Big Data Computing

Master's Degree in Computer Science 2022-2023

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Recap from Last Lectures

- We described linear regression as a powerful technique to predict realvalued 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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• 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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- We may encode the above values as a categorical response variable Y

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

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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 I if the outcome is > 0.5, 0 otherwise
- Still, it is preferable to use a classification method which works by design

LOGISTIC REGRESSION

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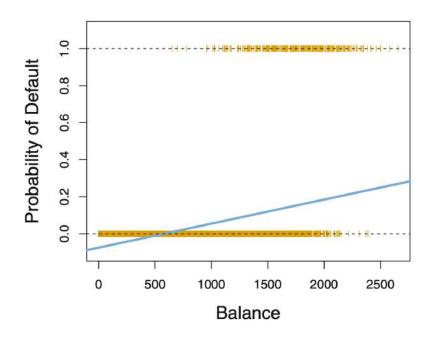
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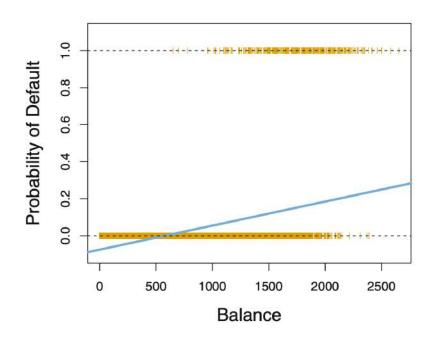
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Logistic Regression instead models the **probability** that Y belongs to one of the two possible outcome values



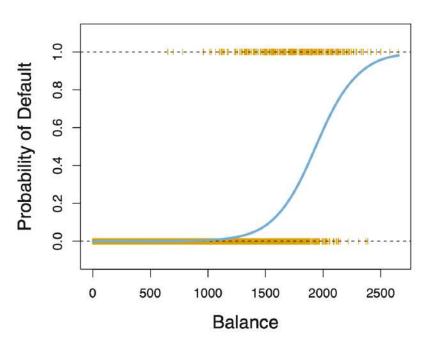
Predicted probability using linear regression (some estimated probabilities are negative!)

Linear Regression



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Linear Regression



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

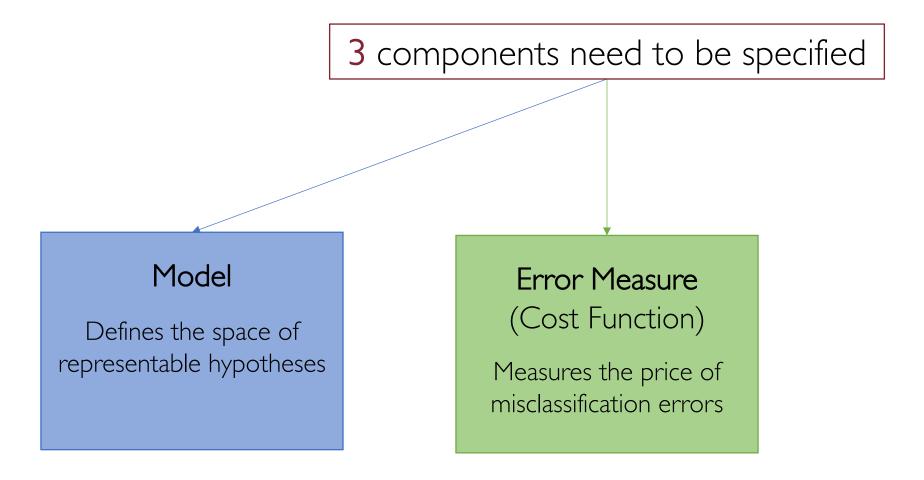
Logistic Regression

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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

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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- $f_{\theta}(x)$ is referred to as (linear) signal

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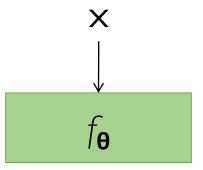
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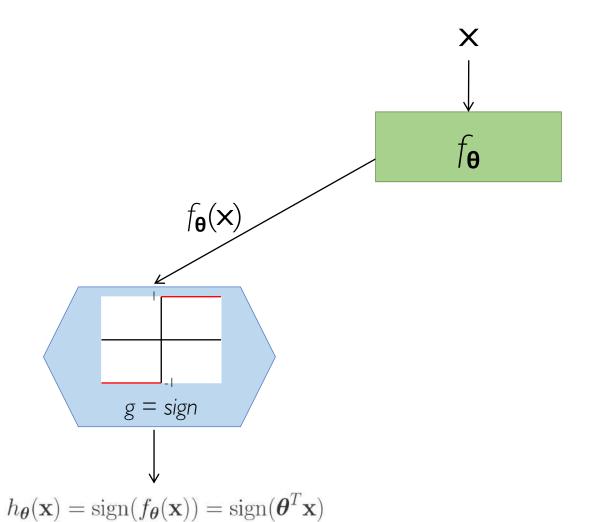
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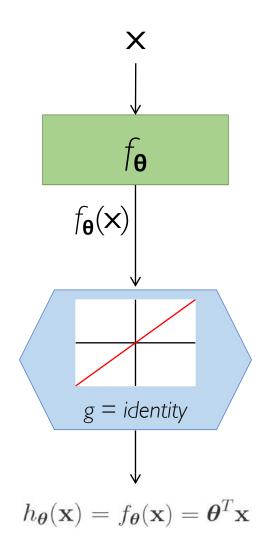
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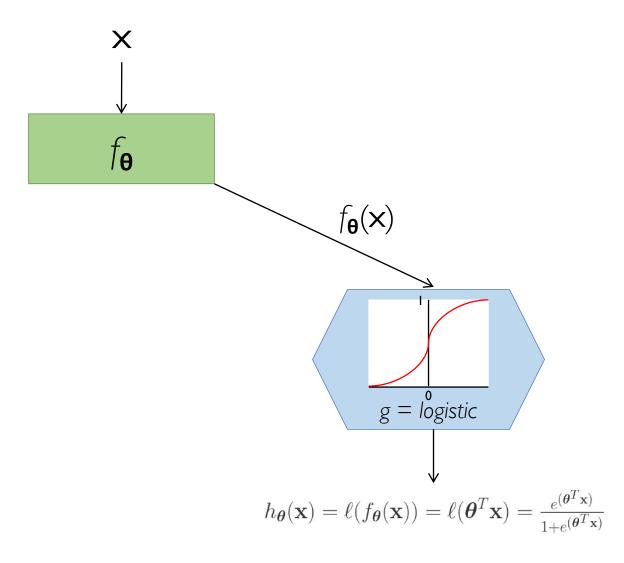
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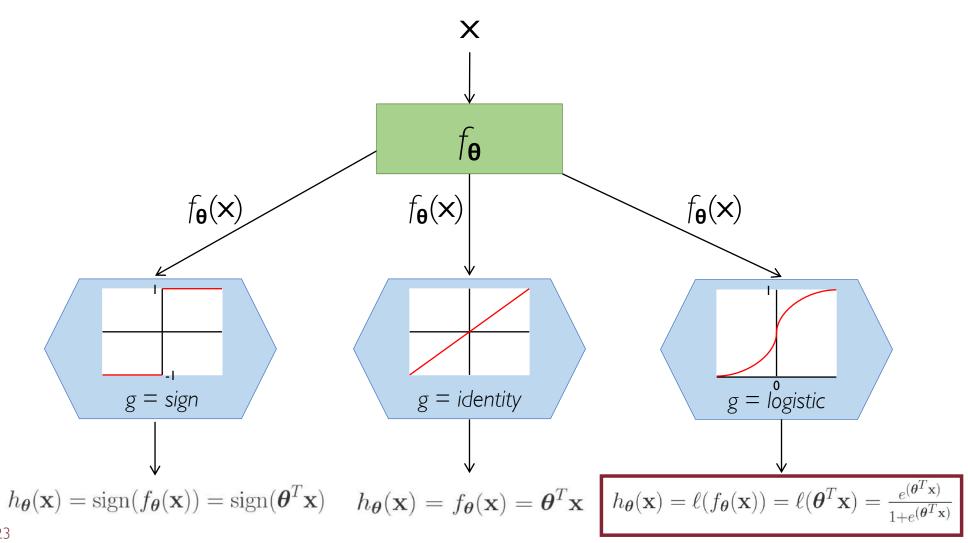
The set of possible hypotheses H changes depending on the parametric model (f_{θ}) and on the thresholding function (g)

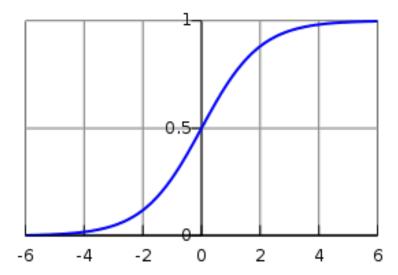




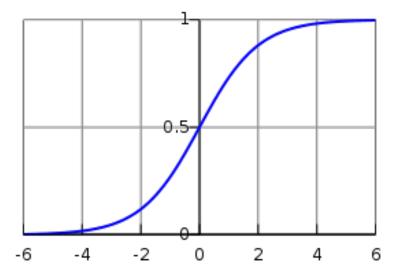






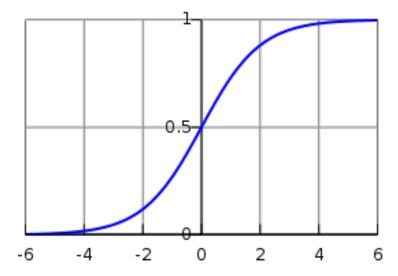


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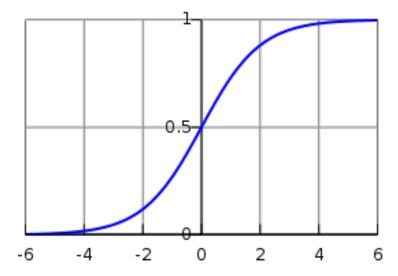
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- Output can be genuinely interpreted as a probability value

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- Other functions may have the same property [e.g., I/π arctan(x) + I/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

• Let p (resp., q = 1-p) be the probability of success (resp., failure) of an event

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- odds(success) = p/q = p/(1-p)
- 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)

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

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

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

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

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

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

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

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

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

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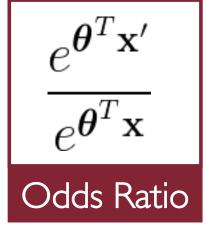
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The ratio of the odds for I-unit increase in x_i

or

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

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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), \dots, (\mathbf{x}_m, y_m)\}\$$

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

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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

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

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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 $h^*_{\theta}(\mathbf{x})$, which in turn is picked from the set of hypotheses defined by logistic function

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

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

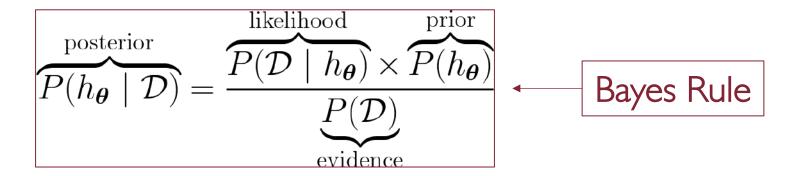
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- How do we estimate $h^*_{\theta}(\mathbf{x})$?
- We will use the same general framework introduced for the supervised learning problem!
- We already fixed the set of hypothesis function to select from
- We still need:
 - A training set D
 - An error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

COST FUNCTION

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



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

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

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

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Maximum Likelihood Estimate (MLE)

Frequentist approach

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MLE returns the set of parameters that maximize the likelihood

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

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MAP returns the set of parameters that maximize the posterior

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

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



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 $h^*_{\theta}(\mathbf{x})$ approximates the true noisy target ϕ

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

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

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

$$h_{\pmb{\theta}}^* = \operatorname{argmax}_{h_{\pmb{\theta}} \in \mathcal{H}} \ P(\ \mathcal{D}\ | h_{\pmb{\theta}})$$

The Likelihood Function

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

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

where ϕ has been replaced with our hypothesis

The Likelihood Function

If we assume the hypothesis is the logistic function

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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:

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

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The Likelihood Function

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

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)\}\$$

The overall likelihood function is computed as:

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

Why Does Likelihood Make Sense?

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

| | $\mathbf{\theta}^{T} \mathbf{x}_{i} > 0$ | $\mathbf{\theta}^{T} \mathbf{x}_{i} < 0$ |
|--------------------|--|--|
| $y_i > 0$ | ≈ | ≈ 0 |
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If the label is disoncordant with the signal then $\ell(y_i\theta^Tx_i)$ approaches to 0

prediction disagrees with the true label

Maximum Likelihood Estimate (MLE)

Find the vector of parameters **0** such that the likelihood function is maximum

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

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

$$\operatorname{argmax}_{m{ heta}} \Bigg(\prod_{i=1}^m \ell(y_i m{ heta}^T \mathbf{x_i}) \Bigg)$$

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

$$\mathrm{argmax}_{\boldsymbol{\theta}} \bigg(\frac{1}{m} \ln \Big(\prod_{i=1}^m \ell(y_i \boldsymbol{\theta}^T \mathbf{x_i}) \Big) \bigg)$$

$$\begin{split} \operatorname{argmax}_{\pmb{\theta}} \bigg(\prod_{i=1}^m \ell(y_i \pmb{\theta}^T \mathbf{x_i}) \bigg) & \operatorname{argmax}_{\pmb{\theta}} \bigg(\frac{1}{m} \ln \Big(\prod_{i=1}^m \ell(y_i \pmb{\theta}^T \mathbf{x_i}) \Big) \bigg) \\ \operatorname{argmax}_{\pmb{\theta}} \bigg(\frac{1}{m} \ln \Big(\prod_{i=1}^m \ell(y_i \pmb{\theta}^T \mathbf{x_i}) \Big) \bigg) &= \operatorname{argmin}_{\pmb{\theta}} \bigg(-\frac{1}{m} \ln \Big(\prod_{i=1}^m \ell(y_i \pmb{\theta}^T \mathbf{x_i}) \Big) \bigg) \end{split}$$

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$$\begin{aligned} \operatorname{argmax}_{\boldsymbol{\theta}} \left(\prod_{i=1}^{m} \ell(y_{i} \boldsymbol{\theta}^{T} \mathbf{x_{i}}) \right) & \operatorname{argmax}_{\boldsymbol{\theta}} \left(\frac{1}{m} \ln \left(\prod_{i=1}^{m} \ell(y_{i} \boldsymbol{\theta}^{T} \mathbf{x_{i}}) \right) \right) \\ \operatorname{argmax}_{\boldsymbol{\theta}} \left(\frac{1}{m} \ln \left(\prod_{i=1}^{m} \ell(y_{i} \boldsymbol{\theta}^{T} \mathbf{x_{i}}) \right) \right) &= \operatorname{argmin}_{\boldsymbol{\theta}} \left(-\frac{1}{m} \ln \left(\ell(y_{1} \boldsymbol{\theta}^{T} \mathbf{x_{i}}) \right) - \dots - \frac{1}{m} \ln \left(\ell(y_{m} \boldsymbol{\theta}^{T} \mathbf{x_{m}}) \right) \right) \\ \operatorname{as}_{k} \ln(a \cdot b) &= k \left(\ln(a) + \ln(b) \right) = k \ln(a) + k \ln(b) \\ &= \operatorname{argmin}_{\boldsymbol{\theta}} \left(\frac{1}{m} \sum_{i=1}^{m} - \ln(\ell(y_{i} \boldsymbol{\theta}^{T} \mathbf{x_{i}})) \right) \\ &= \operatorname{argmin}_{\boldsymbol{\theta}} \left(\frac{1}{m} \sum_{i=1}^{m} \ln \left(\frac{1}{\ell(y_{i} \boldsymbol{\theta}^{T} \mathbf{x_{i}})} \right) \right) \end{aligned}$$

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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:

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

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

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

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

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

$$f_Y(y \mid p) = f_Y(Y = y \mid p) = \begin{cases} p & \text{if } y = 1 \\ q = 1 - p & \text{if } y = -1 \end{cases}$$

Probability mass function of a Bernoullidistributed random variable with **known** parameter *p*

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Probability mass function of a Bernoullidistributed random variable with **known** parameter *p* We plug in a value y for Y and f_Y tells us the **probability** of observing that value **given** the parameter p

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

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

$$\mathcal{L}_{Y}(p \mid y) = f_{Y}(y \mid p) = f_{Y}(Y = y \mid p) = \begin{cases} p & \text{if } y = 1 \\ q = 1 - p & \text{if } y = -1 \end{cases}$$

Likelihood of an observed Bernoullidistributed random variable Y = ywhen the parameter p is **unknown**

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Likelihood of an observed Bernoullidistributed random variable Y = ywhen the parameter p is **unknown** We plug in a value p for the parameter of the distribution and f_Y tells us the **likelihood** of the observed Y = y

The likelihood function does not specify the probability that p is the truth, given the observed sample Y = y

Likelihood Function

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

$$\mathcal{L}_Y(p \mid y_1, \dots, y_m) = \prod_{i=1}^{n} p^{y_i} (1-p)^{1-y_i}$$

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

$$\mathcal{L}_Y(p \mid y_1, \dots, y_m) = \prod_{i=1}^{n} p^{y_i} (1-p)^{1-y_i}$$

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

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

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

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

Substituting p

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

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

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

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

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

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

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

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

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

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

$$y = -1$$

$$y = 0$$

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

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

$$y = 1$$

$$y = 1$$

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

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- We need a more sophisticated learning algorithm!

