Big Data Computing

Master's Degree in Computer Science

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SAPIENZA
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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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- **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?

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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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- In practice, there is no particular reason to choose the encoding above!
- 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
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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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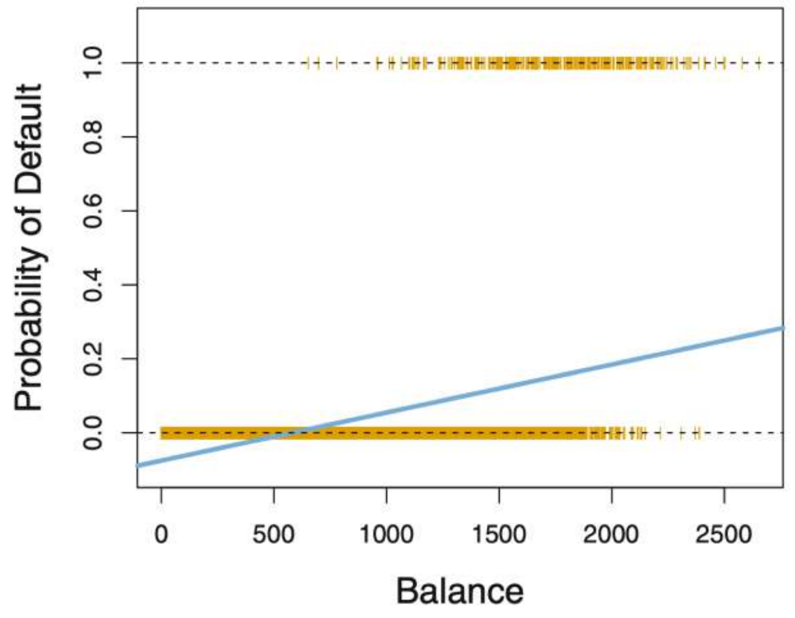
Suppose we want to predict the value of Y from the value of Balance(X)

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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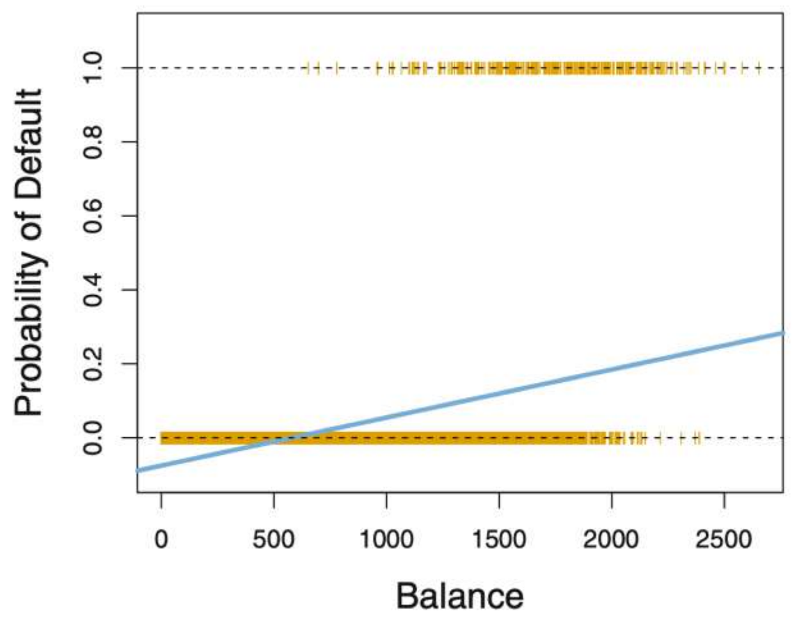

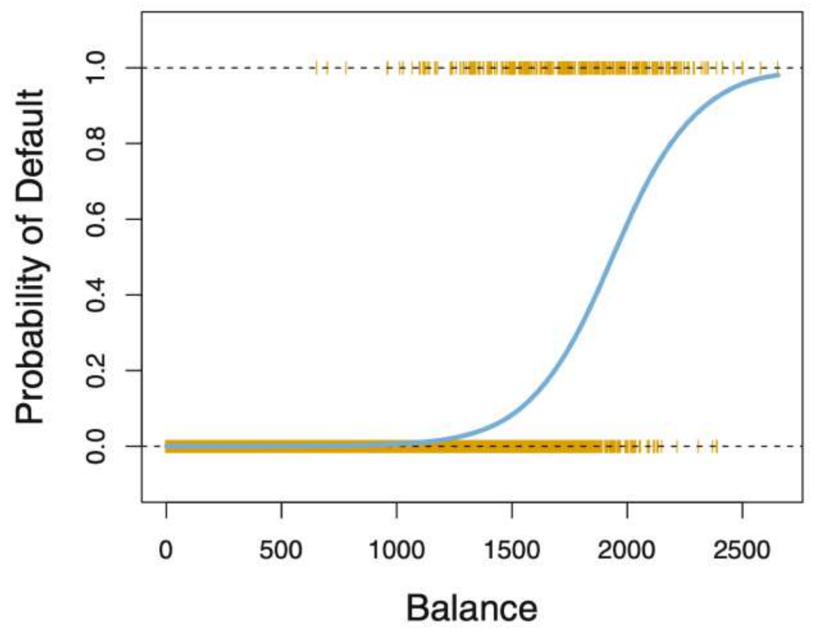

Predicted probability using linear regression
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Linear Regression

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

Defines the space of representable hypotheses

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Error Measure
(Cost Function)

Measures the price of misclassification errors

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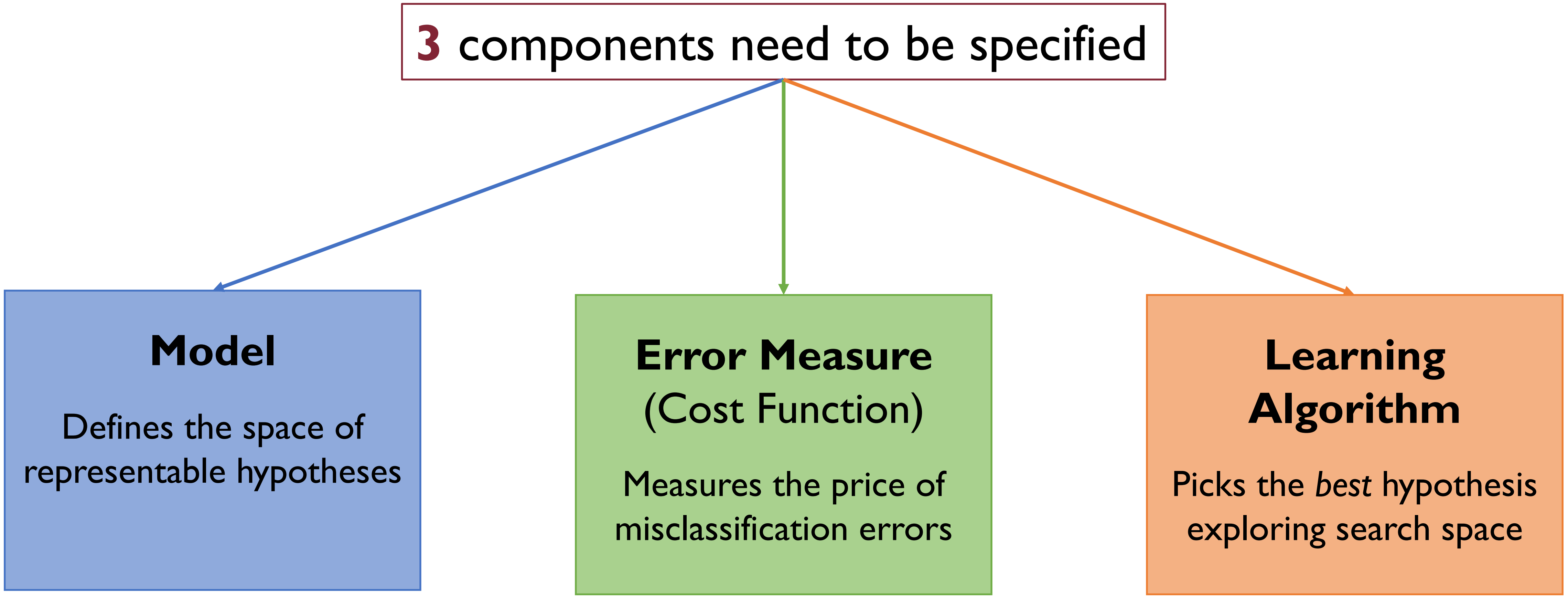

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Model

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 $\mathbf{x} = (x_0, x_1, \ldots, x_{\underset{m}{\cancel{d}}})$ be the $(\overset{m}{\cancel{d}}+1)$-dimensional input

Linear Signal

- Let **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 **θ** so that $\boldsymbol{\theta}^T = (\theta_0, \theta_1, \ldots, \theta_d)$

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

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signal goes from input to output

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

Hypothesis Space (Revisited)

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  f is called the linear signal function
- $h_\theta(\mathbf{x}) = g(f_\theta(\mathbf{x}))$ defines the hypothesis space:

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

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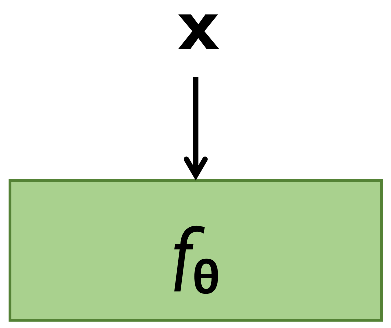
The set of possible hypotheses *H* changes depending on the parametric model (f_θ) and on the **thresholding function** (g)

Filtering (Thresholding)



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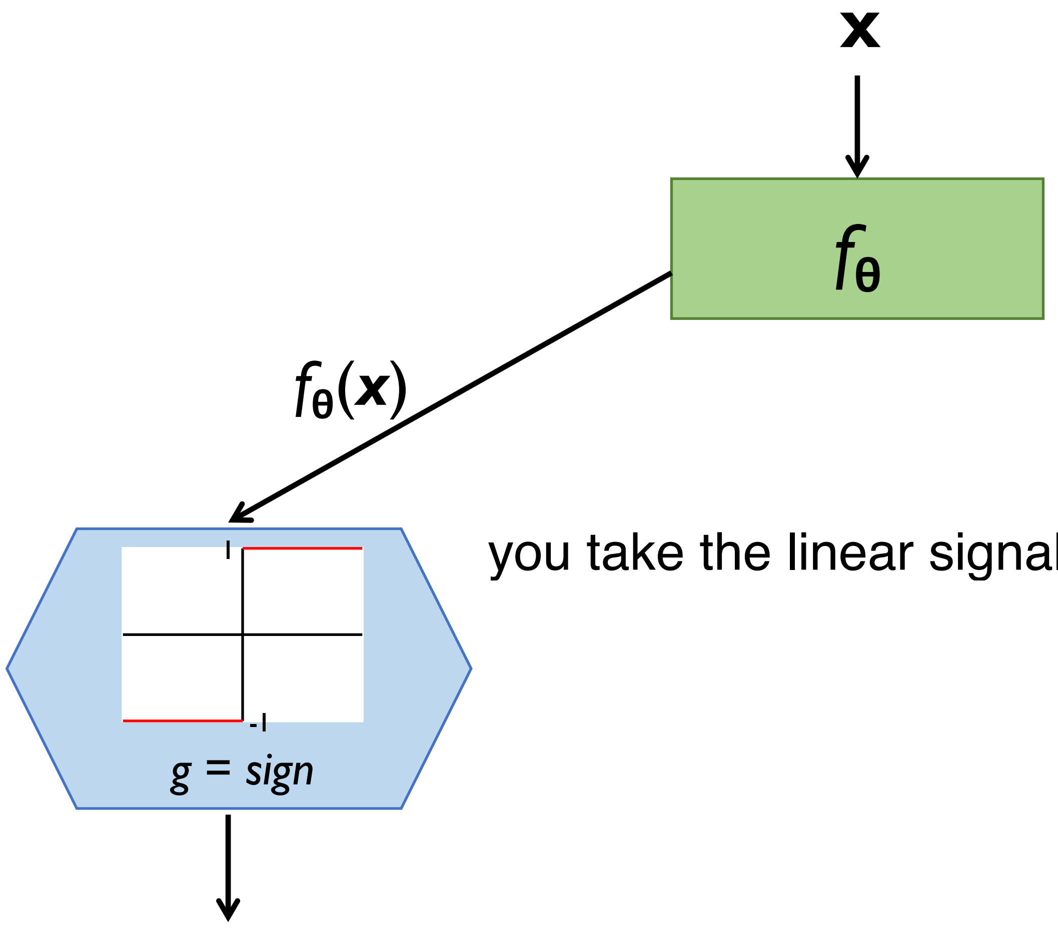

you take the linear signal and then take the sign of the f's output

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

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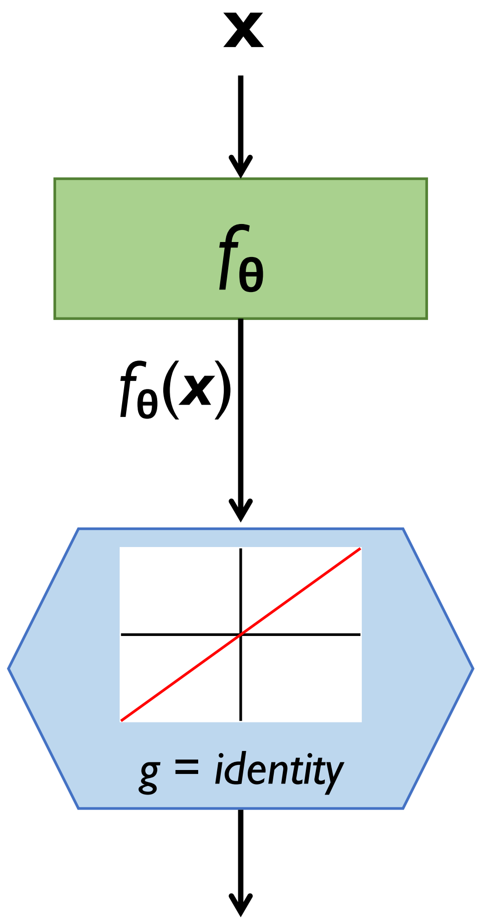

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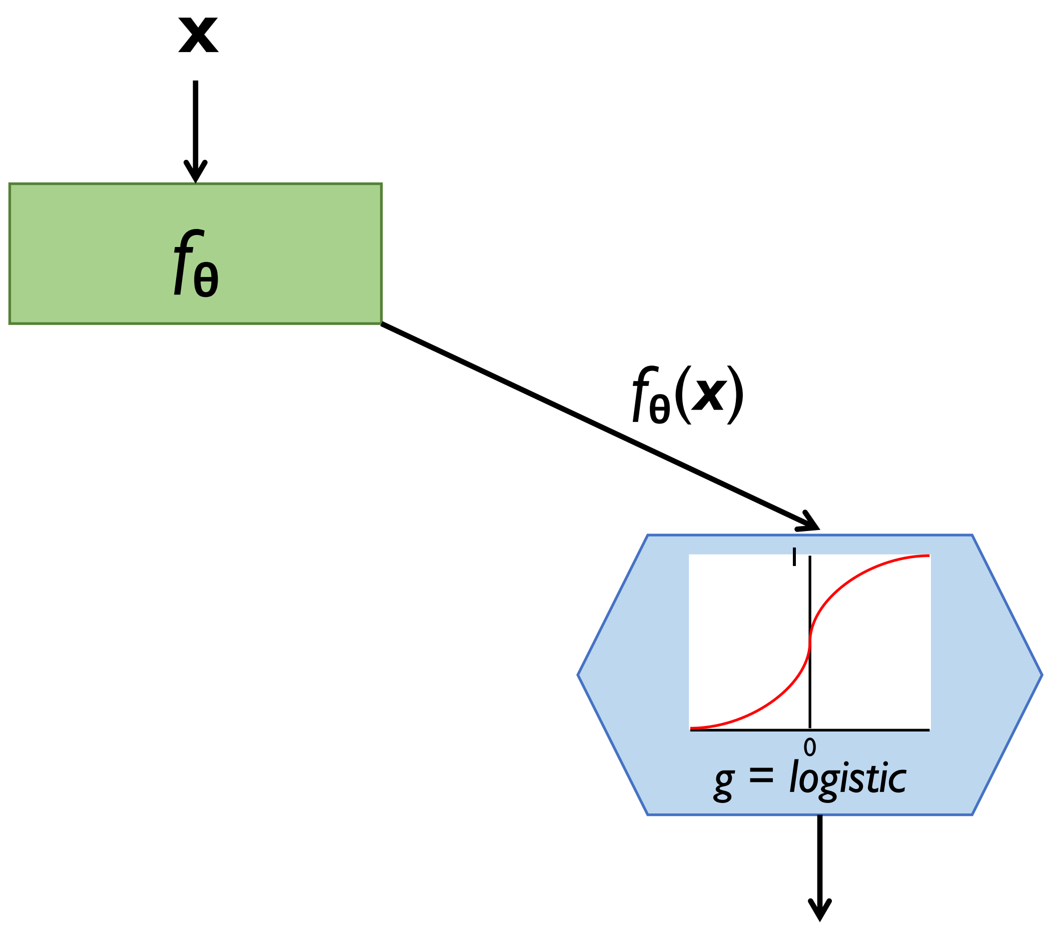

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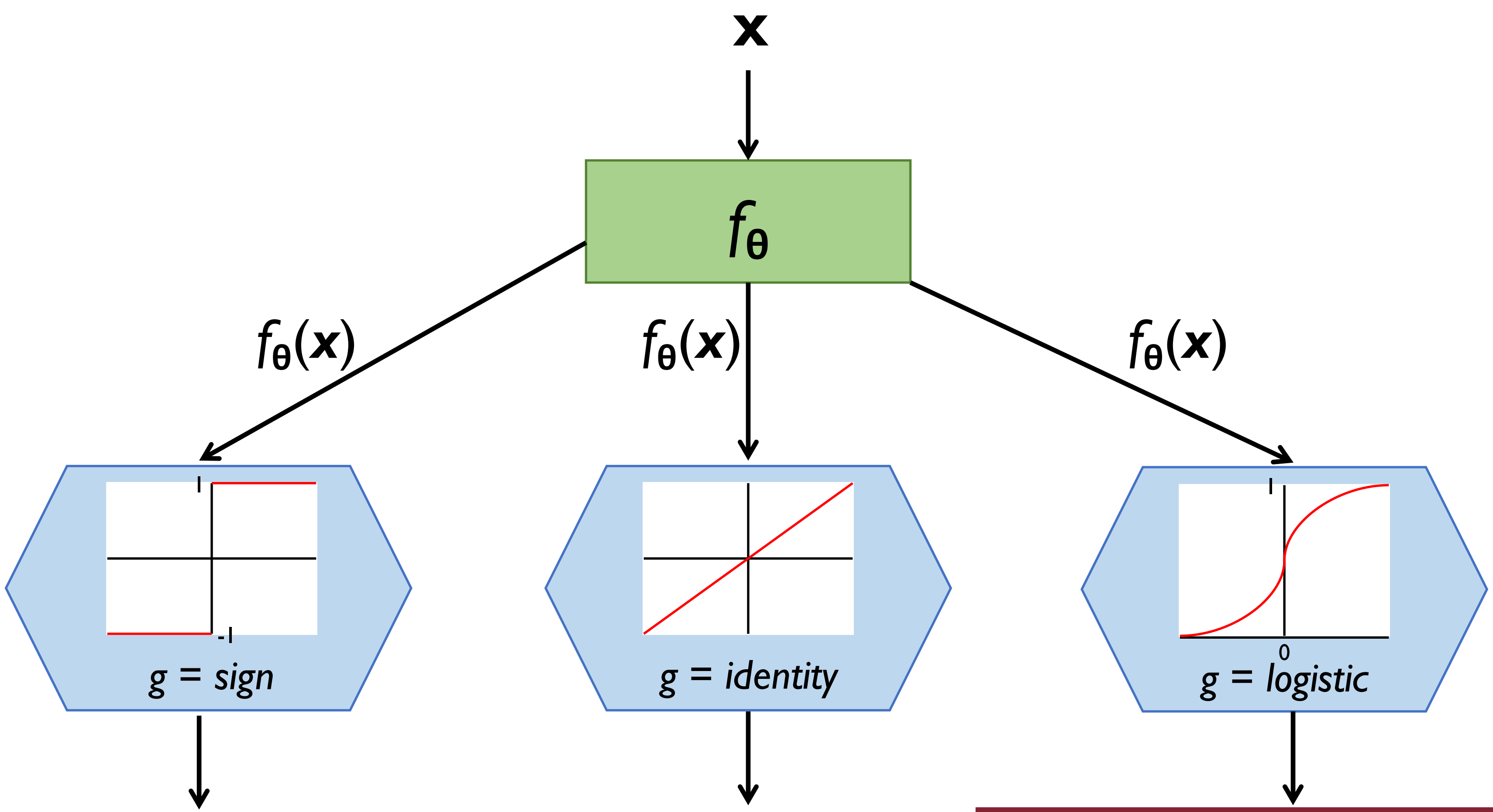

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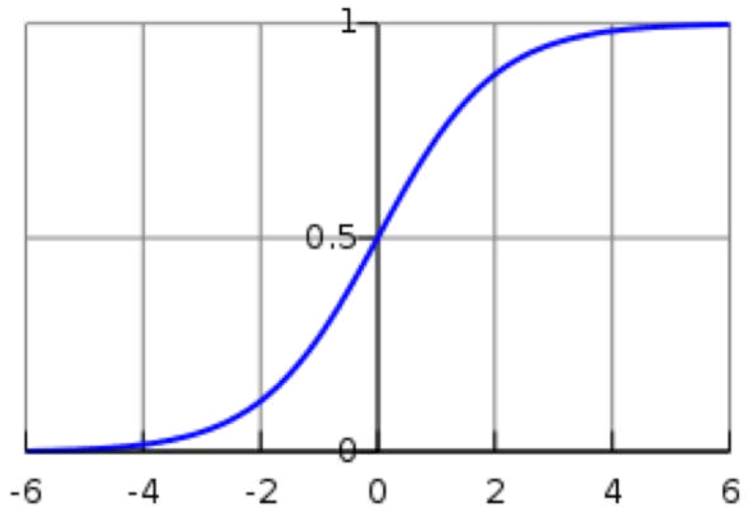
The Logistic Function



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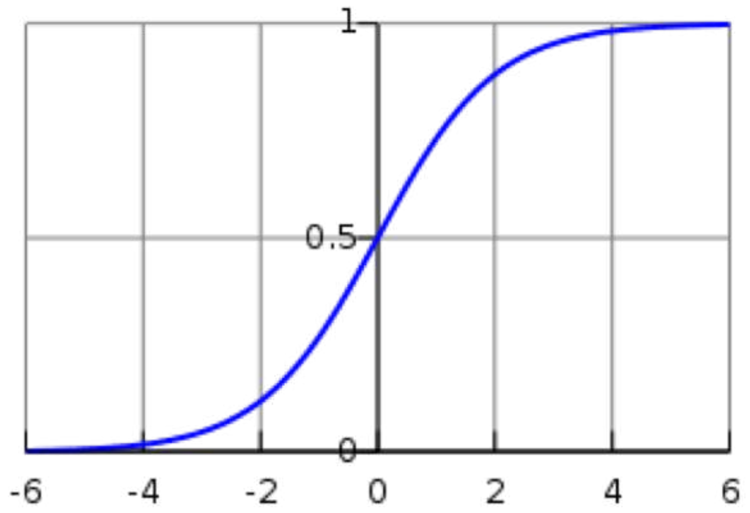

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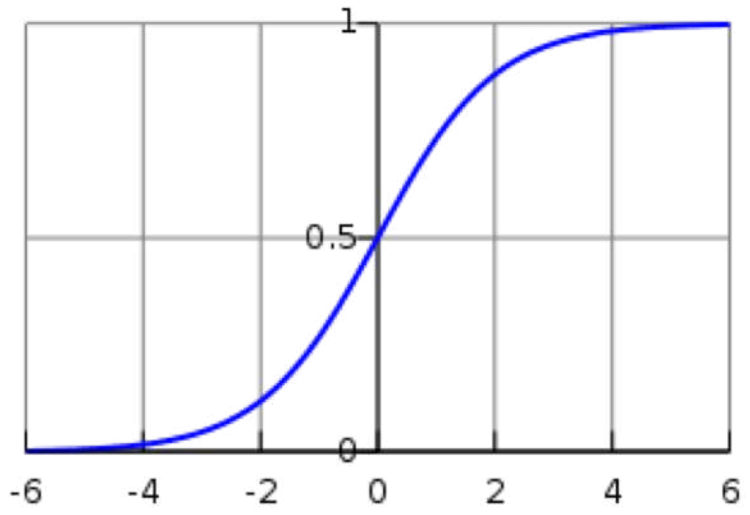

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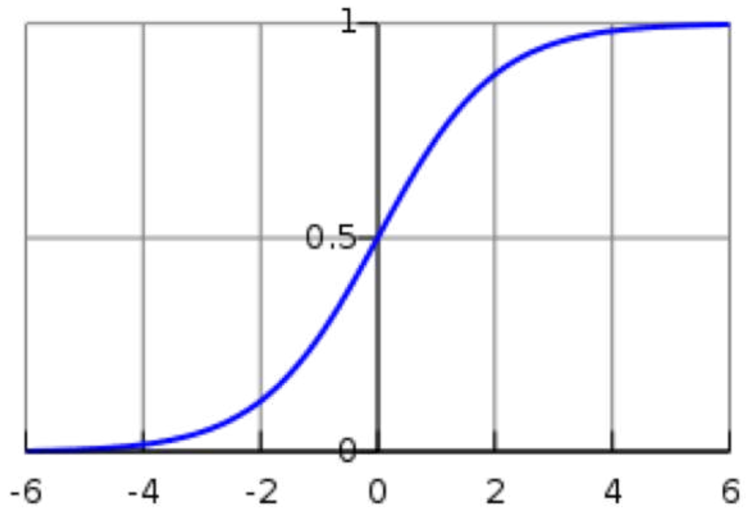

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- When $z = \boldsymbol{\theta}^T\mathbf{x}$ we are applying a *non-linear* transformation to our *linear* signal
- Output can be *genuinely* interpreted as a probability value

Probabilistic Interpretation

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- Other functions may have the same property [e.g., 1/π *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!

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- $odds(failure) = q/p = 1/p/q = 1/odds(success)$
- $logit(p) = ln(odds(success)) = ln(p/q) = ln(p/1-p) = ln(p) - ln(1-p)$

Odds

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

our signal models the natural log of the odds

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

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

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

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

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

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

In order to get p, we plug our regression model into the sigmoid function

Odds Ratio

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

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

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

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

Odds Ratio

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

odds thereself is a ratio

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

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

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

Odds Ratio

odds compute on x'

odds compute on x

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

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

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

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$$= e^{\theta_i}$$

it's the amount of the change

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

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

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no matter the size of the feature, the odds ratio is costant

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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

doesn't depend on the x_i feature

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

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associated with some probability

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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

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

sigmoid apply to the linear signal

Hypothesized Noisy Target

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

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

COST FUNCTION

Finding The Best Hypothesis

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

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

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

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

Flipping the Coin: The Likelihood Function

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

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

Flipping the Coin: The Likelihood Function

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

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

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

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

changes theta

The Likelihood Function

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

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

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:

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

equals to *

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 $\ell(y_i\boldsymbol{\theta}^T\mathbf{x}_i)$ approaches to 1

prediction agrees with the true label

if y =1 and theta transpose x_i applied to logistic functions give us a values close to 1, if the signal is very large, the logstic ouput is closer and closer to 1

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

prediction disagrees with the true label

Maximum Likelihood Estimate (MLE)

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

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

From MLE to In-Sample Error

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

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

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

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

Negative Log-Likelihood

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

Negative Log-Likelihood

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

the log is monotic and then we can apply it, does't change the theta values that

Negative Log-Likelihood

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

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

Negative Log-Likelihood

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

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

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

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

Negative Log-Likelihood

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

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

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

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

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

Cross-Entropy Error

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

Cross-Entropy Error

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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

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

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

y = {-1, +1}

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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

$$Y = \{0, 1\}$$

$$Y \sim \text{Bernoulli}(p)$$

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

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

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

Likelihood Function

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

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

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

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

Negative Log-Likelihood Function

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

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

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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*

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

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

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*

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

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

Substituting *p*

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

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

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

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

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y = 0

Equivalence Between 2 Formulations

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

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)
  - The error measure (cross-entropy)

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

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

Mean Squared Error vs. Cross-Entropy

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

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

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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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we cannot find the the minimazer analiticaly

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

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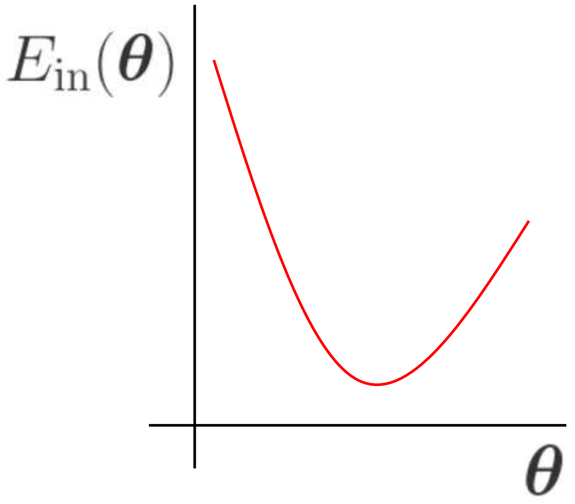
$\Downarrow$

Iterative Solution

(Batch) Gradient Descent

General iterative method for any nonlinear optimization



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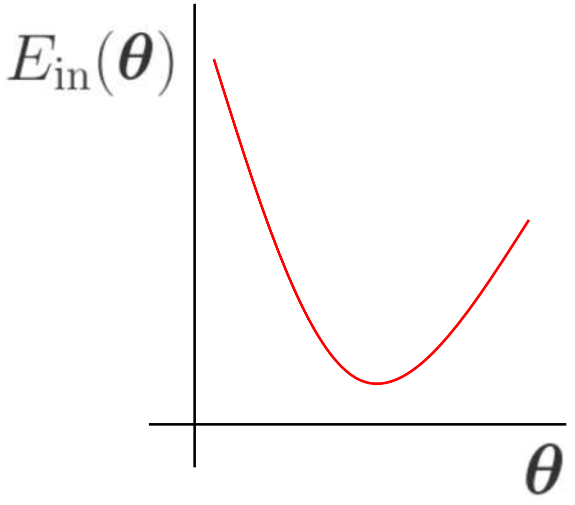


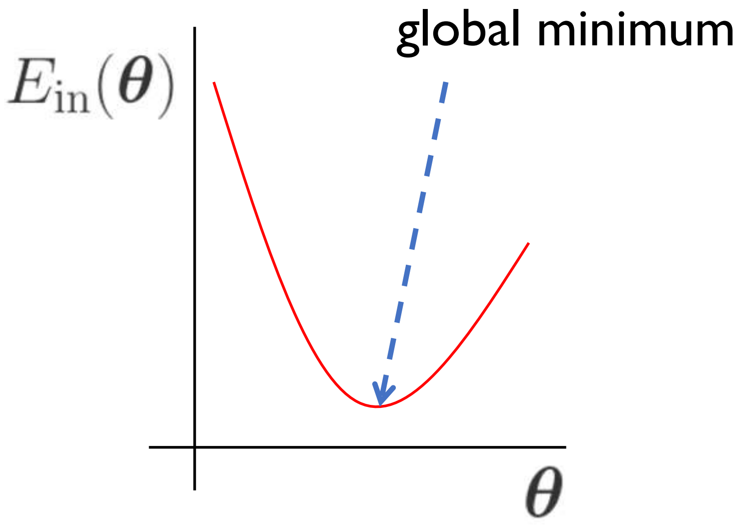
The method **guarantees the convergence to a local minimum**

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

if oyu apply GD to a function to a convex function you get a global minimum, otherwise it is not garanteed that GD can find the best local minimum

(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

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Unit vector representing the direction of the steepest slope

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

unit vector which models the direction

step

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$$\boxed{\text{How do we determine the direction } \mathbf{v}\text{?}}$$

Gradient Descent: The Direction **v**

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

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Gradient Descent: The Direction **v**

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difference of the error, if we have a less value in the time t this implies that the error is better than the t-1

- Concretely, this means moving along the direction which mostly reduces the in-sample error function

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

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

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

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

Gradient Descent: The Direction **v**

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

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

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

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

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

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

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

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Gradient Descent: The Direction **v**

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Gradient Descent: The Direction **v**

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

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

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

The greek letter *nabla* indicates the gradient

Gradient Descent: The Direction **v**

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

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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**

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

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

Gradient Descent: The Direction **v**

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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**

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

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

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

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

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Gradient Descent: The Step η

How the step magnitude η affects the convergence?

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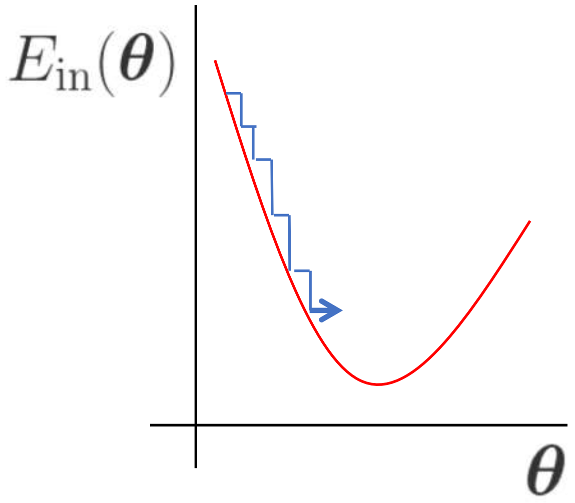
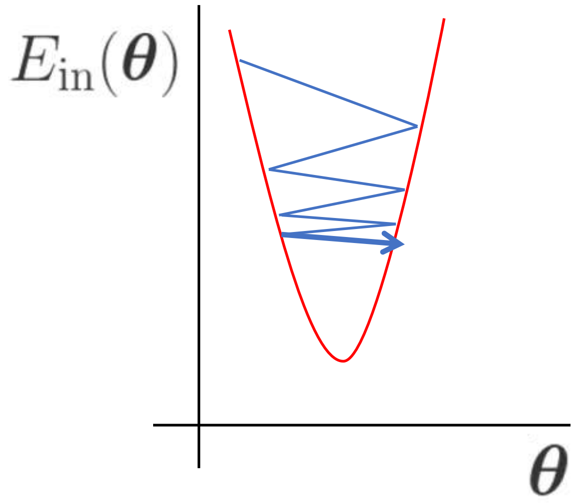


η too small

Gradient Descent: The Step η

How the step magnitude η affects the convergence?



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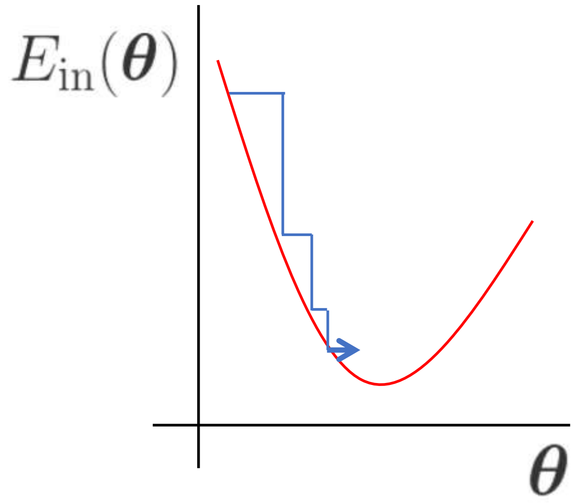
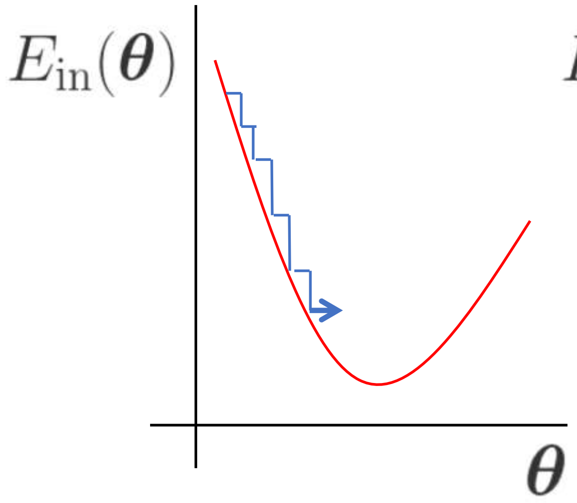


η variable

Gradient Descent: The Step η

How the step magnitude η affects the convergence?



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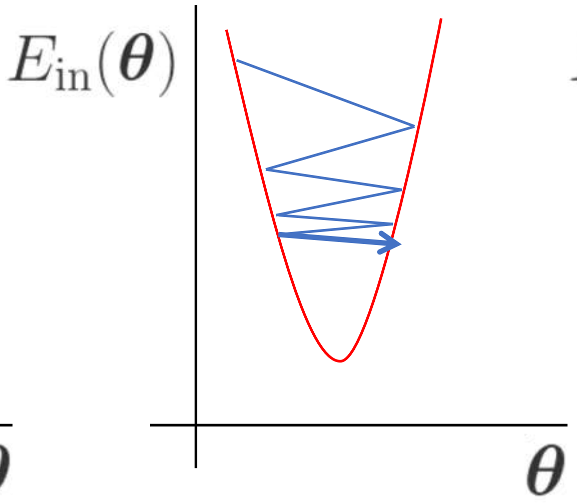

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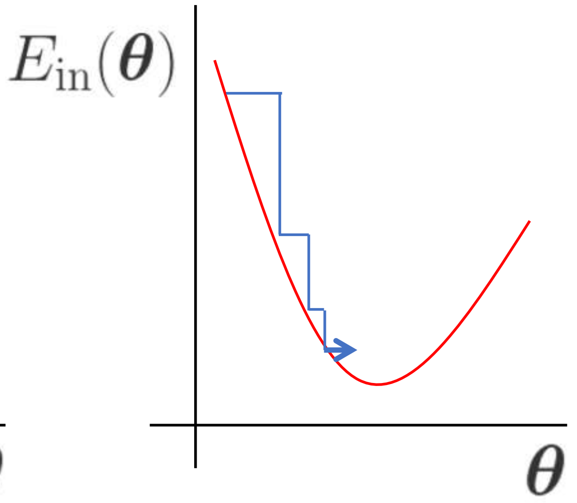

η variable

Rule of thumb

Dynamically change η proportionally to the gradient!

Gradient Descent: The Step η

Remember that at each iteration the update strategy is:

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

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

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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

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

Gradient Descent: The Step η

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Let's take:

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

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

Computing the Gradient of Cross-Entropy

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

chain rule of derivative

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

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3. Return the final vector of parameters **θ**(∞)

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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 $\theta(0)$
- In general, we may get to the local minimum nearest to $\theta(0)$

Gradient Descent: Non-Convex Objectives

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

Gradient Descent: Stopping Criterion

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

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

Gradient Descent: Stopping Criterion

- If the function is convex GD reaches the global minimum when $\nabla E_{in}(\boldsymbol{\theta}(t)) = 0$
- In general, we don't know if eventually the gradient gets to 0 therefore we can use several criteria of termination:
  - stop whenever the difference between two iterations is "small enough" $\rightarrow$ may converge "prematurely"
  - stop when the error equals to ε $\rightarrow$ 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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  - Better local approximation than first-order but each step requires computing the second derivative (Hessian matrix)

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  - Better local approximation than first-order but each step requires computing the second derivative (Hessian matrix)
- Stochastic Gradient Descent (SGD)
  - At each iteration, compute the gradient only from one sample (not the full dataset)
- Regularization
  - Include the L1- or L2-norm of the vector of parameters **θ** 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 $\rightarrow$ iterative Gradient Descent