the same general framework introduced for the supervised learning problem!
- We already fixed the set of hypothesis function to select from
- We still need:
  - A training set D
  - An error measure (cost function) to minimize

COST FUNCTION

Finding The Best Hypothesis

If the hypothesis space H is made of a family of parametric models, $h^*_{\boldsymbol{\theta}}(\mathbf{x})$ can be picked as:

$$h^*_{\boldsymbol{\theta}} = \mathtt{argmax}_{h_{\boldsymbol{\theta}} \in \mathcal{H}} \; P(h_{\boldsymbol{\theta}} \mid \mathcal{D})$$

Finding The Best Hypothesis

If the hypothesis space H is made of a family of parametric models, $h^*_{\boldsymbol{\theta}}(\mathbf{x})$ can be picked as:

$$h^*_{\boldsymbol{\theta}} = \texttt{argmax}_{h_{\boldsymbol{\theta}} \in \mathcal{H}} \; P(h_{\boldsymbol{\theta}} \mid \mathcal{D})$$

That is, we want to maximize the probability of the chosen hypothesis given the data D we observed

Flipping the Coin: The Likelihood Function

We measure the error we are making by assuming that $h^*_{\boldsymbol{\theta}}(\mathbf{x})$ approximates the true noisy target ϕ

Flipping the Coin: The Likelihood Function

We measure the error we are making by assuming that $h^*_{\boldsymbol{\theta}}(\mathbf{x})$ approximates the true noisy target ϕ

How likely is that the observed data D have been generated by our selected hypothesis $h^*_{\boldsymbol{\theta}}(\mathbf{x})$?

Flipping the Coin: The Likelihood Function

We measure the error we are making by assuming that $h^*_{\boldsymbol{\theta}}(\mathbf{x})$ approximates the true noisy target ϕ

How likely is that the observed data D have been generated by our selected hypothesis $h^*_{\boldsymbol{\theta}}(\mathbf{x})$?

Find the hypothesis which maximizes the probability of the observed data D given a particular hypothesis

$$\boxed{h^*_{\boldsymbol{\theta}} = \texttt{argmax}_{h_{\boldsymbol{\theta}} \in \mathcal{H}} P(\mathcal{D} \,|h_{\boldsymbol{\theta}})}$$

The Likelihood Function

Given the generic training example $(\mathbf{x}, y)$ and assuming it has been generated by a hypothesis $h_{\theta}(\mathbf{x})$ the likelihood function is:

$$P(y|\mathbf{x}) = \begin{cases} h_{\theta}(\mathbf{x}) & \text{if } y = +1 \\ 1 - h_{\theta}(\mathbf{x}) & \text{if } y = -1 \end{cases}$$

where ϕ has been replaced with our hypothesis

The Likelihood Function

If we assume the hypothesis is the logistic function

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(\boldsymbol{\theta}^T \mathbf{x})$$

The Likelihood Function

If we assume the hypothesis is the logistic function

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(\boldsymbol{\theta}^T\mathbf{x})$$

And by noticing that logistic function is symmetric, i.e. $\ell(-z) = 1-\ell(z)$, the likelihood for a single example is:

$$\boxed{P(y \mid \mathbf{x}) = \ell(y\boldsymbol{\theta}^T\mathbf{x})}$$

The Likelihood Function

Having access to a full set of *m* i.i.d. training examples *D*

$$\mathcal{D} = \{(\mathbf{x_1}, y_1)\}, \ldots, (\mathbf{x_m}, y_m)\}$$

The overall likelihood function is computed as:

$$\boxed{\prod_{i=1}^{m} P(y_i \mid \mathbf{x_i}) = \prod_{i=1}^{m} \ell(y_i \boldsymbol{\theta}^T \mathbf{x_i})}$$

Why Does Likelihood Make Sense?

How does the likelihood $\ell(y_i\boldsymbol{\theta}^T\mathbf{x}_i)$ changes w.r.t. the sign of y_i and $\boldsymbol{\theta}^T\mathbf{x}_i$?

	$\boldsymbol{\theta}^T\mathbf{x}_i > 0$	$\boldsymbol{\theta}^T\mathbf{x}_i < 0$
$y_i > 0$	≈ 1	≈ 0
$y_i < 0$	≈ 0	≈ 1

Why Does Likelihood Make Sense?

How does the likelihood $\ell(y_i \boldsymbol{\theta}^T \mathbf{x_i})$ changes w.r.t. the sign of y_i and $\boldsymbol{\theta}^T \mathbf{x_i}$?

	$\boldsymbol{\theta}^T \mathbf{x}_i > 0$	$\boldsymbol{\theta}^T \mathbf{x}_i < 0$
$y_i > 0$	≈ 1	≈ 0
$y_i < 0$	≈ 0	≈ 1

If the label is **concordant** with the signal (either positively or negatively) then $\ell(y_i \boldsymbol{\theta}^T \mathbf{x_i})$ approaches to 1

prediction agrees with the true label

Why Does Likelihood Make Sense?

How does the likelihood $\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})$ changes w.r.t. the sign of y_i and $\boldsymbol{\theta}^T\mathbf{x_i}$?

	$\boldsymbol{\theta}^T\mathbf{x}_i > 0$	$\boldsymbol{\theta}^T\mathbf{x}_i < 0$
$y_i > 0$	≈ 1	≈ 0
$y_i < 0$	≈ 0	≈ 1

If the label is **disoncordant** with the signal then $\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})$ approaches to 0

prediction disagrees with the true label

Maximum Likelihood Estimate (MLE)

Find the vector of parameters θ such that the likelihood function is maximum

$$\boxed{\texttt{argmax}_\theta\left(\prod_{i=1}^{m} P(y_i \mid \mathbf{x_i})\right) = \texttt{argmax}_\theta\left(\prod_{i=1}^{m} \ell(y_i \boldsymbol{\theta}^T \mathbf{x_i})\right)}$$

From MLE to In-Sample Error

Given a hypothesis h_θ and a training set D of m labelled samples we are interested in measuring the "in-sample" (i.e. *training*) error

From MLE to In-Sample Error

Given a hypothesis h_θ and a training set D of m labelled samples we are interested in measuring the "in-sample" (i.e. *training*) error

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} e(h_{\boldsymbol{\theta}}(\mathbf{x_i}), y_i)$$

where *e()* measures how "far" the chosen hypothesis is from the true observed value

From MLE to In-Sample Error

Given a hypothesis h_θ and a training set *D* of *m* labelled samples we are interested in measuring the "in-sample" (i.e. *training*) error

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} e(h_{\boldsymbol{\theta}}(\mathbf{x_i}), y_i)$$

where *e()* measures how "far" the chosen hypothesis is from the true observed value

How we can "transform" MLE to the "in-sample" error above?

Negative Log-Likelihood

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\prod_{i=1}^{m} \ell(y_i \boldsymbol{\theta}^T \mathbf{x_i}) \right)$$

Negative Log-Likelihood

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\prod_{i=1}^{m} \ell(y_i \boldsymbol{\theta}^T \mathbf{x}_\mathrm{i})\right)$$

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\boxed{\frac{1}{m}\ln}\left(\prod_{i=1}^{m} \ell(y_i \boldsymbol{\theta}^T \mathbf{x}_\mathrm{i})\right)\right)$$

Negative Log-Likelihood

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)$$

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\boxed{\frac{1}{m}\ln}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\right)$$

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\frac{1}{m}\ln\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\right)=\boxed{\texttt{argmin}_{\boldsymbol{\theta}}\left(-\frac{1}{m}\ln\right.}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\Bigg)$$

Negative Log-Likelihood

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right) \qquad \texttt{argmax}_{\boldsymbol{\theta}}\left(\boxed{\frac{1}{m}\ln}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\right)$$

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\frac{1}{m}\ln\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\right) = \boxed{\texttt{argmin}_{\boldsymbol{\theta}}\left(-\frac{1}{m}\ln\right.}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\Bigg)$$

$$= \texttt{argmin}_{\boldsymbol{\theta}}\left(-\frac{1}{m}\ln\big(\ell(y_1\boldsymbol{\theta}^T\mathbf{x_1})\big)-\ldots-\frac{1}{m}\ln\big(\ell(y_m\boldsymbol{\theta}^T\mathbf{x_m})\big)\right)$$

as $k\ \ln(a\cdot b) = k\big(\ln(a) +\ \ln(b)\big) = k\ \ln(a) + k\ \ln(b)$.

Negative Log-Likelihood

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right) \qquad \texttt{argmax}_{\boldsymbol{\theta}}\left(\boxed{\frac{1}{m}\ln}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\right)$$

$$\texttt{argmax}_{\boldsymbol{\theta}}\left(\frac{1}{m}\ln\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\right)=\boxed{\texttt{argmin}_{\boldsymbol{\theta}}\left(-\frac{1}{m}\ln\right.}\left(\prod_{i=1}^{m}\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})\right)\Bigg)$$

$$=\texttt{argmin}_{\boldsymbol{\theta}}\left(-\frac{1}{m}\ln\left(\ell(y_1\boldsymbol{\theta}^T\mathbf{x_1})\right)-\ldots-\frac{1}{m}\ln\left(\ell(y_m\boldsymbol{\theta}^T\mathbf{x_m})\right)\right)$$

as $k\ \ln(a\cdot b)=k\left(\ln(a)+\ \ln(b)\right)=k\ \ln(a)+k\ \ln(b)$.

$$=\texttt{argmin}_{\boldsymbol{\theta}}\left(\frac{1}{m}\ \sum_{i=1}^{m}\ -\ln(\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i}))\right)$$

$$=\texttt{argmin}_{\boldsymbol{\theta}}\left(\frac{1}{m}\ \sum_{i=1}^{m}\ \ln\left(\frac{1}{\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})}\right)\right)$$

as $-\ln(a)=\ln(\frac{1}{a})$.

Cross-Entropy Error

$$\boxed{\texttt{argmin}_{\boldsymbol{\theta}}\left(\frac{1}{m}\ \sum_{i=1}^{m}\ \ln\left(\frac{1}{\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})}\right)\right)}$$

Cross-Entropy Error

$$\boxed{\mathtt{argmin}_{\theta}\left(\frac{1}{m}\ \sum_{i=1}^{m}\ \ln\left(\frac{1}{\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})}\right)\right)}$$

By noticing that logistic function can be rewritten as follows:

$$\ell(z) = \frac{e^z}{1+e^z} = \frac{1}{e^{-z}+1}$$

We can finally write the "in-sample" error to be minimized:

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m}\ \sum_{i=1}^{m}\ \ln\left(e^{-y_i\boldsymbol{\theta}^T\mathbf{x_i}} + 1\right)$$

Cross-Entropy Error

$$\boxed{\texttt{argmin}_{\boldsymbol{\theta}}\left(\frac{1}{m}\sum_{i=1}^{m}\ln\left(\frac{1}{\ell(y_i\boldsymbol{\theta}^T\mathbf{x_i})}\right)\right)}$$

By noticing that logistic function can be rewritten as follows:

$$\ell(z) = \frac{e^z}{1+e^z} = \frac{1}{e^{-z}+1}$$

We can finally write the "in-sample" error to be minimized:

$$\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m}\ln\left(e^{-y_i\boldsymbol{\theta}^T\mathbf{x_i}}+1\right)}$$

Cross-Entropy Error

Cross-Entropy (a.k.a. Log-Loss) Formulations

2 formulations of cross-entropy can be found depending on the labeling chosen for the (binary) response y

Cross-Entropy (a.k.a. Log-Loss) Formulations

2 formulations of cross-entropy can be found depending on the labeling chosen for the (binary) response y

$$\frac{1}{m}\sum_{i=1}^{m}\ln(e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1)$$

y = {-1, +1}

Cross-Entropy (a.k.a. Log-Loss) Formulations

2 formulations of cross-entropy can be found depending on the labeling chosen for the (binary) response y

$$\frac{1}{m}\sum_{i=1}^{m}\ln(e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1)$$

y = {-1, +1}

$$-\frac{1}{m}\sum_{i=1}^{m}y_i\ln(p)+(1-y_i)\ln(1-p)$$

$$p=\frac{e^{\boldsymbol{\theta}^T\mathbf{x}}}{e^{\boldsymbol{\theta}^T\mathbf{x}}+1}=\frac{1}{1+e^{-\boldsymbol{\theta}^T\mathbf{x}}}$$

y = {0, 1}

Cross-Entropy (a.k.a. Log-Loss) Formulations

$$Y = \{0, 1\}$$
$$Y \sim \text{Bernoulli}(p)$$

$$\boxed{f_Y(y; p)} = \boxed{\mathrm{L}_Y(p; y)} = \begin{cases} p & \text{if } y = 1 \\ q = 1 - p & \text{if } y = 0 \end{cases}$$

Probability density function of a Bernoulli-distributed random variable with known parameter *p*

Likelihood of an observed Bernoulli-distributed random variable (parameter *p* is unknown)

Likelihood Function

Likelihood function of *m* **i.i.d.** observations of Y

$$\mathrm{L}_Y(p; y_1 \ldots y_m) = \prod_{i=1}^{m} p^{y_i}(1-p)^{(1-y_i)}$$

Likelihood Function

Likelihood function of *m* **i.i.d.** observations of Y

$$\mathrm{L}_Y(p; y_1 \ldots y_m) = \prod_{i=1}^{m} p^{y_i}(1-p)^{(1-y_i)}$$

Here the unknown is the parameter *p* and we use the observations $y_1, \ldots, y_m$ to find *p* so as to maximize the likelihood

$$p^* = \mathrm{argmax}_p \left\{ \prod_{i=1}^{m} p^{y_i}(1-p)^{(1-y_i)} \right\}$$

Negative Log-Likelihood Function

$$p^* = \mathrm{argmin}_p \left\{ -\ln\left[\prod_{i=1}^{m} p^{y_i}(1-p)^{(1-y_i)}\right]\right\}$$

Negative Log-Likelihood Function

$$p^* = \text{argmin}_p \left\{ -\ln\left[\prod_{i=1}^{m} p^{y_i}(1-p)^{(1-y_i)} \right] \right\}$$

$$p^* = \text{argmin}_p \left\{ -\sum_{i=1}^{m} \ln\left[p^{y_i}(1-p)^{(1-y_i)} \right] \right\}$$

Negative Log-Likelihood Function

$$p^* = \text{argmin}_p \left\{ -\ln\left[\prod_{i=1}^{m} p^{y_i}(1-p)^{(1-y_i)} \right] \right\}$$

$$p^* = \text{argmin}_p \left\{ -\sum_{i=1}^{m} \ln\left[p^{y_i}(1-p)^{(1-y_i)} \right] \right\}$$

$$p^* = \text{argmin}_p \left\{ -\sum_{i=1}^{m} \ln(p^{y_i}) + \ln\left((1-p)^{(1-y_i)} \right) \right\}$$

Negative Log-Likelihood Function

$$p^* = \operatorname{argmin}_p \left\{ -\sum_{i=1}^{m} \ln(p^{y_i}) + \ln\Big((1-p)^{(1-y_i)}\Big) \right\}$$

Negative Log-Likelihood Function

$$p^* = \text{argmin}_p \left\{ -\sum_{i=1}^{m} \ln(p^{y_i}) + \ln\Big((1-p)^{(1-y_i)}\Big) \right\}$$

$$p^* = \text{argmin}_p \left\{ -\sum_{i=1}^{m} y_i \ln(p) + (1-y_i)\ln(1-p) \right\}$$

Negative Log-Likelihood Function

$$p^* = \text{argmin}_p \left\{ -\sum_{i=1}^{m} \ln(p^{y_i}) + \ln\left((1-p)^{(1-y_i)}\right) \right\}$$

$$p^* = \text{argmin}_p \left\{ \boxed{-\sum_{i=1}^{m} y_i \ln(p) + (1-y_i)\ln(1-p)} \right\}$$

Except for the 1/m factor this is exactly the second formulation we gave for the cross-entropy error

Substituting *p*

$$-\sum_{i=1}^{m} y_i \ln(p) + (1 - y_i)\ln(1 - p)$$

Substituting *p*

$$-\sum_{i=1}^{m} y_i \ln(p) + (1 - y_i)\ln(1 - p)$$

$$-\sum_{i=1}^{m} y_i \ln\left(\boxed{\frac{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1}}\right) + (1 - y_i)\ln\left(1 - \boxed{\frac{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1}}\right)$$

Substituting p

$$-\sum_{i=1}^{m} y_i \ln(p) + (1 - y_i)\ln(1 - p)$$

$$-\sum_{i=1}^{m} y_i \ln\left(\boxed{\frac{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1}}\right) + (1 - y_i)\ln\left(1 - \boxed{\frac{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1}}\right)$$

$$-\sum_{i=1}^{m} y_i[\ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1)] + (1 - y_i)[\ln(1) - \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1)]$$

Substituting *p*

$$-\sum_{i=1}^{m} y_i[\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)] + (1-y_i)[\underbrace{\cancel{\ln(1)}}_{0} - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)]$$

Substituting *p*

$$-\sum_{i=1}^{m} y_i[\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)] + (1-y_i)[\underbrace{\cancel{\ln(1)}}_{0} - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)]$$

$$-\sum_{i=1}^{m} y_i\boldsymbol{\theta}^T\mathbf{x}_i - y_i\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1) - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1) + y_i\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)$$

Substituting p

$$-\sum_{i=1}^{m} y_i[\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)] + (1-y_i)[\underset{0}{\cancel{\ln(1)}} - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)]$$

$$-\sum_{i=1}^{m} y_i\boldsymbol{\theta}^T\mathbf{x}_i \cancel{- y_i\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)} - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1) \cancel{+ y_i\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)}$$

Substituting *p*

$$-\sum_{i=1}^{m} y_i[\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)] + (1-y_i)[\underbrace{\cancel{\ln(1)}}_{0} - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)]$$

$$-\sum_{i=1}^{m} y_i\boldsymbol{\theta}^T\mathbf{x}_i \cancel{- y_i\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)} - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1) \cancel{+ y_i\ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)}$$

$$\boxed{-\sum_{i=1}^{m} y_i\boldsymbol{\theta}^T\mathbf{x}_i - \ln(e^{\boldsymbol{\theta}^T\mathbf{x}_i}+1)}$$

Equivalence Between 2 Formulations

We want to show the 2 formulations below lead to the same function to be minimized

$$\sum_{i=1}^{m} \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1)$$

y = {-1, +1}

$$-\sum_{i=1}^{m} y_i \boldsymbol{\theta}^T \mathbf{x}_i - \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1)$$

y = {0, 1}

Equivalence Between 2 Formulations

We want to show the 2 formulations below lead to the same function to be minimized

$$\boxed{\sum_{i=1}^{m} \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1)} = \boxed{\sum_{i=1}^{m} \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1)}$$

y = -1

y = 0

Equivalence Between 2 Formulations

We want to show the 2 formulations below lead to the same function to be minimized

$$\boxed{\sum_{i=1}^{m} \ln(e^{-\boldsymbol{\theta}^T \mathbf{x}_i} + 1)} \stackrel{?}{=} \boxed{-\sum_{i=1}^{m} \boldsymbol{\theta}^T \mathbf{x}_i - \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i} + 1)}$$

y = 1 y = 1

Equivalence Between 2 Formulations

$$\boxed{\sum_{i=1}^{m} \ln(e^{-\boldsymbol{\theta}^T \mathbf{x}_i} + 1)} = \sum_{i=1}^{m} \ln\left(\frac{1}{e^{\boldsymbol{\theta}^T \mathbf{x}_i}} + 1\right) = \sum_{i=1}^{m} \ln\left(\frac{1 + e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}\right)$$

Equivalence Between 2 Formulations

$$\boxed{\sum_{i=1}^{m} \ln(e^{-\boldsymbol{\theta}^T \mathbf{x}_i} + 1)} = \sum_{i=1}^{m} \ln\left(\frac{1}{e^{\boldsymbol{\theta}^T \mathbf{x}_i}} + 1\right) = \sum_{i=1}^{m} \ln\left(\frac{1 + e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}\right)$$

$$= \sum_{i=1}^{m} \ln(1 + e^{\boldsymbol{\theta}^T \mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i})$$

Equivalence Between 2 Formulations

$$\boxed{\sum_{i=1}^{m} \ln(e^{-\boldsymbol{\theta}^T \mathbf{x}_i} + 1)} = \sum_{i=1}^{m} \ln\left(\frac{1}{e^{\boldsymbol{\theta}^T \mathbf{x}_i}} + 1\right) = \sum_{i=1}^{m} \ln\left(\frac{1 + e^{\boldsymbol{\theta}^T \mathbf{x}_i}}{e^{\boldsymbol{\theta}^T \mathbf{x}_i}}\right)$$

$$= \sum_{i=1}^{m} \ln(1 + e^{\boldsymbol{\theta}^T \mathbf{x}_i}) - \ln(e^{\boldsymbol{\theta}^T \mathbf{x}_i})$$

$$= \boxed{-\sum_{i=1}^{m} \boldsymbol{\theta}^T \mathbf{x}_i - \ln(1 + e^{\boldsymbol{\theta}^T \mathbf{x}_i})}$$

LEARNING ALGORITHM

Picking the Best Hypothesis

- So far, we have defined:
  - The model (logistic function)
  - The error measure (cross-entropy)

Picking the Best Hypothesis

- So far, we have defined:
  - The model (logistic function)
  - The error measure (cross-entropy)

To actually select the best hypothesis, we have to pick the vector of parameters **θ** so that the error measure is minimized

$$\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)}$$

Mean Squared Error vs. Cross-Entropy

In the case of linear regression we have a similar expression for the error measure, i.e. Mean Squared Error (MSE)

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x_i} - y_i\right)^2$$

Mean Squared Error vs. Cross-Entropy

In the case of linear regression we have a similar expression for the error measure, i.e. Mean Squared Error (MSE)

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x_i} - y_i\right)^2$$

Minimising MSE through Ordinary Least Squares (OLS) leads to a **closed-form solution** often referred to as the OLS estimator for **θ**

$$\boxed{\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}}$$

Mean Squared Error vs. Cross-Entropy

The problem is that using Cross-Entropy as error measure we cannot find a closed-form solution to the minimization problem

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)$$

Mean Squared Error vs. Cross-Entropy

The problem is that using Cross-Entropy as error measure we cannot find a closed-form solution to the minimization problem

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)$$

Yet, Cross-Entropy is **convex** w.r.t. the parameters **θ**

Mean Squared Error vs. Cross-Entropy

The problem is that using Cross-Entropy as error measure we cannot find a closed-form solution to the minimization problem

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)$$

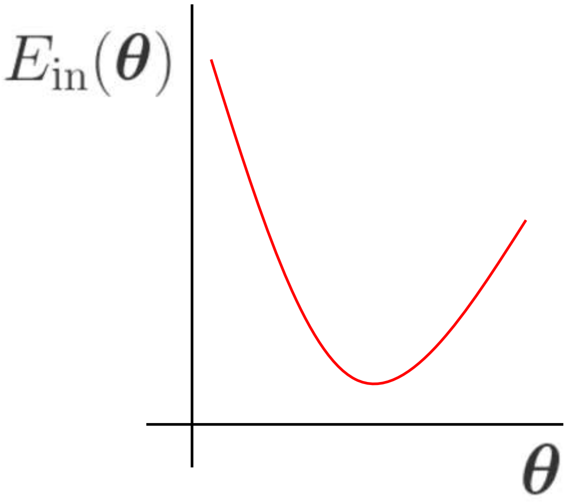
Yet, Cross-Entropy is **convex** w.r.t. the parameters **θ**

$\Downarrow$

Iterative Solution

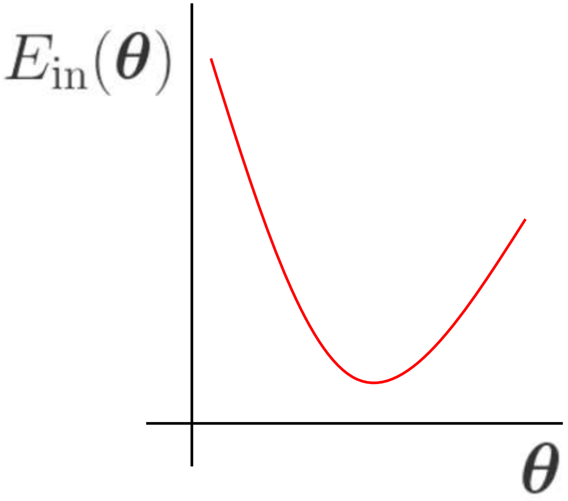
(Batch) Gradient Descent

General iterative method for any nonlinear optimization



(Batch) Gradient Descent

General iterative method for any nonlinear optimization

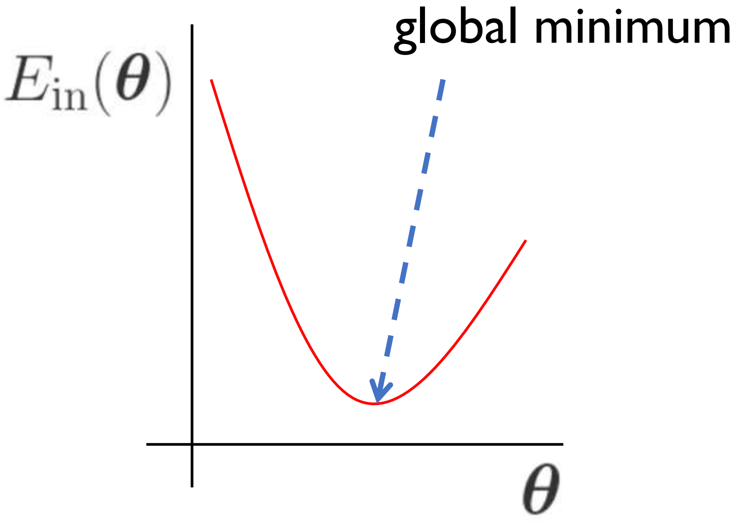


The method **guarantees the convergence to a local minimum**

(Under specific assumptions on the objective function and learning rate)

(Batch) Gradient Descent

General iterative method for any nonlinear optimization



The method **guarantees the convergence to a local minimum**

(Under specific assumptions on the objective function and learning rate)

If the objective function is **convex** (like cross-entropy) then the local minimum is also the **global minimum**

Gradient Descent: The Main Idea

1. At t=0 initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$

Gradient Descent: The Main Idea

1. At $t=0$ initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$
2. Repeat until convergence:
   a. Update the current vector of parameters $\boldsymbol{\theta}(t)$ by taking a "step" along the "steepest" slope: $\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta\mathbf{v}$
   b. Return to 2.

Gradient Descent: The Main Idea

1. At t=0 initialize the (guessed) vector of parameters **θ** to **θ**(0)
2. Repeat until convergence:
   a. Update the current vector of parameters **θ**(t) by taking a "step" along the "steepest" slope: **θ**(t+1) = **θ**(t) + η**v**
   b. Return to 2.

Unit vector representing the direction of the steepest slope

$$\boxed{\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta\mathbf{v}}$$

step

Gradient Descent: The Main Idea

1. At t=0 initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$
2. Repeat until convergence:
   a. Update the current vector of parameters $\boldsymbol{\theta}(t)$ by taking a "step" along the "steepest" slope: $\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta\mathbf{v}$
   b. Return to 2.

Unit vector representing the direction of the steepest slope

$$\boxed{\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta\mathbf{v}}$$

step

How do we determine the direction **v**?

Gradient Descent: The Direction **v**

- We already intuitively said that the direction **v** should be that of the "steepest" slope

Gradient Descent: The Direction **v**

- We already intuitively said that the direction **v** should be that of the "steepest" slope
- Concretely, this means moving along the direction which mostly reduces the in-sample error function

$$\boxed{\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t)) - E_{\text{in}}(\boldsymbol{\theta}(t-1))}$$

Gradient Descent: The Direction **v**

- We already intuitively said that the direction **v** should be that of the "steepest" slope
- Concretely, this means moving along the direction which mostly reduces the in-sample error function

$$\boxed{\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t)) - E_{\text{in}}(\boldsymbol{\theta}(t-1))}$$

We want ΔE_{in} to be **as negative as possible**, which means that we are actually reducing the error w.r.t. the previous iteration t-1

Gradient Descent: The Direction $\mathbf{v}$

$$\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t-1) + \eta \mathbf{v}) - E_{\text{in}}(\boldsymbol{\theta}(t-1))$$

Gradient Descent: The Direction **v**

$$\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t-1) + \eta \mathbf{v}) - E_{\text{in}}(\boldsymbol{\theta}(t-1))$$

Let's first assume we are in the **univariate** case, i.e. **θ** = θ in R

$$\boxed{f = E_{\text{in}}} \qquad \boxed{x_0 = \boldsymbol{\theta}(t-1)} \qquad \boxed{x = \boldsymbol{\theta}(t)}$$

Gradient Descent: The Direction **v**

$$\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t-1) + \eta\mathbf{v}) - E_{\text{in}}(\boldsymbol{\theta}(t-1))$$

Let's first assume we are in the **univariate** case, i.e. **θ** = θ in R

$$\boxed{f = E_{\text{in}}} \qquad \boxed{x_0 = \boldsymbol{\theta}(t-1)} \qquad \boxed{x = \boldsymbol{\theta}(t)}$$

$$\boxed{\delta f = \Delta E_{\text{in}} = f(x) - f(x_0)} \qquad \boxed{\delta x = x - x_0 = \boldsymbol{\theta}(t) - \boldsymbol{\theta}(t-1) = \eta\mathbf{v}}$$

Gradient Descent: The Direction **v**

$$\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t-1) + \eta \mathbf{v}) - E_{\text{in}}(\boldsymbol{\theta}(t-1))$$

Let's first assume we are in the **univariate** case, i.e. **θ** = θ in R

$$\boxed{f = E_{\text{in}}} \qquad \boxed{x_0 = \boldsymbol{\theta}(t-1)} \qquad \boxed{x = \boldsymbol{\theta}(t)}$$

$$\boxed{\delta f = \Delta E_{\text{in}} = f(x) - f(x_0)} \qquad \boxed{\delta x = x - x_0 = \boldsymbol{\theta}(t) - \boldsymbol{\theta}(t-1) = \eta \mathbf{v}}$$

$$\boxed{f'(x_0) = \lim_{\delta x \to 0} \frac{f(x_0+\delta x) - f(x_0)}{\delta x}} \qquad \boxed{f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} \approx \frac{\delta f}{\delta x}}$$

Gradient Descent: The Direction **v**

$$\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t-1) + \eta\mathbf{v}) - E_{\text{in}}(\boldsymbol{\theta}(t-1))$$

Let's first assume we are in the **univariate** case, i.e. **θ** = θ in R

$$\boxed{f = E_{\text{in}}}$$

$$\boxed{x_0 = \boldsymbol{\theta}(t-1)}$$

$$\boxed{x = \boldsymbol{\theta}(t)}$$

$$\boxed{\delta f = \Delta E_{\text{in}} = f(x) - f(x_0)}$$

$$\boxed{\delta x = x - x_0 = \boldsymbol{\theta}(t) - \boldsymbol{\theta}(t-1) = \eta\mathbf{v}}$$

$$\boxed{f'(x_0) = \lim_{\delta x \to 0} \frac{f(x_0+\delta x) - f(x_0)}{\delta x}}$$

$$\boxed{f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} \approx \frac{\delta f}{\delta x}}$$

$$\boxed{\delta f = f(x) - f(x_0) \approx f'(x_0)\delta x = f'(x_0)(x - x_0)}$$

Gradient Descent: The Direction v

$$\boxed{f(x) - f(x_0) \approx f'(x_0)(x - x_0)}$$

Gradient Descent: The Direction v

$$\boxed{f(x) - f(x_0) \approx f'(x_0)(x - x_0)}$$

$$f(x) = \underbrace{f(x_0) + f'(x_0)(x - x_0)}_{\text{First-order Taylor approximation}} \underbrace{+O((x - x_0)^2)}_{\text{Second-order error term}}$$

Gradient Descent: The Direction **v**

$$\boxed{f(x) - f(x_0) \approx f'(x_0)(x - x_0)}$$

$$f(x) = \underbrace{f(x_0) + f'(x_0)(x - x_0)}_{\text{First-order Taylor approximation}} \underbrace{+O((x - x_0)^2)}_{\text{Second-order error term}}$$

To summarize and generalize to the multivariate case of **θ**:

$$\boxed{\delta f = f(x) - f(x_0) = \Delta E_{\text{in}} = \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T \mathbf{v} + O(\eta^2)}$$

The greek letter *nabla* indicates the gradient

Gradient Descent: The Direction **v**

$$\Delta E_{\text{in}} = \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T \mathbf{v} + O(\eta^2)$$

Gradient Descent: The Direction **v**

$$\Delta E_{\text{in}} = \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T \mathbf{v} + O(\eta^2)$$

The unit vector **v** only contributes to the **direction** and not to the magnitude of the iterative step

Gradient Descent: The Direction v

$$\Delta E_{\text{in}} = \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T \mathbf{v} + \cancel{O(\eta^2)}$$

The unit vector **v** only contributes to the **direction** and not to the magnitude of the iterative step

The second-order approximation term is negligible

(when the step size is small)

Gradient Descent: The Direction $\mathbf{v}$

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$

$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

Gradient Descent: The Direction $\mathbf{v}$

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$

$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

$$\mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}||\ \underbrace{||\mathbf{v}||}_{=1}\ cos(\alpha) = ||\mathbf{u}||cos(\alpha)$$

Gradient Descent: The Direction $\mathbf{v}$

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$

$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

$$\mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}|| \underbrace{||\mathbf{v}||}_{=1} cos(\alpha) = ||\mathbf{u}|| cos(\alpha) \qquad -1 \leq cos(\alpha) \leq 1$$

Gradient Descent: The Direction $\mathbf{v}$

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$
$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

$$\mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}|| \underbrace{||\mathbf{v}||}_{=1} cos(\alpha) = ||\mathbf{u}|| cos(\alpha) \qquad -1 \leq cos(\alpha) \leq 1$$

$$-||\mathbf{u}|| \leq \mathbf{u} \cdot \mathbf{v} \leq ||\mathbf{u}||$$
$$-\eta||\mathbf{u}|| \leq \underbrace{\eta \mathbf{u} \cdot \mathbf{v}}_{\Delta E_{\text{in}}} \leq \eta||\mathbf{u}||$$

Gradient Descent: The Direction $\mathbf{v}$

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$

$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

$$\mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}|| \underbrace{||\mathbf{v}||}_{=1} cos(\alpha) = ||\mathbf{u}|| cos(\alpha) \qquad -1 \leq cos(\alpha) \leq 1$$

$$-||\mathbf{u}|| \leq \mathbf{u} \cdot \mathbf{v} \leq ||\mathbf{u}||$$

$$-\eta||\mathbf{u}|| \leq \underbrace{\eta \mathbf{u} \cdot \mathbf{v}}_{\Delta E_{\text{in}}} \leq \boxed{\eta||\mathbf{u}||}$$

The most **positive** ΔE_{in} when $\cos(\alpha) = 1$ (i.e., $\alpha = 0°$)

Both error and step vectors have the same direction

Gradient Descent: The Direction v

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$
$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

$$\mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}|| \underbrace{||\mathbf{v}||}_{=1} cos(\alpha) = ||\mathbf{u}|| cos(\alpha) \qquad -1 \leq cos(\alpha) \leq 1$$

$$-||\mathbf{u}|| \leq \mathbf{u} \cdot \mathbf{v} \leq ||\mathbf{u}||$$
$$\boxed{-\eta||\mathbf{u}||} \leq \underbrace{\eta \mathbf{u} \cdot \mathbf{v}}_{\Delta E_{\text{in}}} \leq \eta||\mathbf{u}||$$

The most **negative** ΔE_{in} when cos(α) = -1 (i.e., α = 180°)

The error and step vectors have opposite direction

Gradient Descent: The Direction **v**

At each iteration t, we want the unit vector **v** which makes exactly **the most negative** ΔE_{in}

$$\eta \mathbf{u} \cdot \mathbf{v} = -\eta ||\mathbf{u}||$$

Gradient Descent: The Direction **v**

At each iteration t, we want the unit vector **v** which makes exactly **the most negative** ΔE_{in}

$$\eta \mathbf{u} \cdot \mathbf{v} = -\eta ||\mathbf{u}||$$

$$\mathbf{u} \cdot \mathbf{v} = -||\mathbf{u}||$$
$$\mathbf{u}^T \cdot \mathbf{u} \cdot \mathbf{v} = -||\mathbf{u}||\mathbf{u}^T$$

$$\mathbf{v} = -\frac{||\mathbf{u}||\mathbf{u}^T}{||\mathbf{u}||^2} = -\frac{\mathbf{u}^T}{||\mathbf{u}||} = -\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))}{\nabla ||E_{\text{in}}(\boldsymbol{\theta}(t-1))||}$$

Gradient Descent: The Direction **v**

At each iteration t, we want the unit vector **v** which makes exactly **the most negative** ΔE_{in}

$$\eta \mathbf{u} \cdot \mathbf{v} = -\eta ||\mathbf{u}||$$

$$\mathbf{u} \cdot \mathbf{v} = -||\mathbf{u}||$$

$$\mathbf{u}^T \cdot \mathbf{u} \cdot \mathbf{v} = -||\mathbf{u}||\mathbf{u}^T$$

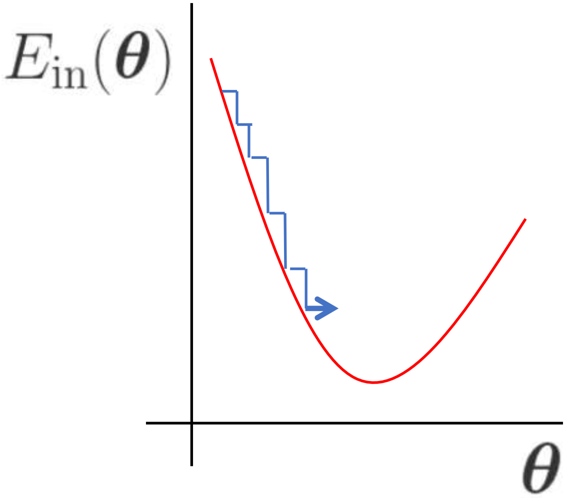
$$\mathbf{v} = -\frac{||\mathbf{u}||\mathbf{u}^T}{||\mathbf{u}||^2} = -\frac{\mathbf{u}^T}{||\mathbf{u}||} = \boxed{-\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))}{\nabla ||E_{\text{in}}(\boldsymbol{\theta}(t-1))||}}$$

Gradient Descent: The Step η

How the step magnitude η affects the convergence?

Gradient Descent: The Step η

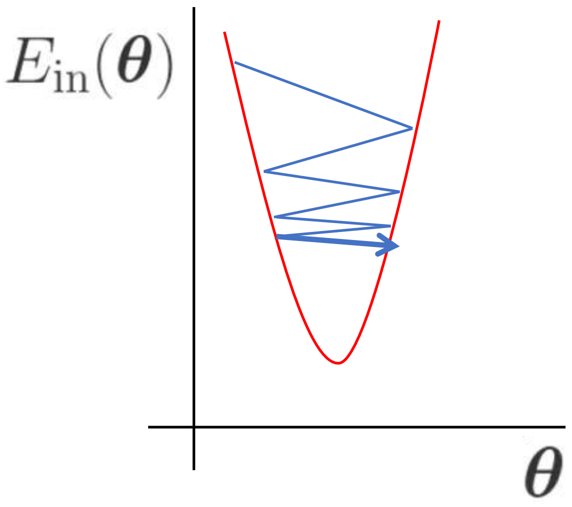
How the step magnitude η affects the convergence?



η too small

Gradient Descent: The Step η

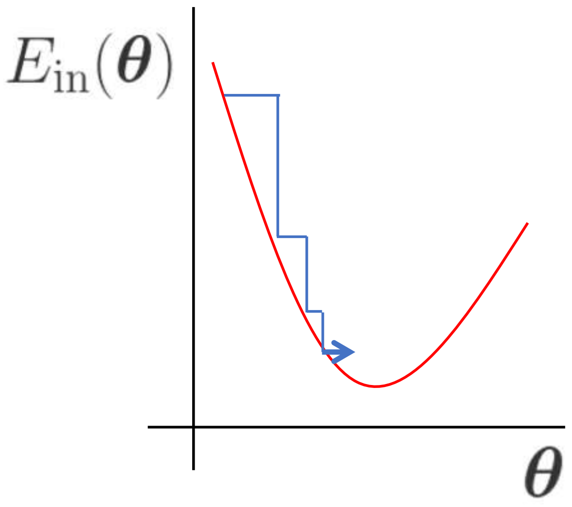
How the step magnitude η affects the convergence?



η too large

Gradient Descent: The Step η

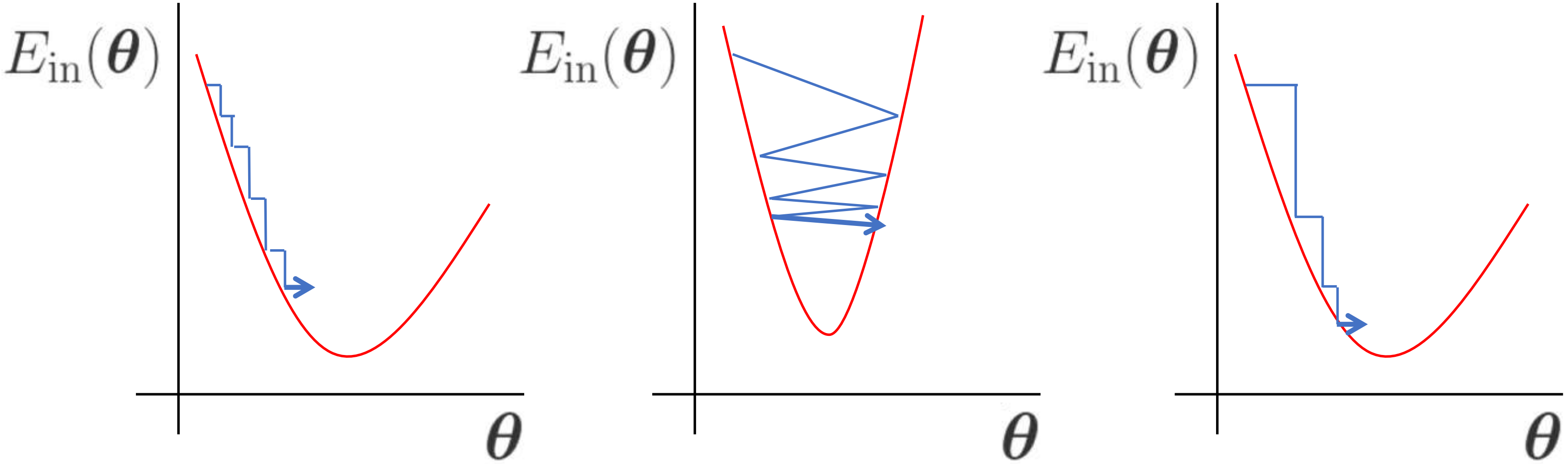
How the step magnitude η affects the convergence?



η variable

Gradient Descent: The Step η

How the step magnitude η affects the convergence?



η too small | η too large | η variable

Rule of thumb

Dynamically change η proportionally to the gradient!

Gradient Descent: The Step η

Remember that at each iteration the update strategy is:

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta \mathbf{v}$$

$$\mathbf{v} = -\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

Gradient Descent: The Step η

Remember that at each iteration the update strategy is:

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta \mathbf{v}$$

$$\mathbf{v} = -\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

At each iteration t, the step η is fixed

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

Gradient Descent: The Step η

Instead of having a fixed η at each iteration, use a variable η_t as function of η

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta_t \mathbf{v} \qquad \eta_t = \eta k$$

Gradient Descent: The Step η

Instead of having a fixed η at each iteration, use a variable η_t as function of η

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta_t \mathbf{v} \qquad \eta_t = \eta k$$

Let's take: $$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta k \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

Gradient Descent: The Step η

Instead of having a fixed η at each iteration, use a variable η_t as function of η

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta_t \mathbf{v} \qquad \eta_t = \eta k$$

Let's take: $$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta k \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \boxed{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|} \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

Gradient Descent: The Step η

Instead of having a fixed η at each iteration, use a variable η_t as function of η

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta_t \mathbf{v} \qquad \eta_t = \eta k$$

Let's take: $$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta k \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \cancel{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|} \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\cancel{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}}$$

$$\boxed{\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t))}$$

Computing the Gradient of Cross-Entropy

$$\nabla E_{\text{in}}(\boldsymbol{\theta}) = \nabla \left[\frac{1}{m} \sum_{i=1}^{m} \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

Computing the Gradient of Cross-Entropy

$$\nabla E_{\text{in}}(\boldsymbol{\theta}) = \nabla \left[\frac{1}{m} \sum_{i=1}^{m} \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

$$= \left[\frac{1}{m} \sum_{i=1}^{m} \nabla \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

Computing the Gradient of Cross-Entropy

$$\nabla E_{\text{in}}(\boldsymbol{\theta}) = \nabla \left[\frac{1}{m} \sum_{i=1}^{m} \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

$$= \left[\frac{1}{m} \sum_{i=1}^{m} \nabla \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right] = \left[\frac{1}{m} \sum_{i=1}^{m} \frac{1}{e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1} \nabla (e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

chain rule of derivative

Computing the Gradient of Cross-Entropy

$$\nabla E_{\text{in}}(\boldsymbol{\theta}) = \nabla \left[\frac{1}{m} \sum_{i=1}^{m} \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

$$= \left[\frac{1}{m} \sum_{i=1}^{m} \nabla \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right] = \left[\frac{1}{m} \sum_{i=1}^{m} \frac{1}{e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1} \nabla (e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

chain rule of derivative

$$= \frac{1}{m} \sum_{i=1}^{m} \frac{-y_i \mathbf{x}_i e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i}}{e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1}$$

Computing the Gradient of Cross-Entropy

$$\nabla E_{\text{in}}(\boldsymbol{\theta}) = \nabla\left[\frac{1}{m}\sum_{i=1}^{m}\ln(e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1)\right]$$

$$= \left[\frac{1}{m}\sum_{i=1}^{m}\nabla\ln(e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1)\right] = \left[\frac{1}{m}\sum_{i=1}^{m}\frac{1}{e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1}\nabla(e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1)\right]$$

chain rule of derivative

$$= \frac{1}{m}\sum_{i=1}^{m}\frac{-y_i\mathbf{x}_i e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}}{e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1} = \boxed{-\frac{1}{m}\sum_{i=1}^{m}\frac{y_i\mathbf{x}_i}{1+e^{y_i\boldsymbol{\theta}^T\mathbf{x}_i}}}$$

Gradient Descent: The Algorithm

1. At t=0 initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$

Gradient Descent: The Algorithm

1. At t=0 initialize the (guessed) vector of parameters **θ** to **θ**(0)
2. For t = 0, 1, 2, … until stop:
   a. Compute the gradient of the cross-entropy error $\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)}$

$$\boxed{\nabla E_{\text{in}}(\boldsymbol{\theta}(t)) = -\frac{1}{m} \sum_{i=1}^{m} \frac{y_i \mathbf{x}_i}{1 + e^{y_i \boldsymbol{\theta}(t)^T \mathbf{x}_i}}}$$

Gradient Descent: The Algorithm

1. At t=0 initialize the (guessed) vector of parameters **θ** to **θ**(0)
2. For t = 0, 1, 2, … until stop:
   a. Compute the gradient of the cross-entropy error $\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)}$

$$\boxed{\nabla E_{\text{in}}(\boldsymbol{\theta}(t)) = -\frac{1}{m} \sum_{i=1}^{m} \frac{y_i \mathbf{x}_i}{1 + e^{y_i \boldsymbol{\theta}(t)^T \mathbf{x}_i}}}$$

   b. Update the vector of parameters: $\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \nabla E_{in}(\boldsymbol{\theta}(t))$
   c. Return to 2.

Gradient Descent: The Algorithm

1. At t=0 initialize the (guessed) vector of parameters **θ** to **θ**(0)
2. For t = 0, 1, 2, … until stop:
   a. Compute the gradient of the cross-entropy error $\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)}$

$$\boxed{\nabla E_{\text{in}}(\boldsymbol{\theta}(t)) = -\frac{1}{m}\sum_{i=1}^{m} \frac{y_i \mathbf{x}_i}{1 + e^{y_i \boldsymbol{\theta}(t)^T \mathbf{x}_i}}}$$

   b. Update the vector of parameters: **θ**(t+1) = **θ**(t) - η ∇E$_{\text{in}}$(**θ**(t))
   c. Return to 2.
3. Return the final vector of parameters **θ**(∞)

Gradient Descent: Initialization

- How do we choose the initial value of the parameters $\theta(0)$?

Gradient Descent: Initialization

- How do we choose the initial value of the parameters $\theta(0)$?
- Typically, random initialization!

Gradient Descent: Initialization

- How do we choose the initial value of the parameters $\theta(0)$?
- Typically, random initialization!
- If the function is convex we are guaranteed to reach the global minimum no matter what is the initial value of $\theta(0)$

Gradient Descent: Initialization

- How do we choose the initial value of the parameters $\theta(0)$?
- Typically, random initialization!
- If the function is convex we are guaranteed to reach the global minimum no matter what is the initial value of $\theta(0)$
- In general, we may get to the local minimum nearest to $\theta(0)$

Gradient Descent: Non-Convex Objectives

- GD can still be used to try to optimize **non-convex** objectives

Gradient Descent: Non-Convex Objectives

- GD can still be used to try to optimize **non-convex** objectives
- Problem: non-convex functions may have several local minima

Gradient Descent: Non-Convex Objectives

- GD can still be used to try to optimize **non-convex** objectives
- Problem: non-convex functions may have several local minima
- A bad initialization might cause GD to end up into a "bad" local minimum and miss "better" ones (or even the global if it exists)

Gradient Descent: Non-Convex Objectives

- GD can still be used to try to optimize **non-convex** objectives
- Problem: non-convex functions may have several local minima
- A bad initialization might cause GD to end up into a "bad" local minimum and miss "better" ones (or even the global if it exists)
- Solution (heuristic): repeating GD 100÷1,000 times each time with a different θ(0) may reduce the chance the above issue occurs

Gradient Descent: Stopping Criterion

- If the function is convex GD reaches the global minimum when

$\nabla E_{in}(\boldsymbol{\theta}(t)) = 0$

Gradient Descent: Stopping Criterion

- If the function is convex GD reaches the global minimum when $\nabla E_{in}(\boldsymbol{\theta}(t)) = 0$
- In general, we don't know if eventually the gradient gets to 0 therefore we can use several criteria of termination:
  - stop whenever the difference between two iterations is "small enough" → may converge "prematurely"
  - stop when the error equals to ε → may not converge if the target error is not achievable
  - stop after T iterations
  - combinations of the above in practice works…

Gradient Descent: Advanced Topics

- Gradient Descent using second-order approximation
  - Better local approximation than first-order but each step requires computing the second derivative (Hessian matrix)

Gradient Descent: Advanced Topics

- Gradient Descent using second-order approximation
  - Better local approximation than first-order but each step requires computing the second derivative (Hessian matrix)
- Stochastic Gradient Descent (SGD)
  - At each iteration, compute the gradient only from one sample (not the full dataset)

Gradient Descent: Advanced Topics

- Gradient Descent using second-order approximation
  - Better local approximation than first-order but each step requires computing the second derivative (Hessian matrix)
- Stochastic Gradient Descent (SGD)
  - At each iteration, compute the gradient only from one sample (not the full dataset)
- Regularization
  - Include the L1- or L2-norm of the vector of parameters $\boldsymbol{\theta}$ in the cross-entropy error to avoid overfitting

Take-Home Message of Today

- Logistic Regression is a powerful tool for predicting binary variables through probability of each class

Take-Home Message of Today

- Logistic Regression is a powerful tool for predicting binary variables through probability of each class
- It fits a regression line between input (features) and output (logarithm of the odds), assuming probability takes the form of a sigmoid function

Take-Home Message of Today

- Logistic Regression is a powerful tool for predicting binary variables through probability of each class
- It fits a regression line between input (features) and output (logarithm of the odds), assuming probability takes the form of a sigmoid function
- Parameter estimation is typically done via MLE (i.e., by minimizing Cross-Entropy error)

Take-Home Message of Today

- Logistic Regression is a powerful tool for predicting binary variables through probability of each class
- It fits a regression line between input (features) and output (logarithm of the odds), assuming probability takes the form of a sigmoid function
- Parameter estimation is typically done via MLE (i.e., by minimizing Cross-Entropy error)
- No closed-form solution → iterative Gradient Descent