Big Data Computing

Master's Degree in Computer Science

2020-2021

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)

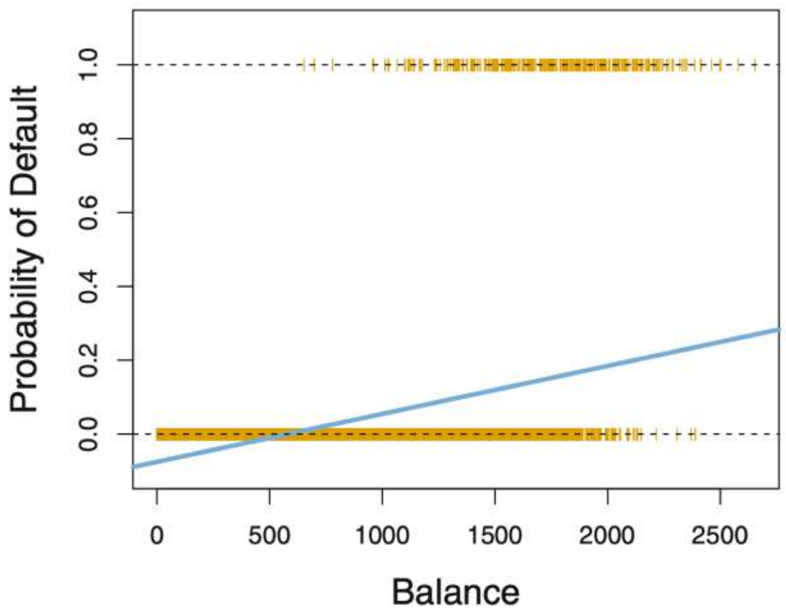
Consider a binary response Default(Y) taking on two values: Yes or No

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

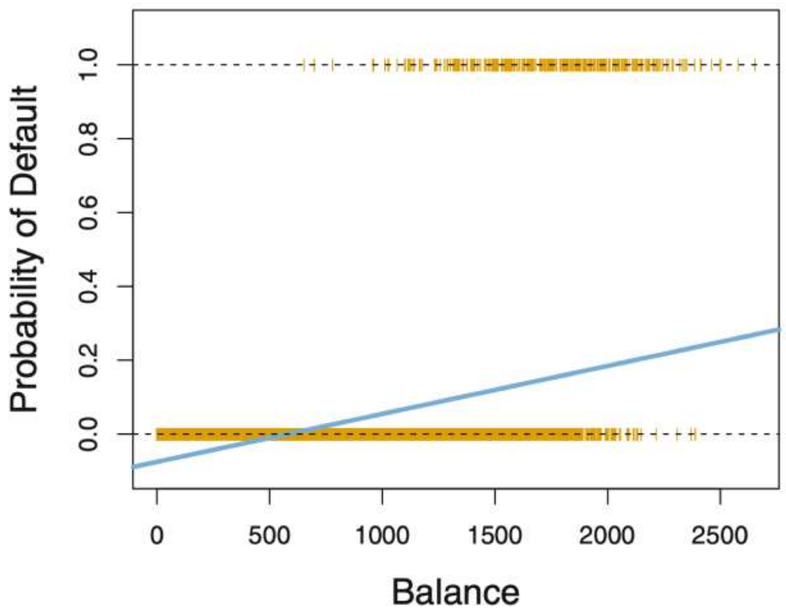
Example: Default(Y) vs. Balance(X)

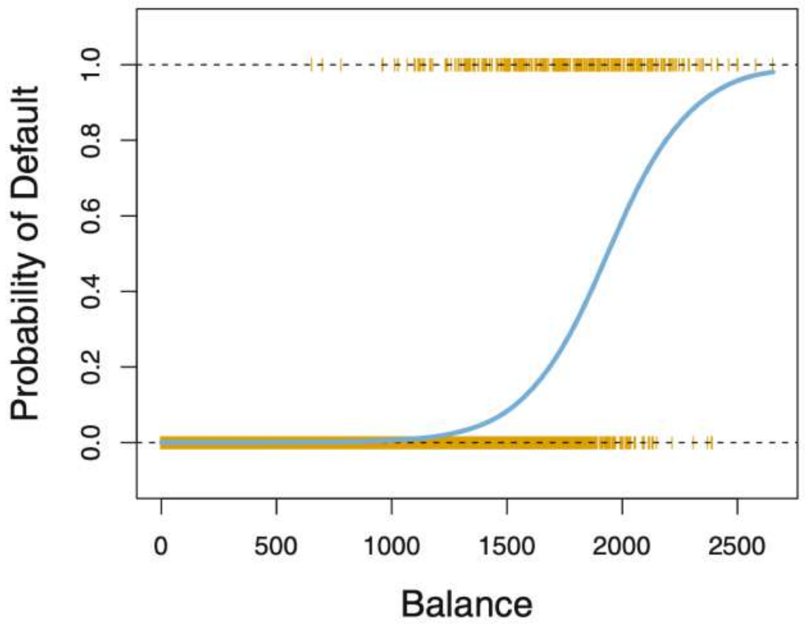


Predicted probability using linear regression
(some estimated probabilities are negative!)

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

3 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 **x** = (x_0, x_1, …, x_d) be the (d+1)-dimensional input
- Let *F* be the family of real-valued functions parametrized by **θ** so that $\boldsymbol{\theta}^T$ = (θ_0, θ_1, …, θ_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 **x** with the parameters **θ**

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 $\boldsymbol{\theta}$
- $f_{\boldsymbol{\theta}}(\mathbf{x})$ 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*
- $h_{\boldsymbol{\theta}}(\mathbf{x}) = g(f_{\boldsymbol{\theta}}(\mathbf{x}))$ defines the hypothesis space:

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

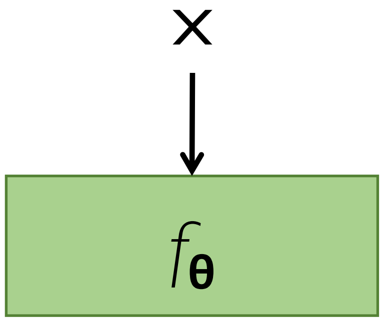
Hypothesis Space (Revisited)

- 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*
- $h_{\boldsymbol{\theta}}(\mathbf{x}) = g(f_{\boldsymbol{\theta}}(\mathbf{x}))$ defines the hypothesis space:

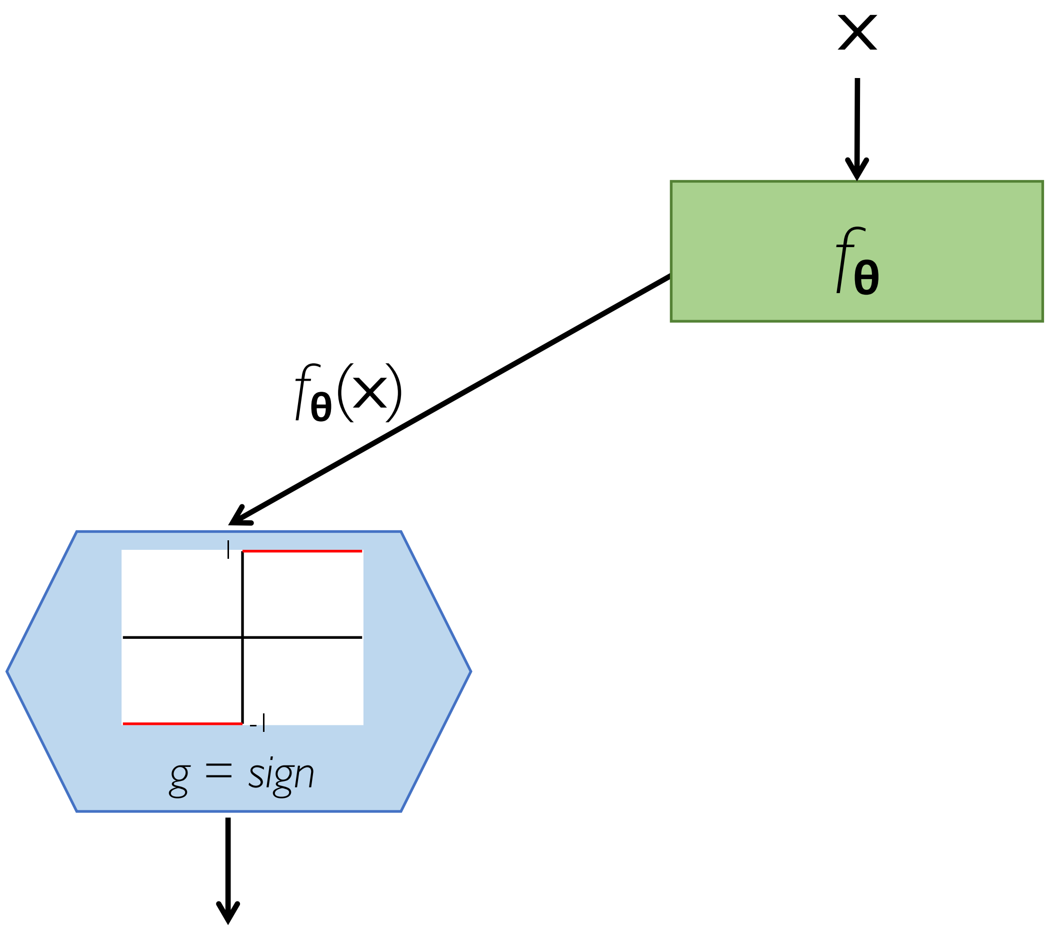
$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : \mathbb{R}^{d+1} \longmapsto \mathbb{R} \mid h_{\boldsymbol{\theta}}(\mathbf{x}) = g(f_{\boldsymbol{\theta}}(\mathbf{x})) = g(\boldsymbol{\theta}^T\mathbf{x}) = g\big(\sum_{i=0}^{d} \theta_i x_i\big)\}$$

The set of possible hypotheses *H* changes depending on the parametric model ($f_{\boldsymbol{\theta}}$) and on the thresholding function (*g*)

Filtering (Thresholding)

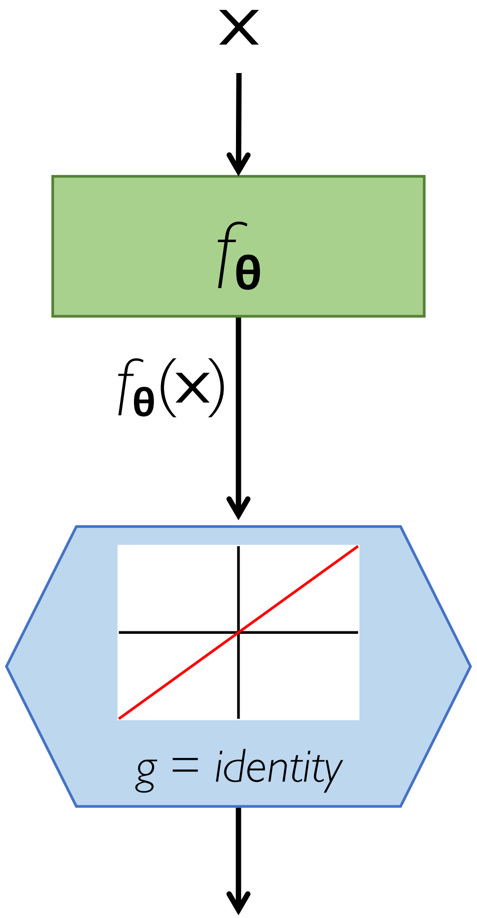


Filtering (Thresholding)



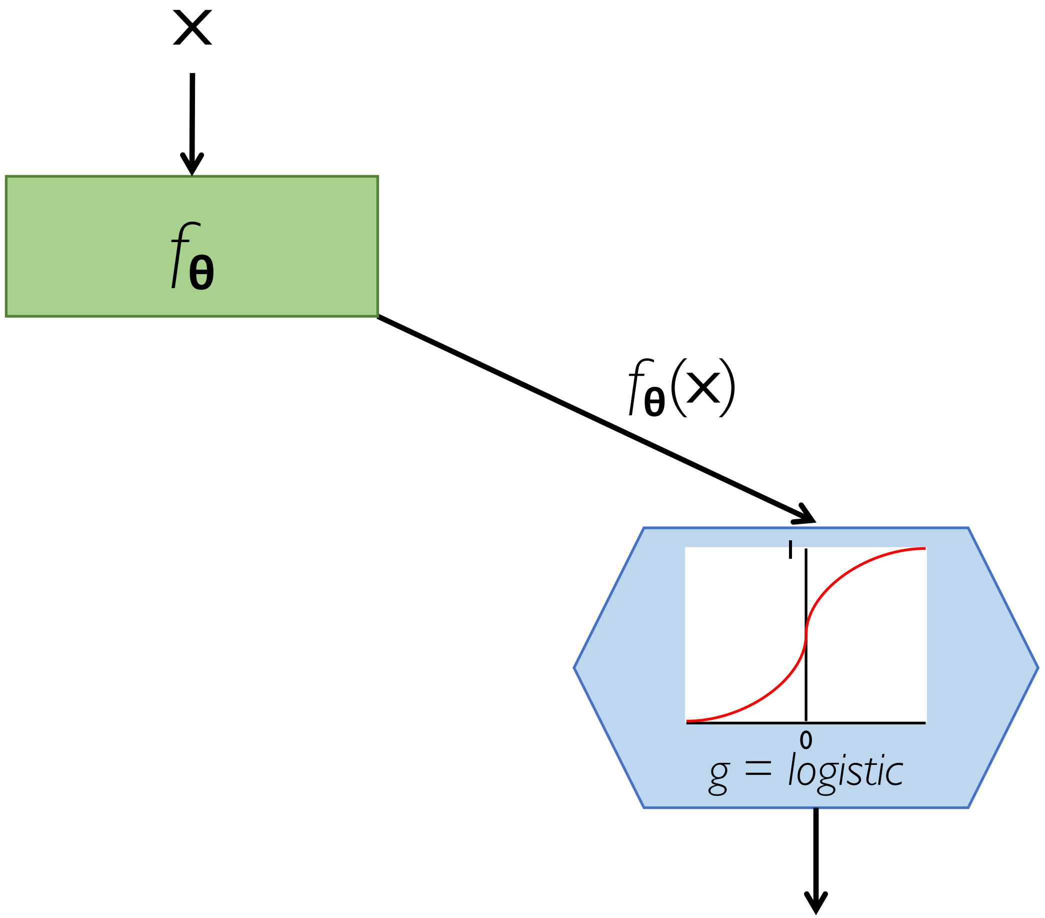
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \mathrm{sign}(f_{\boldsymbol{\theta}}(\mathbf{x})) = \mathrm{sign}(\boldsymbol{\theta}^T\mathbf{x})$$

Filtering (Thresholding)



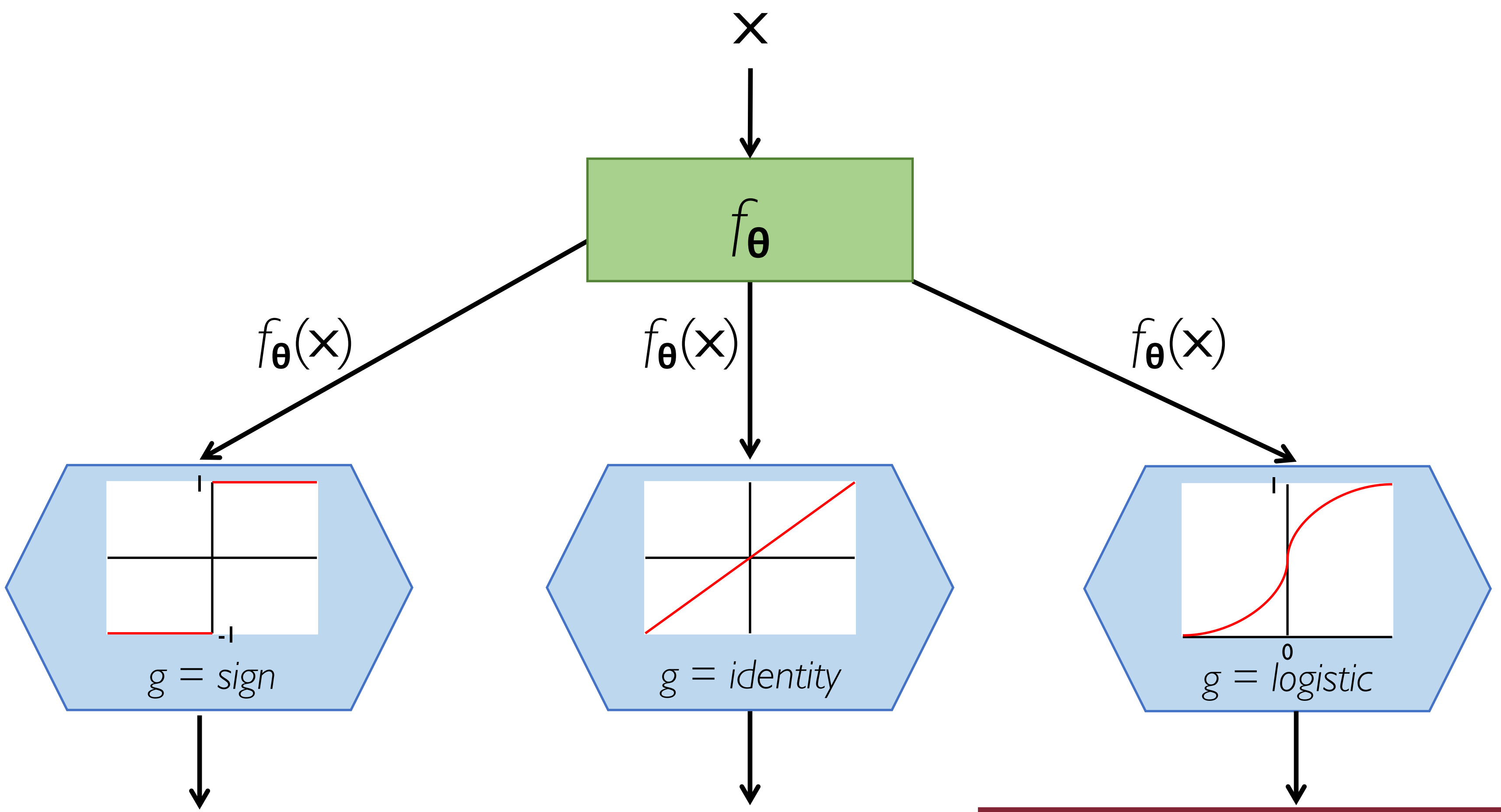
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = f_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T\mathbf{x}$$

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)

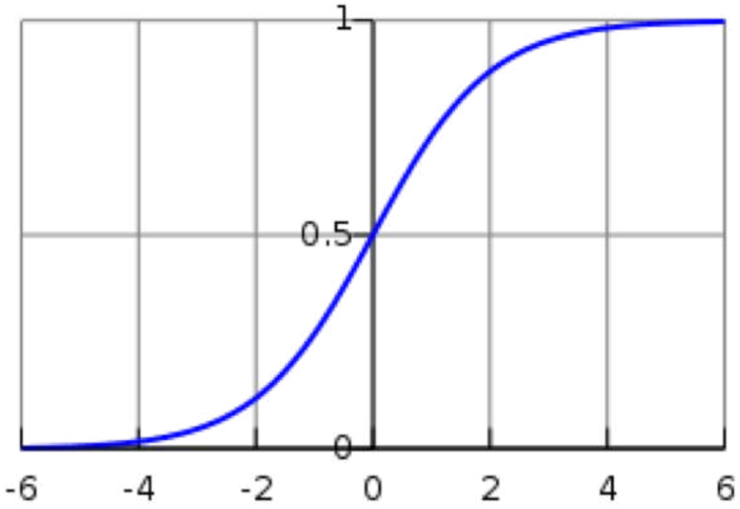


$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \mathrm{sign}(f_{\boldsymbol{\theta}}(\mathbf{x})) = \mathrm{sign}(\boldsymbol{\theta}^T\mathbf{x})$$

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

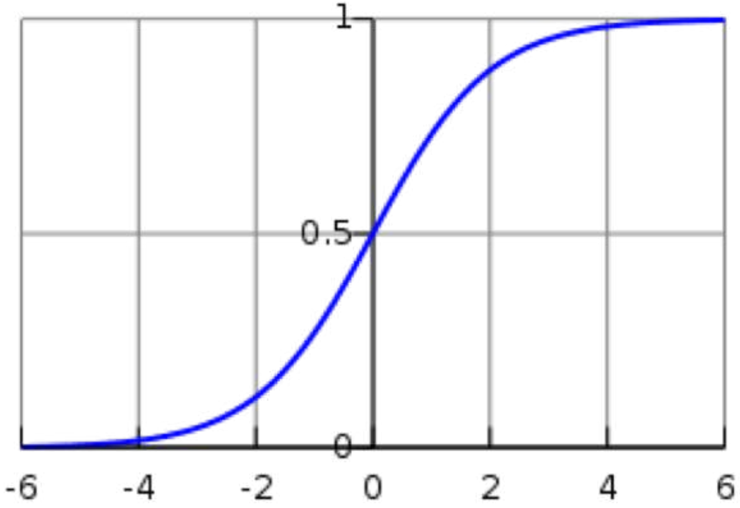
$$\boxed{h_{\boldsymbol{\theta}}(\mathbf{x}) = \ell(f_{\boldsymbol{\theta}}(\mathbf{x})) = \ell(\boldsymbol{\theta}^T\mathbf{x}) = \frac{e^{(\boldsymbol{\theta}^T\mathbf{x})}}{1+e^{(\boldsymbol{\theta}^T\mathbf{x})}}}$$

The Logistic Function



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

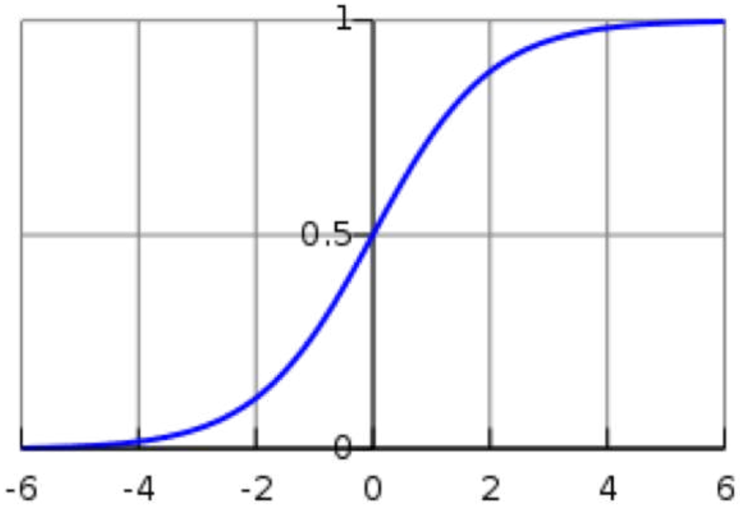
The Logistic Function



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

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

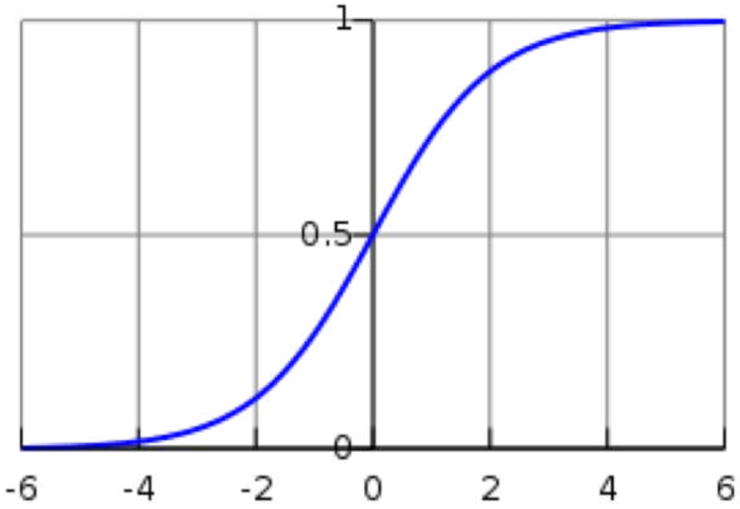
The Logistic Function



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

- 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., $1/\pi$ *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!

Additional Notes

https://github.com/gtolomei/big-data-computing/raw/master/extra/Notes_on_Logistic_Regression.pdf

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!

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

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:

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

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

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

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

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

From Odds to Probability

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

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

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

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

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

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

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 $\mathbf{x}$ and the odds computed at a different point $\mathbf{x}'$

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 $\mathbf{x}$ as input it always outputs either $y = +1$ or $y = -1$ (mutually exclusive)

Deterministic vs. Noisy Target

- Deterministic function: given $\mathbf{x}$ as input it always outputs either $y = +1$ or $y = -1$ (mutually exclusive)
- Noisy target function: given $\mathbf{x}$ 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 $\mathbf{x}$ as input it always outputs either $y = +1$ or $y = -1$ (mutually exclusive)
- Noisy target function: given $\mathbf{x}$ 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

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

Bayes Rule

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

2 main ways to find the estimate of the best hypothesis parameters $\boldsymbol{\theta}^*$

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\boxed{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

2 main ways to find the estimate of the best hypothesis parameters $\boldsymbol{\theta}^*$

Maximum Likelihood Estimate (MLE)

Frequentist approach

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\boxed{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

2 main ways to find the estimate of the best hypothesis parameters $\boldsymbol{\theta}^*$

Maximum A Posteriori (MAP)

Bayesian approach

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

2 main ways to find the estimate of the best hypothesis parameters $\boldsymbol{\theta}^*$

Maximum Likelihood Estimate (MLE)

Frequentist approach

Maximum A Posteriori (MAP)

Bayesian approach

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

MLE returns the set of parameters that maximize the likelihood

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

Finding The Best Hypothesis

$$\overbrace{P(h_{\boldsymbol{\theta}} \mid \mathcal{D})}^{\text{posterior}} = \frac{\overbrace{P(\mathcal{D} \mid h_{\boldsymbol{\theta}})}^{\text{likelihood}} \times \overbrace{P(h_{\boldsymbol{\theta}})}^{\text{prior}}}{\underbrace{P(\mathcal{D})}_{\text{evidence}}}$$

MAP returns the set of parameters that maximize the posterior

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

$$= \texttt{argmax}_{h_{\boldsymbol{\theta}} \in \mathcal{H}} \frac{P(\mathcal{D} \mid h_{\boldsymbol{\theta}}) \times P(h_{\boldsymbol{\theta}})}{P(\mathcal{D})}$$

$$= \texttt{argmax}_{h_{\boldsymbol{\theta}} \in \mathcal{H}} P(\mathcal{D} \mid h_{\boldsymbol{\theta}}) \times P(h_{\boldsymbol{\theta}})$$

MLE vs. MAP

MLE is just a special case of MAP where priors are uniform

(i.e., every hypothesis is equiprobable)

MLE vs. MAP

MLE is just a special case of MAP where priors are uniform

(i.e., every hypothesis is equiprobable)

Both MLE and MAP are point estimators: they return a single value for the optimal parameter vector $\boldsymbol{\theta}^*$

MLE vs. MAP

MLE is just a special case of MAP where priors are uniform

(i.e., every hypothesis is equiprobable)

Both MLE and MAP are point estimators: they return a single value for the optimal parameter vector $\boldsymbol{\theta}^*$

Note

A full Bayesian estimation is also possible, where the full posterior distribution (i.e., probability density/mass function) is estimated, although this turns out to be often computationally intractable

MLE: Maximizing The Likelihood Function

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

MLE: Maximizing 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 $h^{*}_{\boldsymbol{\theta}}(\mathbf{x})$?

MLE: Maximizing 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

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

The Likelihood Function

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

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

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 $\ell(y_i \theta^T x_i)$ 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 $\ell(y_i\theta^T x_i)$ 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

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

From MLE to In-Sample Error

Given a hypothesis $h_{\boldsymbol{\theta}}$ 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 $h_{\boldsymbol{\theta}}$ 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 $h_{\boldsymbol{\theta}}$ 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

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

Negative Log-Likelihood

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

Negative Log-Likelihood

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

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

Negative Log-Likelihood

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

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

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

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

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

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

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:

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

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

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

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

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

Negative Log-Likelihood Function

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

Negative Log-Likelihood Function

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

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

Negative Log-Likelihood Function

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

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

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

Negative Log-Likelihood Function

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

Negative Log-Likelihood Function

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

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

Negative Log-Likelihood Function

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

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

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*

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

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

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

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

$y = \{-1, +1\}$

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

$y = \{0, 1\}$

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

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

$\boxed{y = 1}$ $\boxed{y = 1}$

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 $\boldsymbol{\theta}^*$ 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 $\boldsymbol{\theta}$

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

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

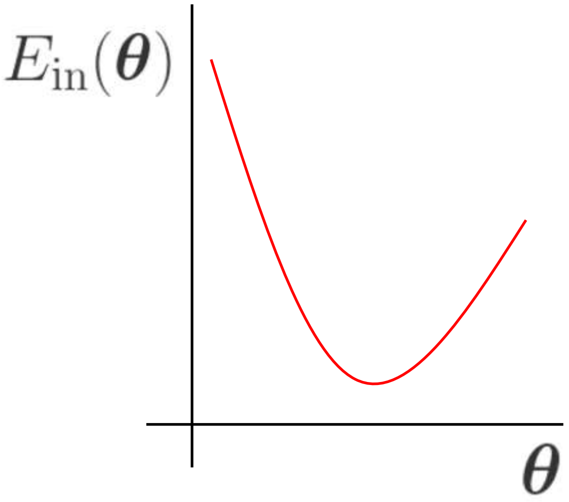
Yet, Cross-Entropy is convex w.r.t. the parameters $\boldsymbol{\theta}$

$\Downarrow$

Iterative Solution

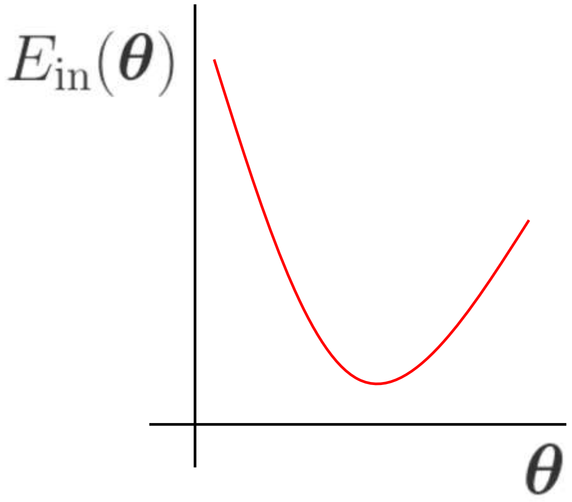
(Batch) Gradient Descent

General iterative method for any nonlinear optimization



(Batch) Gradient Descent

General iterative method for any nonlinear optimization

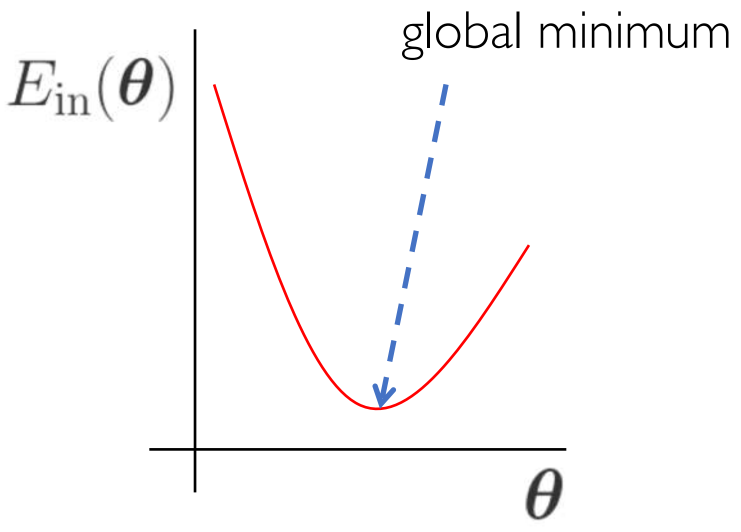


The method **guarantees the convergence to a local minimum**

(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: $\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta \mathrm{v}$
   b. Return to 2.

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

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

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

Let's first assume we are in the univariate case, i.e., $\boldsymbol{\theta} = \vartheta$ 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., $\boldsymbol{\theta} = \vartheta$ 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., $\boldsymbol{\theta} = \vartheta$ in R

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

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

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

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

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

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

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

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., $\boldsymbol{\theta} = \vartheta$ 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 $\boldsymbol{\theta}$:

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

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 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 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 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 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 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}

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

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

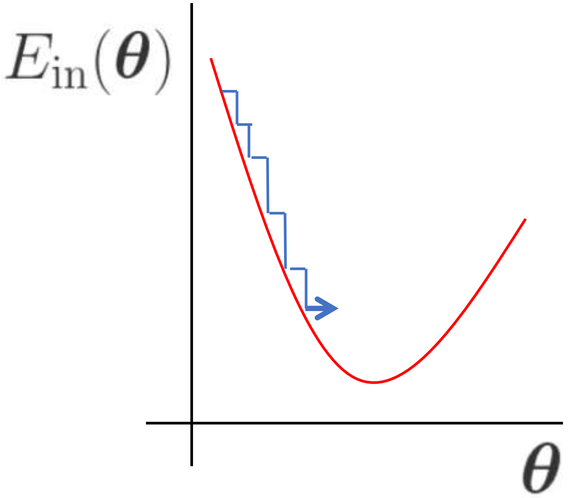
$$\mathbf{v} = -\frac{||\mathbf{u}||\mathbf{u}^T}{||\mathbf{u}||^2} = -\frac{\mathbf{u}^T}{||\mathbf{u}||} = \boxed{-\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))}{||\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))||}}$$

Gradient Descent: The Step η

How the step magnitude η affects the convergence?

Gradient Descent: The Step η

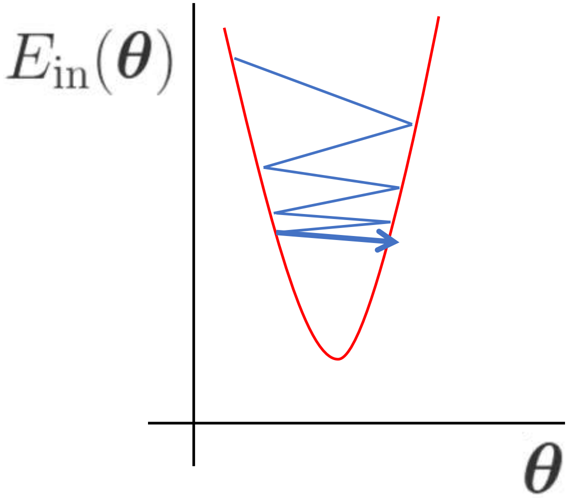
How the step magnitude η affects the convergence?



η too small

Gradient Descent: The Step η

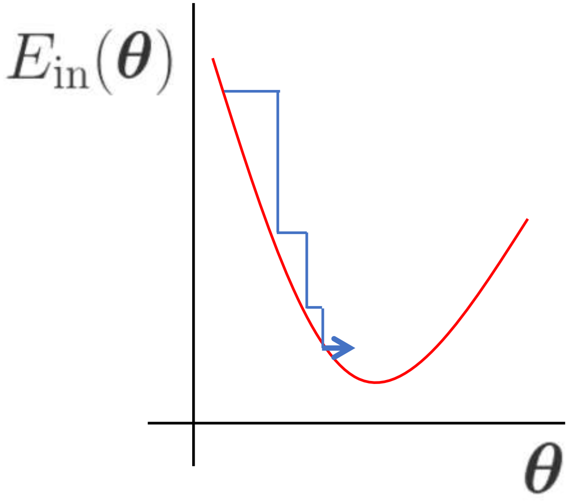
How the step magnitude η affects the convergence?



η too large

Gradient Descent: The Step η

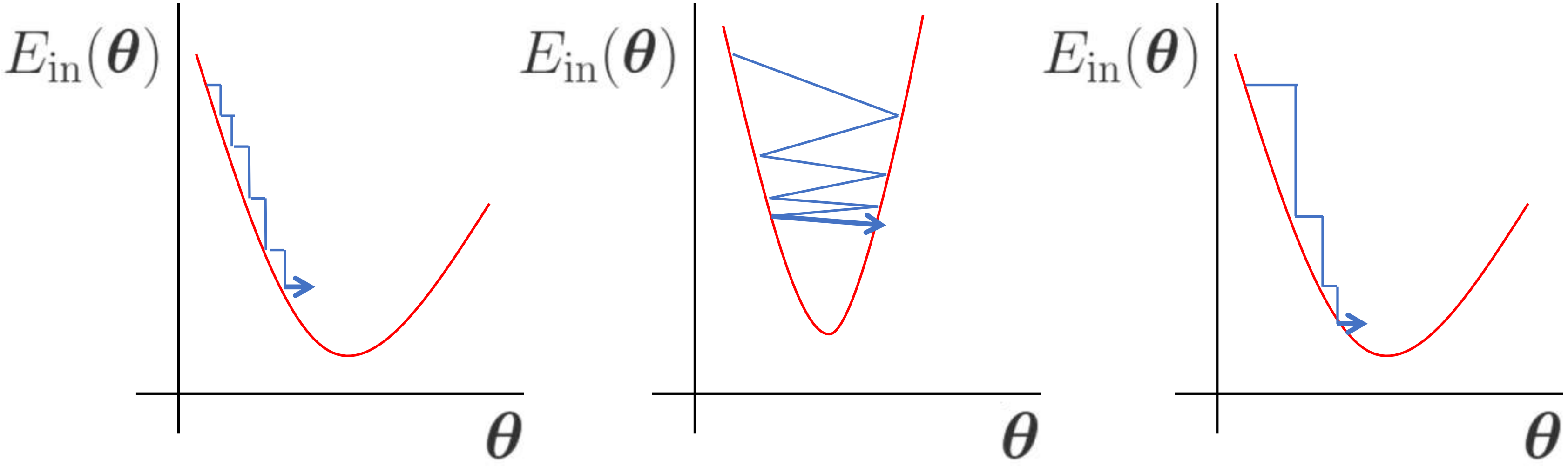
How the step magnitude η affects the convergence?



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

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

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

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

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

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 $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$
2. For $t = 0, 1, 2, \ldots$ 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 $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$
2. For $t = 0, 1, 2, \ldots$ 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: $\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t))$
   c. Return to 2.

Gradient Descent: The Algorithm

1. At $t = 0$ initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$
2. For $t = 0, 1, 2, \ldots$ 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: $\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t))$
   c. Return to 2.
3. Return the final vector of parameters $\boldsymbol{\theta}(\infty)$

Gradient Descent: Initialization

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

Gradient Descent: Initialization

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

Gradient Descent: Initialization

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

Gradient Descent: Initialization

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

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 $\boldsymbol{\theta}(0)$ 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 vs. Mini-Batch Gradient Descent (SGD vs. MBGD)
  - At each iteration, compute the gradient only from one instance (SGD) or a sample of k instances (MBGD) rather than 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 vs. Mini-Batch Gradient Descent (SGD vs. MBGD)
  - At each iteration, compute the gradient only from one instance (SGD) or a sample of k instances (MBGD) rather than 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