Big Data Computing

Master's Degree in Computer Science

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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)

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- 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

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- 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

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- Different (and still legitimate) encodings will produce different models

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- 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)

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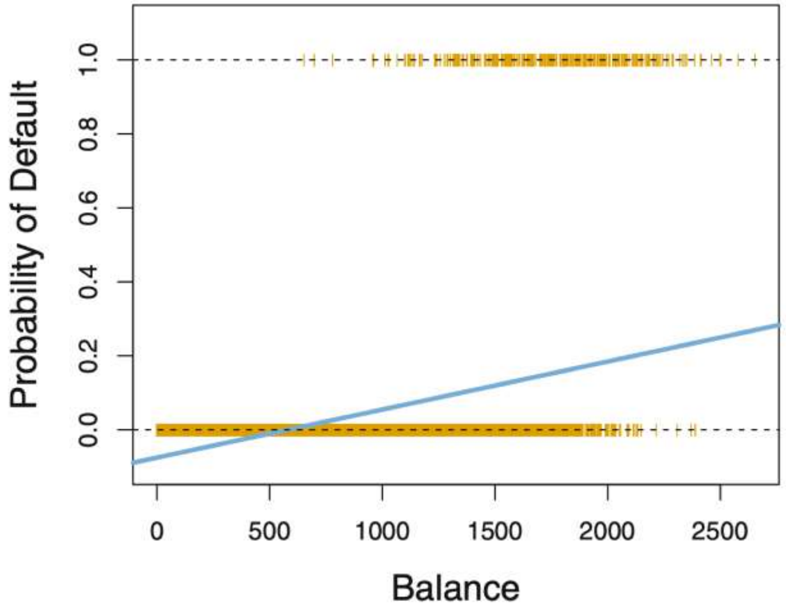
Suppose we want to predict the value of Y from the value of Balance(X)

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

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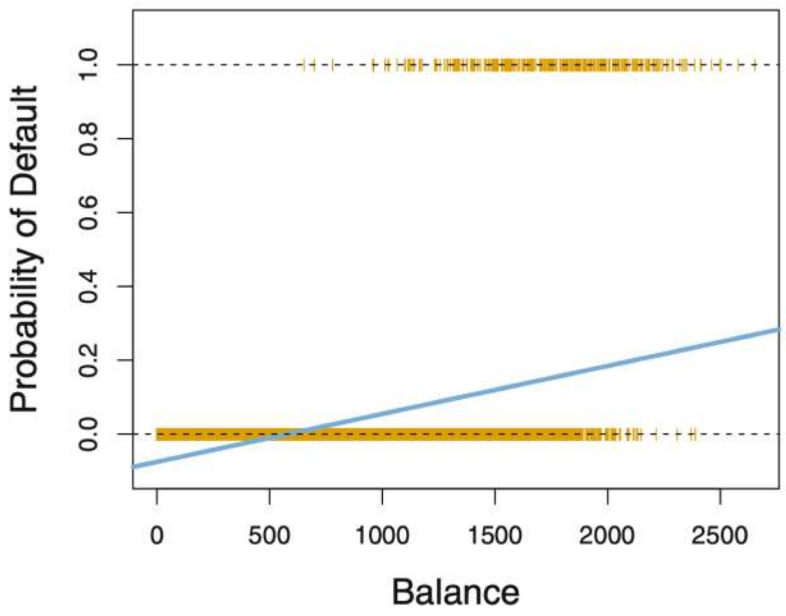

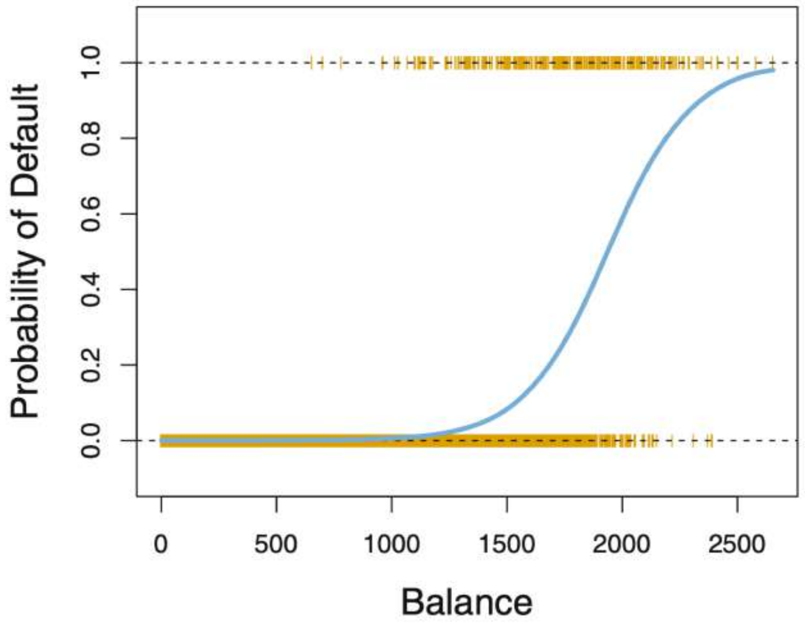

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Linear Regression

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

Logistic Regression

General Concepts

3 components need to be specified

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Model

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Learning Algorithm

Picks the best hypothesis exploring search space

MODEL

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

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- 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)

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

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

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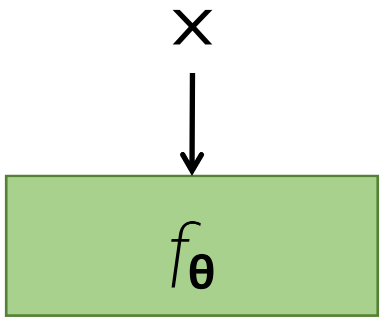
The set of possible hypotheses H changes depending on the parametric model ($f_{\boldsymbol{\theta}}$) and on the thresholding function (g)

Filtering (Thresholding)



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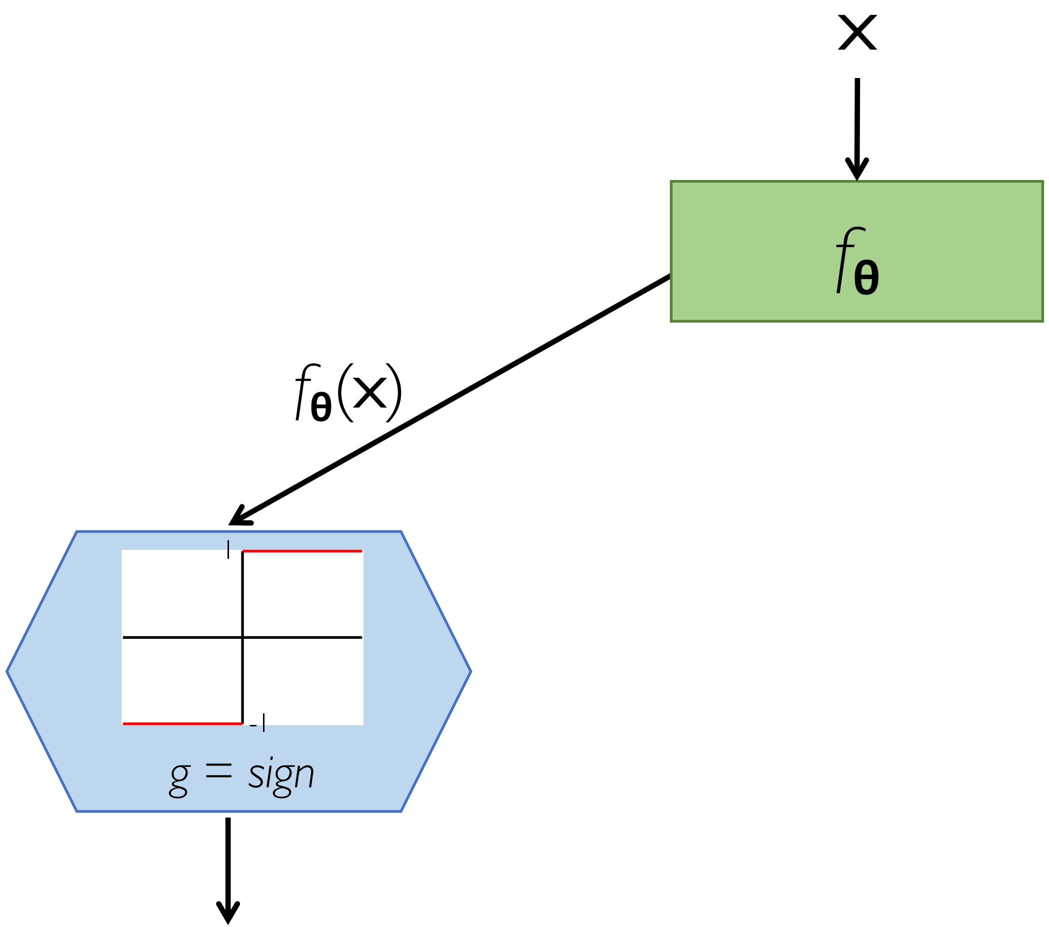

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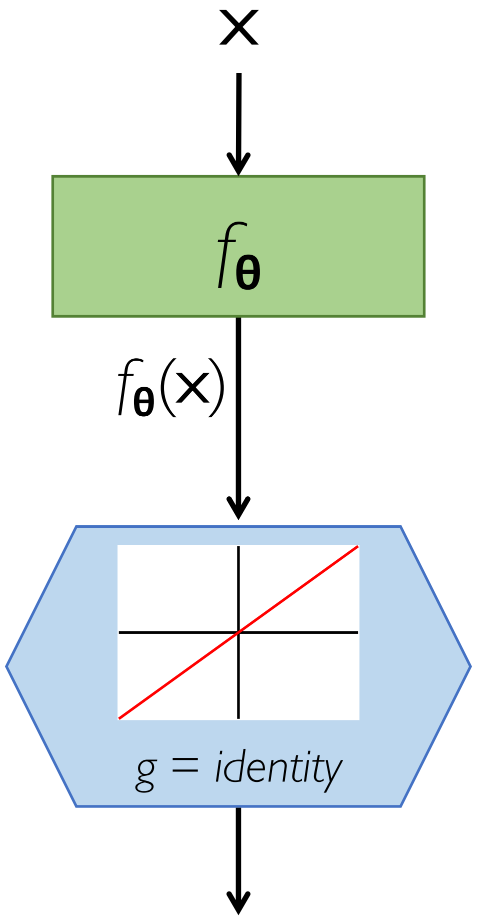

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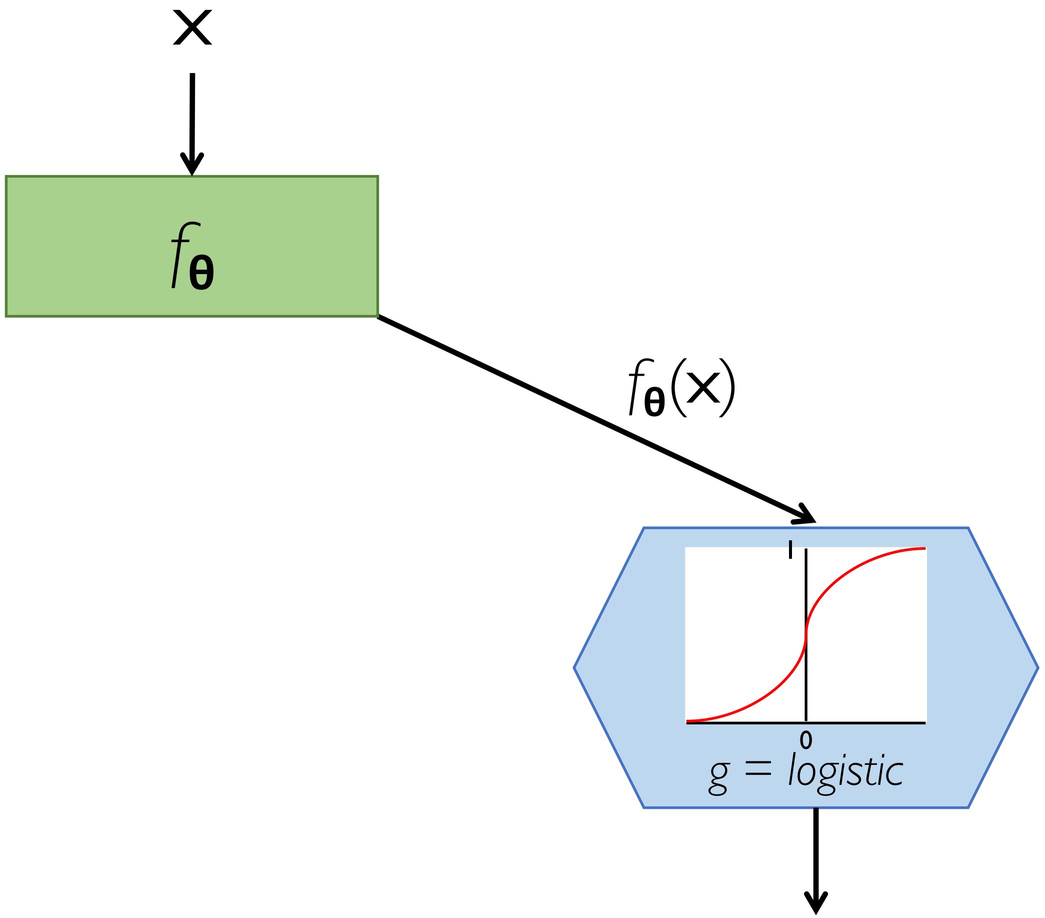

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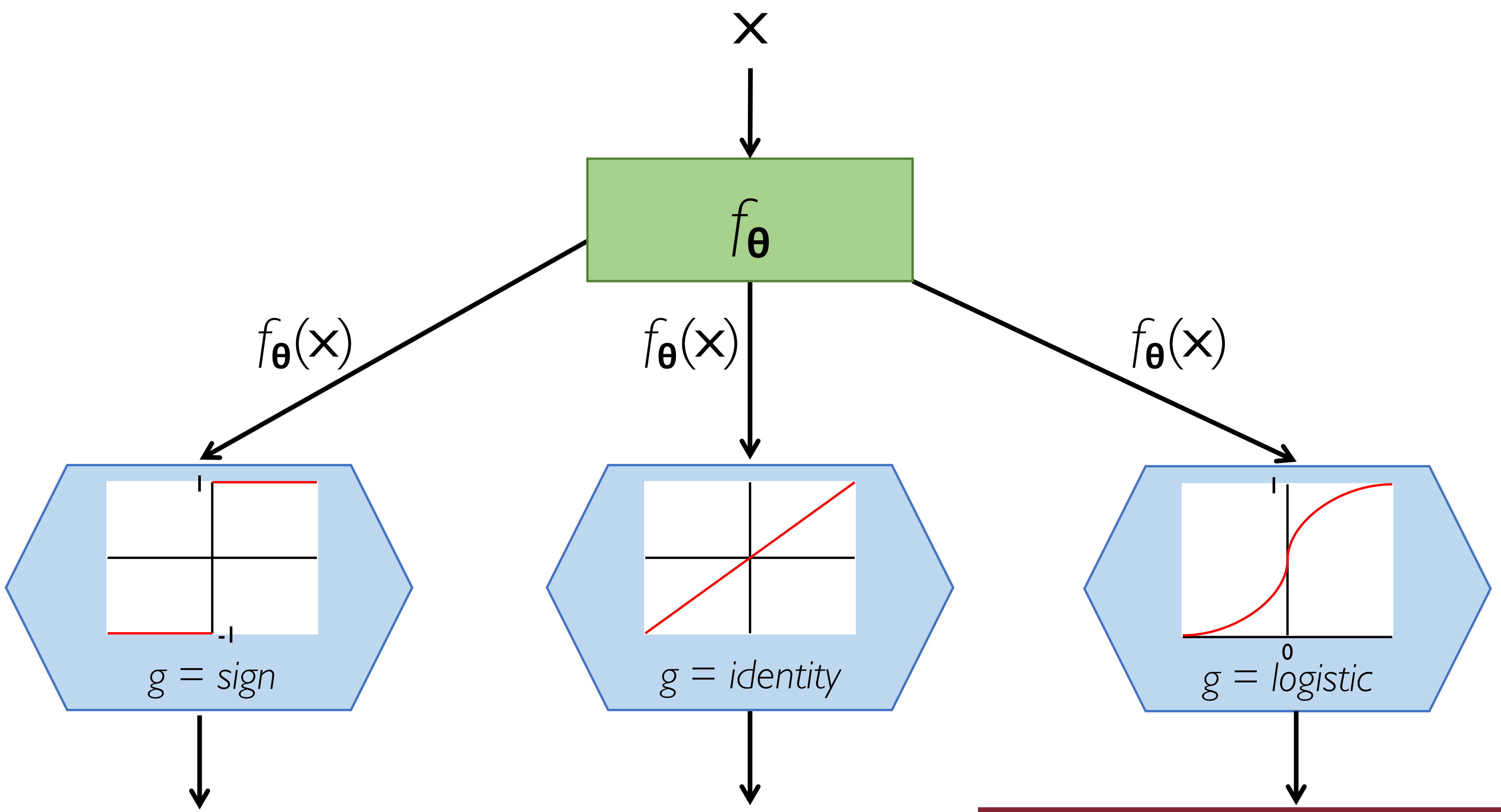

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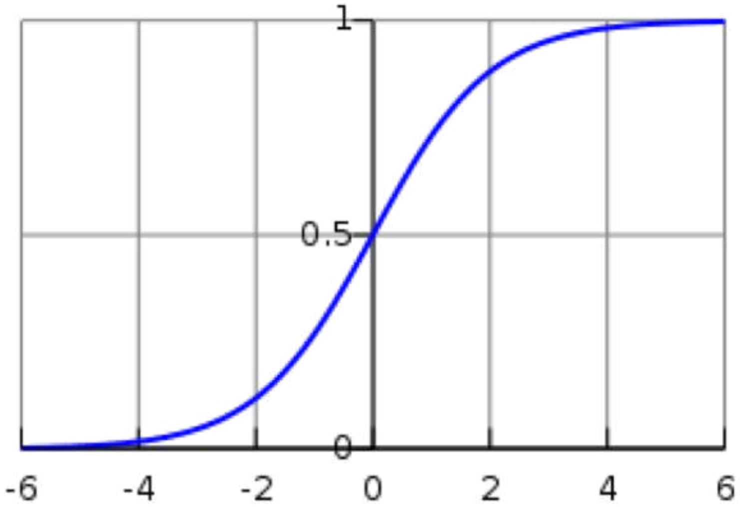
The Logistic Function



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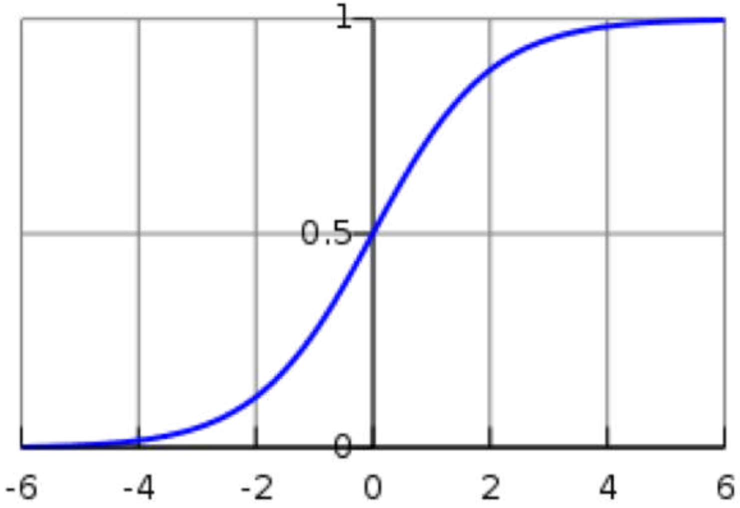

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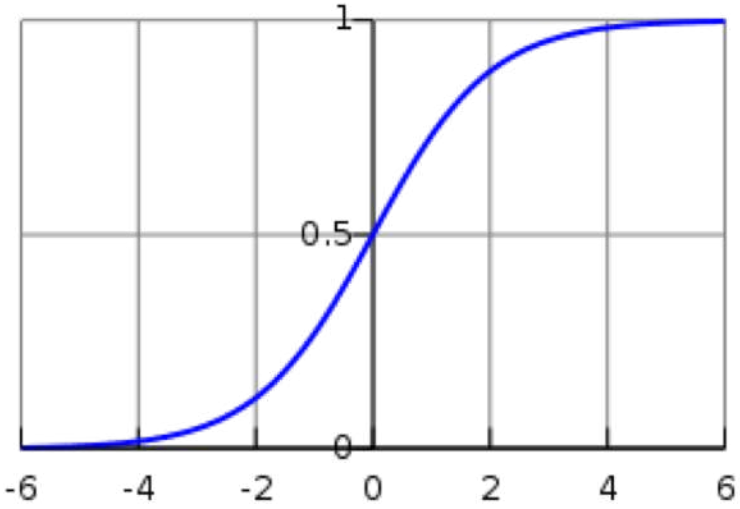

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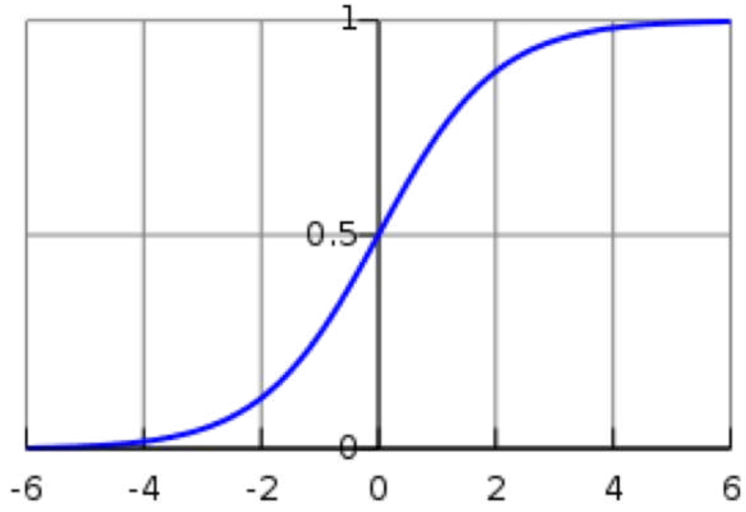

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- Output can be *genuinely* interpreted as a probability value

Probabilistic Interpretation

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- Other functions may have the same property [e.g., $1/\pi$ *arctan(x) + 1/2*]

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- 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

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- $odds(failure) = q/p = 1/p/q = 1/odds(success)$
- $logit(p) = ln(odds(success)) = ln(p/q) = ln(p/1\text{-}p) = ln(p) - ln(1\text{-}p)$

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

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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

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

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

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

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

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

Odds Ratio

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

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

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Let's measure the ratio between the odds computed at a certain input $\mathbf{x}$ and the odds computed at a different point $\mathbf{x}'$

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

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

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

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$$= e^{\theta_i}$$

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

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

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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!

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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)

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Goal

$\phi: \mathbb{R}^{d+1} \rightarrow [0,1]$ 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 $h^*_{\boldsymbol{\theta}}(\mathrm{x})$?

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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

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

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Bayes Rule

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

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Maximum Likelihood Estimate (MLE)

Frequentist approach

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MLE returns the set of parameters that maximize the likelihood

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

Finding The Best Hypothesis

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MAP returns the set of parameters that maximize the posterior

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

MLE vs. MAP

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

(i.e., every hypothesis is equiprobable)

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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

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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 $h_{\boldsymbol{\theta}}(\mathbf{x})$ 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

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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
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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

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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

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

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

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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

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

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

Negative Log-Likelihood

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

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

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

Negative Log-Likelihood

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

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

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

Cross-Entropy Error

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

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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:

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

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Cross-Entropy Error

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

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

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

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

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

$y = \{0, 1\}$

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

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

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

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

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

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

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

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*

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

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

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

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

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

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LEARNING ALGORITHM

Picking the Best Hypothesis

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

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  - The model (logistic function)
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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)

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

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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

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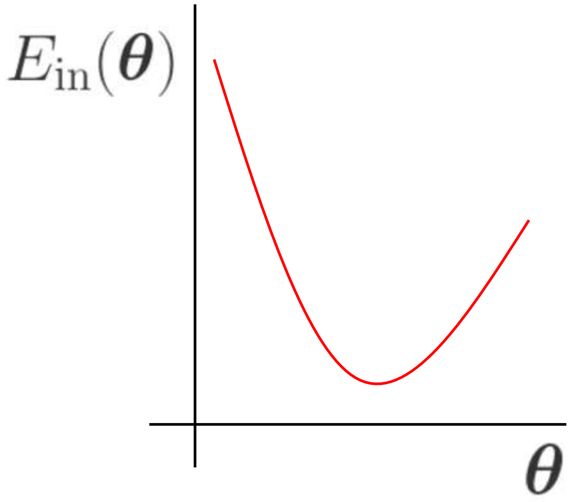
$\Downarrow$

Iterative Solution

(Batch) Gradient Descent

General iterative method for any nonlinear optimization



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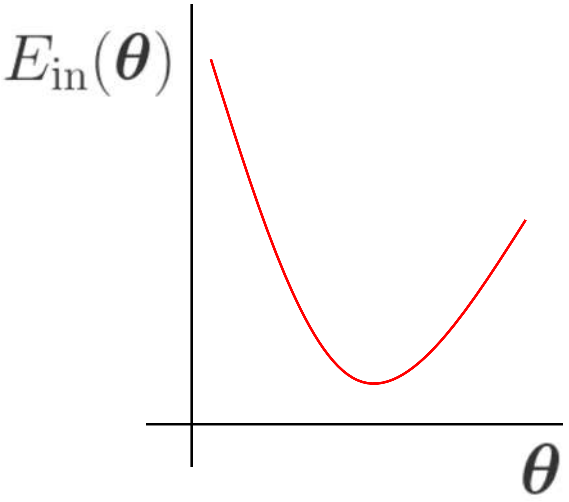

The method **guarantees the convergence to a local minimum**

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

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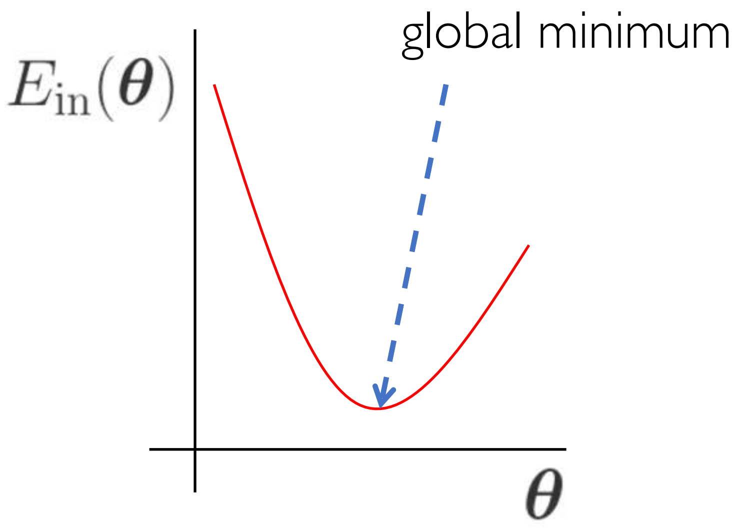

The method **guarantees the convergence to a local minimum**

(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 $\boldsymbol{\theta}(0)$

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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

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

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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

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

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

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

Gradient Descent: The Direction v

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

Gradient Descent: The Direction v

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

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

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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

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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

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

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

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

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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

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

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

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

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

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}

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

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

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

Gradient Descent: The Direction v

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

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Gradient Descent: The Step η

How the step magnitude η affects the convergence?

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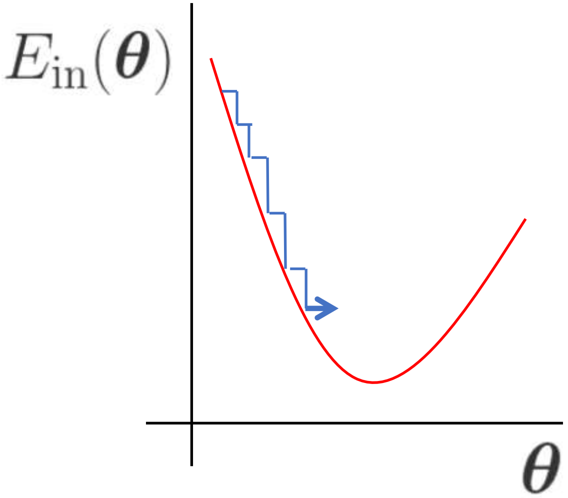
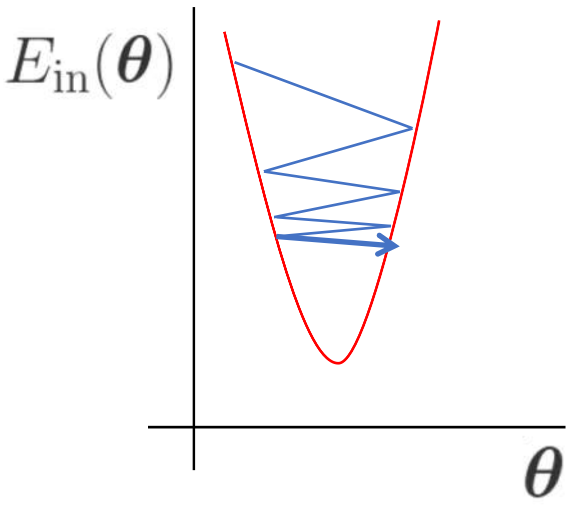


η too small

Gradient Descent: The Step η

How the step magnitude η affects the convergence?



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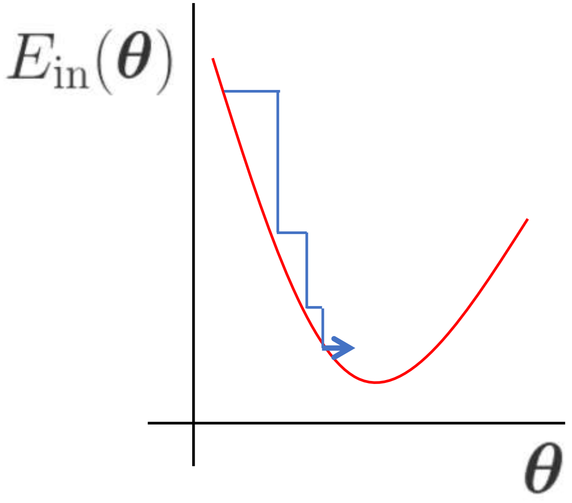
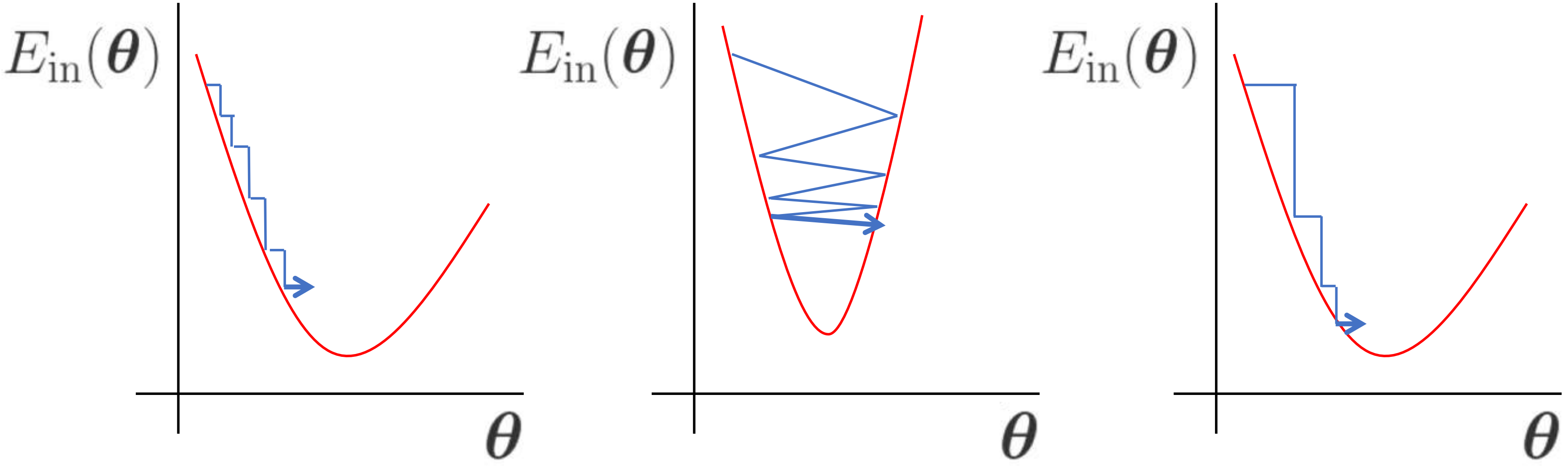


η variable

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

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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

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

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Gradient Descent: The Step η

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

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Computing the Gradient of Cross-Entropy

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

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chain rule of derivative

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3. Return the final vector of parameters $\boldsymbol{\theta}(\infty)$

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- 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 $\boldsymbol{\theta}(0)$

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- 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

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- 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…

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- 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

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- 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