UNIVERSITÄT
ZU KÖLN

Machine Learning: Logistic Regression

VL Sprachliche Informationsverarbeitung

Nils Reiter
nils.reiter@uni-koeln.de

December 5, 2024
Winter term 2024/25

INSTITUT FÜR
DIGITAL HUMANITIES
UNIVERSITÄT ZU KÖLN

Recap: Machine Learning so Far

- Naive Bayes
  - "Classical machine learning"
  - Binary classification method
  - Manually defined features (e.g., some tokens appearing in an e-mail)
- Evaluation
  - Accuracy, precision, recall, F-score
  - Baseline

Section 1

Linear/Logistic Regression

Regression

- Regression
  - Prediction of numeric values (e.g., future COVID-19 cases; number of nouns in a text, ...)
  - Based on some input features (e.g., "R-Wert", number of past cases, ...)

Regression

- Regression
  - Prediction of numeric values (e.g., future COVID-19 cases; number of nouns in a text, ...)
  - Based on some input features (e.g., "R-Wert", number of past cases, ...)
- Linear
  - The relation between input features and output values is linear
  - Math: $y = a_1x_1 + a_2x_2 + \cdots + a_nx_n + b$

Regression

- Regression
  - Prediction of numeric values (e.g., future COVID-19 cases; number of nouns in a text, …)
  - Based on some input features (e.g., "R-Wert", number of past cases, …)
- Linear
  - The relation between input features and output values is linear
  - Math: $y = a_1x_1 + a_2x_2 + \cdots + a_nx_n + b$
- Logistic
  - Relation between input and output follows a logistic equation σ:
    - $0 \leq \sigma(x) \leq 1$, for all values of x
    - They can be interpreted as probabilities

Linear Regression

Example

- Input: Number of words in a (narrative, prose) text
- Output: Number of literary characters in the text
  (in the sense of “Figur”, not in the sense of “Zeichen”)

Linear Regression

Example

- Input: Number of words in a (narrative, prose) text
- Output: Number of literary characters in the text
  (in the sense of "Figur", not in the sense of "Zeichen")
- Linear equation (with one input variable): $y = ax + b$
  - With x being the number of tokens and y the number of characters

Linear Regression

The data set

x (# pages)	y (# characters)
10	3
105	5
150	8
210	12
250	7
295	13

Linear Regression

The data set

x (# pages)	y (# characters)
10	3
105	5
150	8
210	12
250	7
295	13

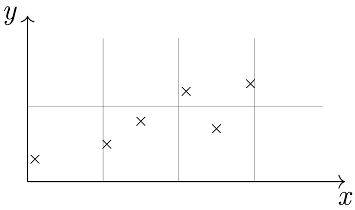


Figure: Data set, each $\times$ represents a text (x: text length, y: num. of characters)

Linear Regression

The data set

x (# pages)	y (# characters)
10	3
105	5
150	8
210	12
250	7
295	13

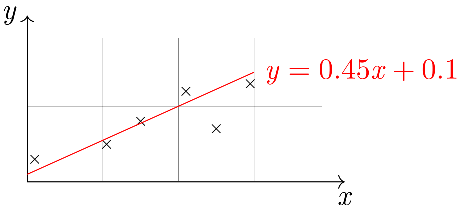
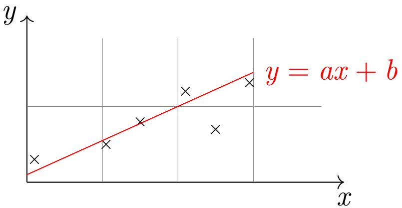


Figure: Data set, each $\times$ represents a text (x: text length, y: num. of characters)

Linear Regression

The Task



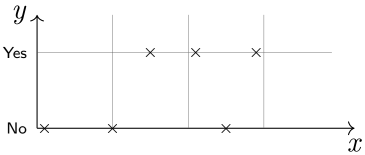
The Model

- Linear regression with one variable (= univariate linear regression)
- Prediction (hypothesis function): $y = h_{a,b}(x) = ax + b$
- How to set parameters a and b? ➔training algorithm

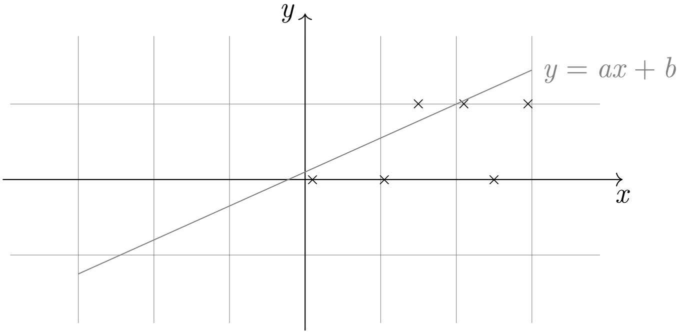
From Regression to Classification

- Example task: Given the number of words in an e-mail, is it spam?

x (# words)	y (# spam)
10	No
100	No
150	Yes
210	Yes
250	No
290	Yes

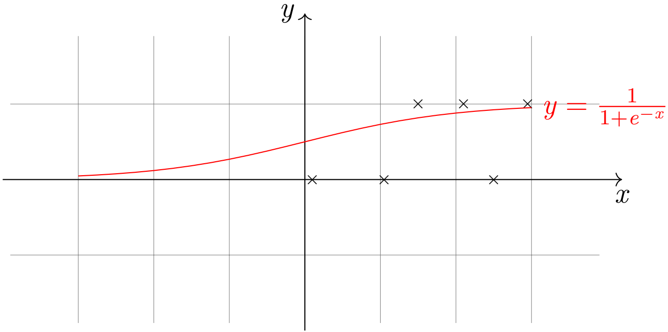


Fitting an Equation



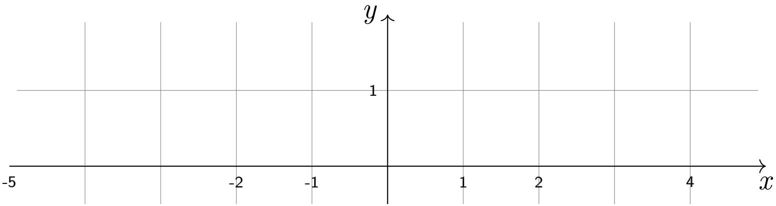
linear equation

Fitting an Equation



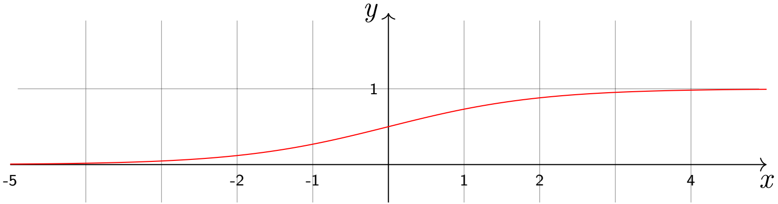
logistic function

The Logistic Function



$$y = \frac{1}{1+e^{-(ax+b)}} \qquad \text{(general form)}$$

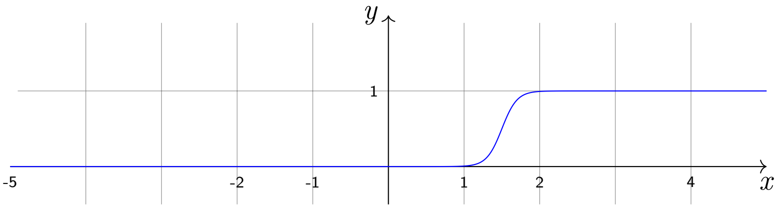
The Logistic Function



$y = \frac{1}{1+e^{-(ax+b)}}$ (general form)

$y = \frac{1}{1+e^{-(1*x+0)}}$

The Logistic Function

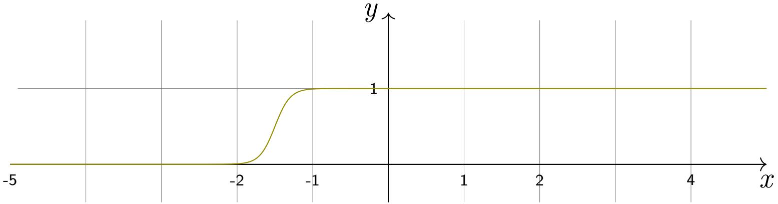


$$y = \frac{1}{1+e^{-(ax+b)}} \qquad \text{(general form)}$$

$$y = \frac{1}{1+e^{-(1*x+0)}}$$

$$y = \frac{1}{1+e^{-(10*x-15)}}$$

The Logistic Function



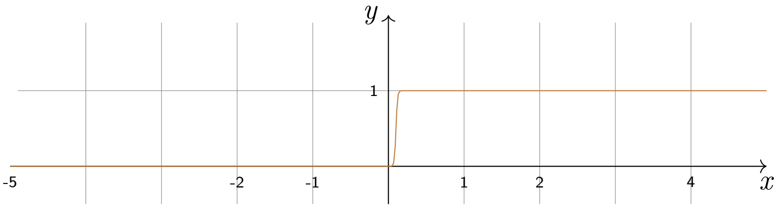
$$y = \frac{1}{1+e^{-(ax+b)}} \qquad \text{(general form)}$$

$$y = \frac{1}{1+e^{-(1*x+0)}}$$

$$y = \frac{1}{1+e^{-(10*x-15)}}$$

$$y = \frac{1}{1+e^{-(10*x+15)}}$$

The Logistic Function



$$y = \frac{1}{1+e^{-(ax+b)}}$$ (general form)

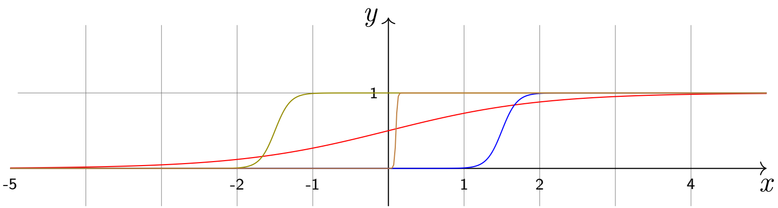
$$y = \frac{1}{1+e^{-(1*x+0)}}$$

$$y = \frac{1}{1+e^{-(10*x-15)}}$$

$$y = \frac{1}{1+e^{-(10*x+15)}}$$

$$y = \frac{1}{1+e^{-(100*x-10)}}$$

The Logistic Function



$$y = \frac{1}{1+e^{-(ax+b)}} \qquad \text{(general form)}$$

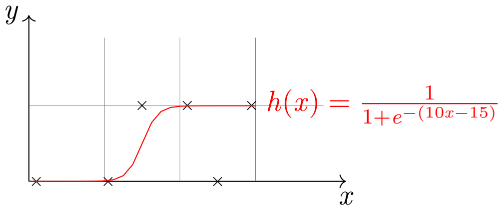
$$y = \frac{1}{1+e^{-(1*x+0)}}$$

$$y = \frac{1}{1+e^{-(10*x-15)}}$$

$$y = \frac{1}{1+e^{-(10*x+15)}}$$

$$y = \frac{1}{1+e^{-(100*x-10)}}$$

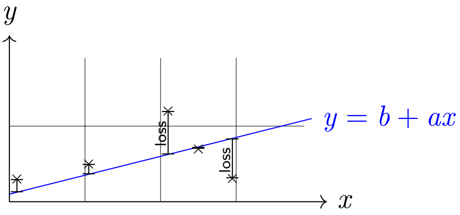
Parameter Fitting

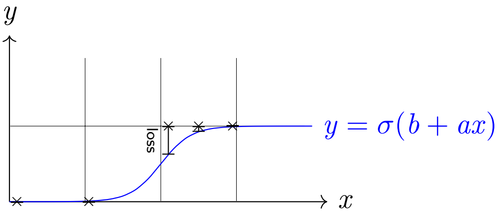


- Linear equations can be wrapped in a logistic one
  - $\sigma(x) = \frac{1}{1+e^{-x}} \quad \rightarrow \quad y = \sigma(ax + b)$
- Same parameters to be tuned (a and b)
- $e = \sum_{n=0}^{\infty} \frac{1}{n!} = 2.71828$ (Euler's number)

Summary: Linear/Logistic Regression

(With a single variable)





- Logistic/linear regression is half of the math of deep learning

- Remaining question: How to learn parameters a and b?

Generalization to More Parameters

- Example: Classify Spam/Not Spam based on number of words from keyword list (e.g., "profit")
- Features: $x_1, x_2, x_3, \ldots$
- Logistic regression model: $y = \sigma(w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3)$
  - I.e., one w parameter for each feature, and an additional constant w_0
- Parameter vector: $\vec{w} = \langle w_0, w_1, w_2, \ldots \rangle$
- Input vector: $\vec{x} = \langle x_1, x_2, x_3, \ldots \rangle$

Section 2

Practice

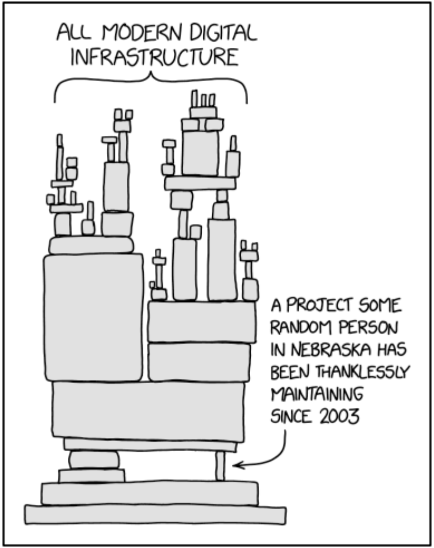


Figure: XKCD 2347

Doing Logistic Regression in Practice

- Many implementations in for many programming languages
- Python scikit-learn
- General structure (convention)
  - Data loading
    - Typical variable names: `x_train`, `y_train`, `x_test`, `y_test`
  - Preprocessing
  - Model initialisation (or loading if its pre-trained)
  - Model training (function often called `fit()`)
  - Model evaluation

demo

Hausaufgabe 4 (bis 19.12.)

Trainieren Sie ein logistisches Regressionsmodell, um handgeschriebene Ziffern zu erkennen. Die Ziffern wurden handgeschrieben, schwarz/weiß eingescannt und die Bilder dann als 28x28-Matritzen mit Graustufeninformationen bereitgestellt. Es handelt sich nur um Nullen und Einsen, und ist damit eine binäre Klassifikationsaufgabe. Sie finden die Trainings- und Testdaten hier, und hier ein Python-Skript, mit einer Funktion zum Einlesen der Daten. Verwenden Sie die Bibliothek scikit-learn für das eigentliche Training (und schauen Sie sich ruhig ein bisschen um, was die Bibliothek sonst so bereithält).

Section 3

Gradient Descent

Learning Regression Models

- How to select the parameters w_0, w_1 such that the hypothesis function describes the data points as best as possible?
- Learning algorithm *Gradient Descent*

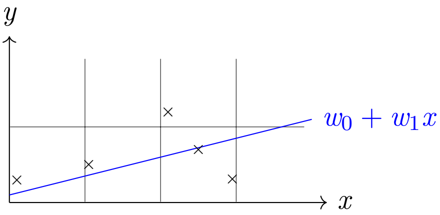
Learning Regression Models

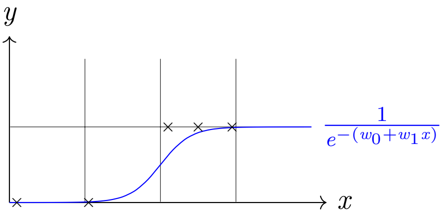
- How to select the parameters w_0, w_1 such that the hypothesis function describes the data points as best as possible?
- Learning algorithm *Gradient Descent*

Gradient descent is half of the algorithms of deep learning

Loss: Intuition

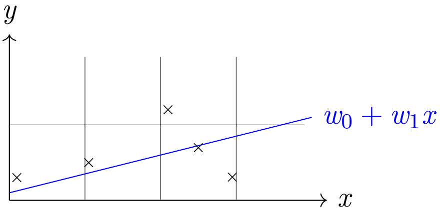
The *loss* measures the ‘wrongness’ of values for w_0 and w_1

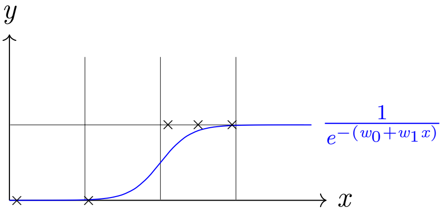




Loss: Intuition

The *loss* measures the 'wrongness' of values for w_0 and w_1

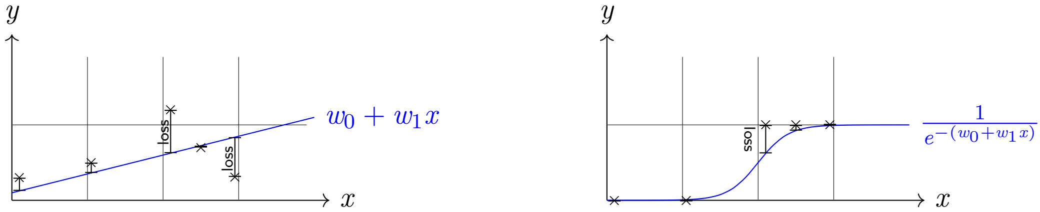




- How big is the gap between a hypothesis (= the) and the data?
- Is $\vec{w} = \langle 0.3, 0.5 \rangle$ or $\vec{w} = \langle 0.4, 0.4 \rangle$ better?

Loss: Intuition

The *loss* measures the ‘wrongness’ of values for w_0 and w_1

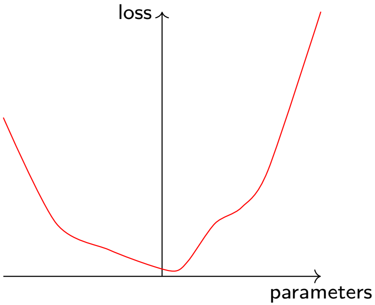


- How big is the gap between a hypothesis (= the) and the data?
- Is $\vec{w} = \langle 0.3, 0.5 \rangle$ or $\vec{w} = \langle 0.4, 0.4 \rangle$ better?

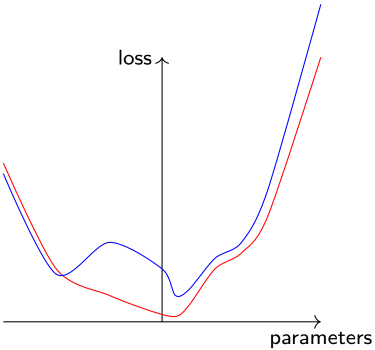
Gradient Descent: Intuition

- Loss should be as small as possible
- Total loss can be calculated for given parameters $\vec{w} = (w_0, w_1)$ (and with respect to a data set!)
- Idea:
    - Make many iterations
    - In each iteration, change $\vec{w}$ towards to make the loss smaller
    - We use the derivative of the loss function to know how $\vec{w}$ needs to be changed

Loss function: Intuition



Loss function: Intuition



Function should be convex!
If not, we might get stuck in local minimum

Loss Function with More Parameters

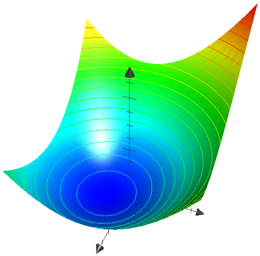


Figure: The loss function in our setting visualised

- Searching for the a, b settings with minimal loss
- $=$ Searching for the minimum!

Hypothesis vs. Loss Function

Hypothesis function h

- Calculates outcome for a single instance based on
  - Feature values $\vec{x}$
  - Parameter values $\vec{w}$

Loss function J

- Calculates 'wrongness' of h based on
  - Parameter values $\vec{w}$
  - A data set consisting of many instances with
    - Feature values $\vec{x}$
    - Correct outcomes Y

Loss Function

Definition

Loss function depends on hypothesis function

Linear hypothesis function

- $h(x) = w_0 + w_1 x_1$
- Loss: Mean squared error

Loss Function

Definition

Loss function depends on hypothesis function

Linear hypothesis function

- $h(x) = w_0 + w_1 x_1$
- Loss: Mean squared error

Logistic hypothesis function

- $h(x) = \sigma(w_0 + w_1 x_1) = \frac{1}{e^{-(w_0 + w_1 x_1)}}$
- Loss: (Binary) cross-entropy loss

Loss Function

Definition for Linear Regression

- The loss function is a function on parameter values a and b (for a given hypothesis function and data set)
  - Hypothesis function: $h_{\vec{w}} = w_1 x + w_0$

$\vec{w} = (w_0, w_1)$: parameters $h_{\vec{w}}$: hypothesis function m: number of items

$$J(\vec{w}) =$$

Loss Function

Definition for Linear Regression

- The loss function is a function on parameter values a and b
  (for a given hypothesis function and data set)
  - Hypothesis function: $h_{\vec{w}} = w_1 x + w_0$

$\vec{w} = (w_0, w_1)$: parameters $h_{\vec{w}}$: hypothesis function m: number of items

$$J(\vec{w}) = \qquad h_{\vec{w}}(x_i) - y_i$$

- Calculate the loss for item i

Loss Function

Definition for Linear Regression

- The loss function is a function on parameter values a and b (for a given hypothesis function and data set)
  - Hypothesis function: $h_{\vec{w}} = w_1 x + w_0$

$\vec{w} = (w_0, w_1)$: parameters $h_{\vec{w}}$: hypothesis function m: number of items

$$J(\vec{w}) = \qquad (h_{\vec{w}}(x_i) - y_i)^2$$

- Calculate the loss for item i
- Square the error

Loss Function

Definition for Linear Regression

- The loss function is a function on parameter values a and b
  (for a given hypothesis function and data set)
  - Hypothesis function: $h_{\vec{w}} = w_1 x + w_0$

$\vec{w} = (w_0, w_1)$: parameters $h_{\vec{w}}$: hypothesis function m: number of items

$$J(\vec{w}) = \sum_{i=1}^{m} (h_{\vec{w}}(x_i) - y_i)^2$$

- Calculate the loss for item i
- Square the error
- Sum them up

Loss Function

Definition for Linear Regression

- The loss function is a function on parameter values a and b
  (for a given hypothesis function and data set)
  - Hypothesis function: $h_{\vec{w}} = w_1 x + w_0$

$\vec{w} = (w_0, w_1)$: parameters $h_{\vec{w}}$: hypothesis function m: number of items

$$J(\vec{w}) = \frac{1}{m} \sum_{i=1}^{m} (h_{\vec{w}}(x_i) - y_i)^2$$

- Calculate the loss for item i
- Square the error
- Sum them up
- Divide by the number of items
  - Known as: *Mean squared error*

Loss Function

Definition for Linear Regression

- The loss function is a function on parameter values a and b
  (for a given hypothesis function and data set)
  - Hypothesis function: $h_{\vec{w}} = w_1 x + w_0$

$\vec{w} = (w_0, w_1)$: parameters $h_{\vec{w}}$: hypothesis function m: number of items

$$J(\vec{w}) = \frac{1}{2} \frac{1}{m} \sum_{i=1}^{m} (h_{\vec{w}}(x_i) - y_i)^2$$

- Calculate the loss for item i
- Square the error
- Sum them up
- Divide by the number of items
  - Known as: *Mean squared error*
- Divide by two
  - out of convenience, because derivation

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

$$J(\vec{w}) = \qquad h_{\vec{w}}(x_i) + \qquad (1 - h_{\vec{w}}(x_i))$$

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

$$J(\vec{w}) = \qquad \log h_{\vec{w}}(x_i) + \qquad \log\left(1 - h_{\vec{w}}(x_i)\right)$$

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

$$J(\vec{w}) = \qquad y_i \log h_{\vec{w}}(x_i) + (1 - y_i) \log (1 - h_{\vec{w}}(x_i))$$

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
    - I.e., for each instance, one of the summands is 0

$$J(\vec{w}) = -\frac{1}{m}\sum_{i=0}^{m} y_i \log h_{\vec{w}}(x_i) + (1 - y_i)\log\left(1 - h_{\vec{w}}(x_i)\right)$$

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

$$J(\vec{w}) = -\frac{1}{m}\sum_{i=0}^{m} \underbrace{y_i \log h_{\vec{w}}(x_i)}_{0 \text{ iff } y_i=0} + \underbrace{(1-y_i)\log(1-h_{\vec{w}}(x_i))}_{0 \text{ iff } y_i=1}$$

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

y_i	$h_{\vec{w}}(x_i) + \epsilon$	$y_i \log h_{\vec{w}}(x_i) + (1 - y_i) \log(1 - h_{\vec{w}}(x_i))$
0	1.0000001	-23.2535
0	0	0

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

y_i	$h_{\vec{w}}(x_i) + \epsilon$	$y_i \log h_{\vec{w}}(x_i) + (1 - y_i) \log(1 - h_{\vec{w}}(x_i))$
0	1.0000001	−23.2535
0	0	0
1	1	0
1	0.0000001	−23.2535

Loss function

Definition for Logistic Regression

- Two cases: $y_i = 0$ or $y_i = 1$ – y_i: real outcome for instance i
  - I.e., for each instance, one of the summands is 0

y_i	$h_{\vec{w}}(x_i) + \epsilon$	$y_i \log h_{\vec{w}}(x_i) + (1 - y_i) \log(1 - h_{\vec{w}}(x_i))$
0	1.0000001	-23.2535
0	0	0
1	1	0
1	0.0000001	-23.2535
1	0.8	-0.3219281
1	0.2	-2.321928

Caveat: $\log 0$ is undefined – add $\epsilon = 0.0000001$ if needed

Misunderstandings about Loss

- Loss values are not an evaluation measure
- It is meaningless to report loss values in the same way as accuracy or precision

Misunderstandings about Loss

- Loss values are not an evaluation measure
- It is meaningless to report loss values in the same way as accuracy or precision
- Because it's not scaled
- When used to compare, scale not important

Misunderstandings about Loss

- Loss values are not an evaluation measure
- It is meaningless to report loss values in the same way as accuracy or precision
- Because it's not scaled
- When used to compare, scale not important

Example

x	y
10	3
105	5
150	8
210	12
250	7
295	13

Table: Lower Loss Value

x	y
10	30
105	50
150	80
210	120
250	70
295	130

Table: Higher Loss Value

Summary

Regression

- Fitting parameters to a data distribution
  - Linear R: Numeric prediction algorithm
    - Prediction model: $h_{\vec{w}}(x) = w_0 + w_1 x$
  - Logistic R: Classification algorithm (because we interpret results as probabilities)
    - Prediction model: $h_{\vec{w}}(x) = \frac{1}{e^{-(w_0 + w_1 x)}}$
- Learning algorithm: Gradient descent

Gradient Descent

- Initialise $\vec{w}$ with random values (e.g., 0)
- Repeat:
  - Find the direction to the minimum by taking the derivative
  - Change $\vec{w}$ accordingly, using a learning rate η
  - Stop when $\vec{w}$ don't change anymore

References I