NUS | Computing
National University of Singapore

CS4248: Natural Language Processing

Lecture 5 — Introduction into Connectionist Machine Learning

Announcements

- Project
  - Project teams announced (check your team and update us per our announcement if you see anything amiss)
  - Project's Intermediate Update Rubric / Template is available
    (Find in "Canvas > Files > Project" or live version (best bet) at https://bit.ly/cs4248-2320-iu-template)
- Assignment
  - A2: Text Classification competition, restricted to ML algorithms taught (Naive Bayes and Logistic Regression)
  - Emphasis on Natural Language Feature Engineering
- Questions, help, and communications
  - The Teaching Team is here to help but we cannot do the assessment for you
  - Please acknowledge that TA cannot answer every question about assignments and the project
    (of you really think there is a problem with the communications, you can always send us (Min/Chris) an email)
  - If an email or Canvas post does not get replied to in 2-3 days, you are welcome to follow up

Outline

- **Generative vs. Discriminative Classifiers**

- Logistic Regression
  - Setup as Probabilistic Classifier
  - Cross-Entropy Loss Function
  - Gradient Descent
  - Overfitting & Regularization
  - Multiclass Logistic Regression

- Towards Neural Networks
  - Motivation: XOR Problem
  - Basic Neural Network Architecture

Text Classification (well, for classification, in general)

- Formal setup
  - X — set of all documents; $x \in X$ — a single document
  - Y — set of all classes (or class labels); $y \in Y$ — a single class (or class label)
  - Mapping h from input space X to output space Y ➜ $h : X \to Y$

➜ Find best $\hat{h}$ to approximate the true mapping h

We find $\hat{h}$ by <u>learning</u> $\hat{h}$ from the data
➜ **Supervised (Machine) Learning**

- Probabilistic Classifiers (e.g., Naive Bayes)

Instead of $\hat{h} : X \to Y$, learn $\hat{P}(Y|X)$ (or $\hat{P}(y|x)$ for an $\langle x, y \rangle$ pair)

Text Classification — Probabilistic Classifiers

- Common goal: Learn $P(y|x)$
  - Learn $P(y|x)$ from the data

- Two basic approaches

(1) Generative Classifiers

- Learn joint probability $P(x, y)$
- Apply Bayes Rule to get $P(y|x)$

$$\rightarrow \hat{y} = \underset{y \in Y}{\operatorname{argmax}} \overbrace{P(x|y)P(y)}^{= P(x,y) \propto P(y|x)}$$

(2) Discriminative Classifiers

- Learn $P(y|x)$ directly

$$\rightarrow \hat{y} = \underset{y \in Y}{\operatorname{argmax}} P(y|x)$$

Generative vs. Discriminative Classifiers — Intuition

- Task: Train a classifier to distinguish zebra from elephants images

Source: Wiki Common (CC BY-SA 4.0): zebra, elephant

Generative vs. Discriminative Classifiers — Intuition

- Generative classifier
  - Builds 2 models what zebra and elephant images look like

Feature x_i	P(x_i, zebra)	P(x_i, elephant)
"is grey"	0.32	0.95
"is striped"	0.99	0.08
"long nose"	0.40	0.98
"four legs"	0.88	0.99
…	…	…

  - Models allow to assign a "zebra probability" and an "elephant probability" to any image (using Bayes Rule)
  - Givan a new image: Run both models and see which fits better

Generative vs. Discriminative Classifiers — Intuition

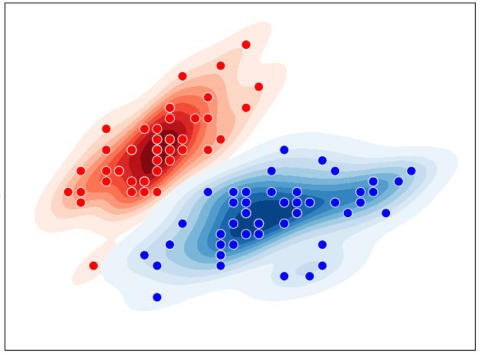
- Discriminative classifier
  - Tries to distinguish zebra and elephant images
  - Does not model how zebra and elephant images "look like"

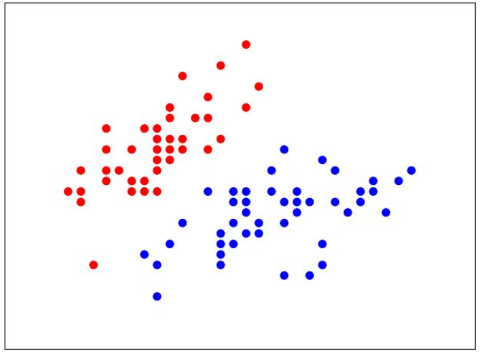
Question: How could we quickly distinguish zebras from elephants?

Generative vs. Discriminative Classifiers

Generative classifier

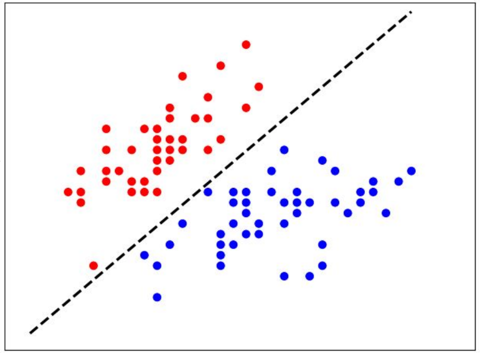
- Learn data distribution of each class
- Classifies new data item by comparing the item with each class distribution





Discriminative classifier

- Learn the decision boundaries between classes
- Classifies new data item based on in which "region" the new item falls



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Linear Models

- Underlying assumption:
  - There exists linear relationship between $x^{(j)}$ and dependent variable $y^{(j)}$

$$\hat{y}^{(j)} = h_\theta\left(x^{(j)}\right) = f\left(b + \theta_1 x_1^{(j)} + \theta_2 x_2^{(j)} + \cdots + \theta_n x_n^{(j)}\right)$$

$$= f\left(\left[\sum_{i=1}^{n} \theta_i x_i^{(j)}\right] + b\right)$$

Predicted value which is hopefully close to $y^{(j)}$

$$\theta = \underbrace{\{b, \theta_1, \theta_2, \ldots, \theta_n\}}, \; b \in \mathbb{R}, \; \theta_i \in \mathbb{R}$$

These are the parameters we need to learn
➜ Learning = finding the "right" parameter values

Linear Models — More User-Friendly Notation

- Vector representation
  - **Bias Trick:** Introduce constant feature $x_0^{(j)}$

$$h_\theta\left(x^{(j)}\right) = f\left(\theta_0 \underbrace{x_0^{(j)}}_{=1} + \theta_1 x_1^{(j)} + \theta_2 x_2^{(j)} + \cdots + \theta_n x_n^{(j)}\right)$$

  - Represent $x^{(j)}$ with new constant feature

$$x^{(j)} = \left(1, x_1^{(j)}, x_2^{(j)}, \ldots, x_n^{(j)}\right)$$

  - Rewrite linear relationship using vectors representing $x^{(j)}$ and θ

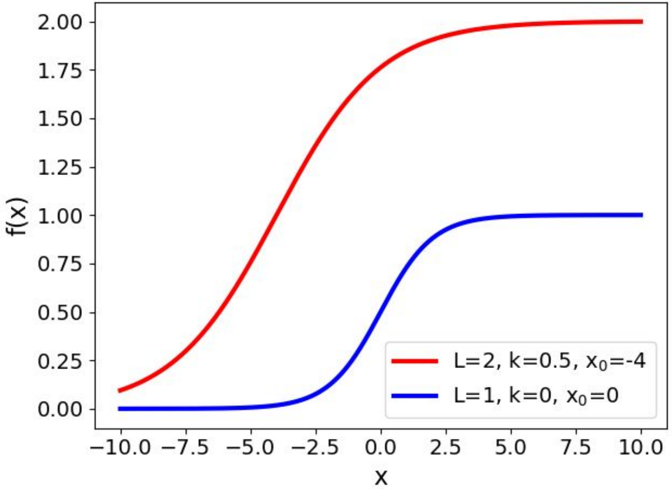
$$h\left(x^{(j)}\right) = f\left(\theta^T x^{(j)}\right) \qquad \theta = \{\theta_0, \theta_1, \theta_2, \ldots, \theta_n\},\ \theta_i \in \mathbb{R}$$

Note: Throughout the rest of the slide, we drop to superscript in $x^{(j)}$ and $y^{(j)}$ if there is no ambiguity.

Logistic Regression

- Logistic Regression ➜ Real-valued predictions interpreted as probability
  - Function *f* is the standard **Logistic Function** (Sigmoid function)

$$f(x) = \frac{L}{1 + e^{-k(x - x_0)}} \xrightarrow{L=1,\ k=1,\ x_0=0} f(x) = \frac{1}{1 + e^{-x}}$$



Logistic Regression — Probabilistic Interpretation

- $\hat{y}$ interpreted as a probability

$$\hat{y} = h_\theta(x) = f(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}} \qquad \text{with} \quad \hat{y} \in [0, 1]$$

➜ $\hat{y} = h_\theta(x)$ is the estimated probability that $y = 1$ given x and θ

$$\hat{y} = P(y = 1 | x, \theta)$$

➜ Given only discrete 2 outcomes: $P(y = 1 | x, \theta) + P(y = 0 | x, \theta) = 1$

$$\hat{y} = 1 - P(y = 0 | x, \theta)$$

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Logistic Regression — Runthrough (Part 1)

- Sentiment Analysis for movie reviews

"It's hokey. There are no surprises, the writing is poor. So why was it so enjoyable? For one thing, the cast is great. Another nice touch is the music. I was overcome with the urge to get off the couch and start dancing. It sucked me in, and it'll do the same to you."

Feature	Description	Value
x_1	Number of positive words	
x_2	Number of negative words	
x_3	1 if "no" in text; 0 otherwise	
x_4	Number of 1st & 2nd person pronouns	
x_5	1 if "!" in text; 0 otherwise	
x_6	*ln* of word/token count	

Side notes:

- Naive Bayes and Logistic Regression require feature engineering as they do not combine primitive features into composite ones.
- The 6 features on the left are chosen for simplicity; in practice these can be the tf-idf weights

Logistic Regression — Runthrough (Part 1)

- Step 1: Extract feature values

"It's hokey. There are no surprises, the writing is poor. So why was it so enjoyable? For one thing, the cast is great. Another nice touch is the music. I was overcome with the urge to get off the couch and start dancing. It sucked me in, and it'll do the same to you."

Feature	Description	Value
x_1	Number of positive words	3
x_2	Number of negative words	2
x_3	1 if "no" in text; 0 otherwise	1
x_4	Number of 1st & 2nd person pronouns	3
x_5	1 if "!" in text; 0 otherwise	0
x_6	*ln* of word/token count	ln(66) = 4.19

In-Lecture Activity (5 mins)

- Question: What might be other useful features for a sentiment classifier?
  - Bonus: Briefly discuss how easy/difficult it would be to extract your features
  - Post your features to the Canvas Discussion
    (individually or as a group; include all group members' names in the post)

Logistic Regression — Runthrough (Part 1)

- Step 2: Factor in weights θ
  - Let's assume some oracle gave us those weights
  - It's time to include the bias using the "bias trick"

Feature	Description	Value	Weight θ_i
x_0	Bias b	1	0.1
x_1	Number of positive words	3	2.5
x_2	Number of negative words	2	-5.0
x_3	1 if "no" in text; 0 otherwise	1	-1.2
x_4	Number of 1st & 2nd person pronouns	3	0.5
x_5	1 if "!" in text; 0 otherwise	0	2.0
x_6	*ln* of word/token count	4.19	0.7

Logistic Regression — Runthrough (Part 1)

- Step 4: Compute linear signal (sum of weighted features)

Feature	Description	Value	Weight θ_i	$\theta_i x_i$
x_0	Bias *b*	1	0.1	0.1
x_1	Number of positive words	3	2.5	7.5
x_2	Number of negative words	2	-5.0	-10.0
x_3	1 if "no" in text; 0 otherwise	1	-1.2	-1.2
x_4	Number of 1st & 2nd person pronouns	3	0.5	1.5
x_5	1 if "!" in text; 0 otherwise	0	2.0	0
x_6	*ln* of word/token count	4.19	0.7	2.933

$$\sum = 0.833$$

Vector notation:

$$x = (1, 3, 2, 1, 3, 0, 4.19)^T$$

$$\theta = (0.1, 2.5, -5.0, -1.2, 0.5, 2.0, 0.7)^T$$

➜ $\theta^T x = 0.833$

Logistic Regression — Runthrough (Part 1)

$$\boxed{\theta^T x = 0.833}$$

- Step 4: Compute probabilities

$$P(+|x) = P(y=1|x,\theta) = \sigma(\theta^T x) = \frac{1}{1+e^{-\theta^T x}} = \frac{1}{1+e^{-0.833}} = 0.7$$

$$P(-|x) = P(y=0|x,\theta) = 1 - P(y=1|x,\theta) = 0.3$$

$$\Downarrow$$

$P(+|x) > 0.5$ ➜ $\hat{y} = +\ (\text{positive})$

Classify movie review as "positive"

Logistic Regression

- So, where did the values for θ come from?
  (in the example, they were simply given to us)
  - Of course, different θ values would have resulted in different probabilities

- Break down into 2 questions

  (1) *How can we quantify how good a set of θ values is?*

  ➜ **Loss function** (also: cost function, error function)

  (2) *How can we systematically find the best θ values?*

  ➜ **Gradient Descent** (numerical method to minimize loss function)

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Logistic Regression — Loss Function

- Intuition: A set of values for θ is good if
  - the correct label y (0 or 1; coming from the dataset)
  - the model's estimated label $\hat{y} = \sigma(\theta^T x)$

  are similar for all $\langle x, y \rangle$ pairs

➜ Find θ that **minimizes the difference** between $\hat{y}$ and y

$L(\hat{y}, y)$ = how much $\hat{y}$ differs from y

Logistic Regression — Loss Function

$$\boxed{\hat{y} = \frac{1}{1 + e^{-\theta^T x}}}$$

- Goal: Maximize probability of the correct label $P(y|x)$

$$\hat{y} = P(y = 1|x, \theta) = 1 - P(y = 0|x, \theta)$$

- Intermediate step: Combine both case into one formula
  - $P(y|x)$ is a Bernoulli distribution (2 discrete outcomes)

$$P(y|x) = \begin{cases} \hat{y} & , y = 1 \\ 1 - \hat{y} & , y = 0 \end{cases}$$

➜ Combine into: $\boxed{P(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}}$

Logistic Regression — Loss Function

$$\hat{y} = \frac{1}{1 + e^{-\theta^T x}}$$

- Goal: Maximize probability of the correct label $P(y|x)$

  - Find θ that **maximizes**

$$P(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}$$

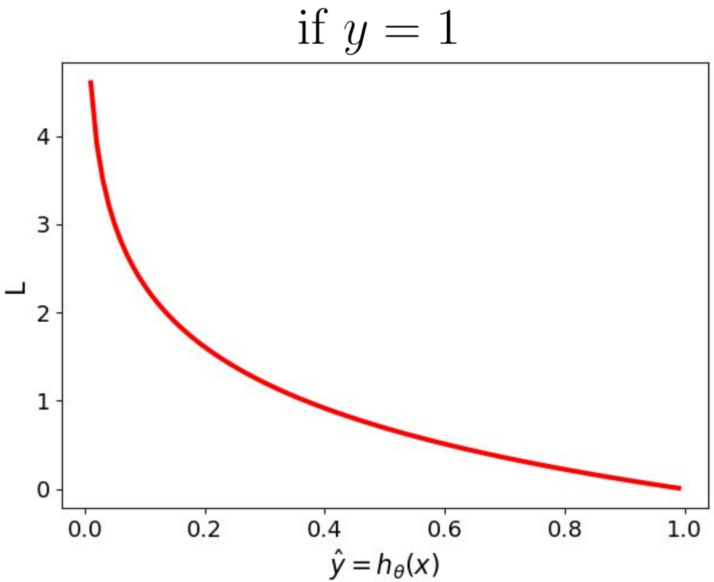
$$\log P(y|x) = \log \left[\hat{y}^y (1 - \hat{y})^{1-y}\right]$$
$$= y \log \hat{y} + (1 - y) \log (1 - \hat{y})$$

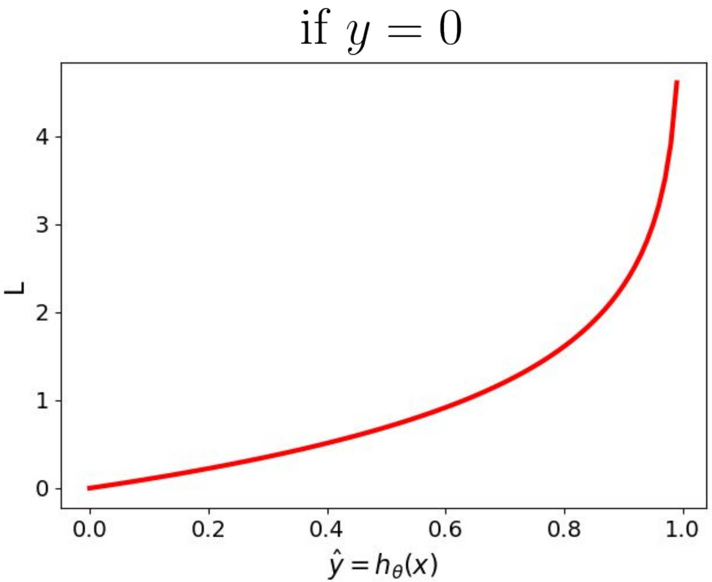
  - Find θ that **minimizes**

$$L_{CE}(\hat{y}, y) = -P(y|x) = \underbrace{-\left[y \log \hat{y} + (1 - y) \log (1 - \hat{y})\right]}_{\textbf{Cross-Entropy Loss}}$$

Cross-Entropy Loss — Visualization

$$L_{CE}(\hat{y}, y) = -\left[y \log \hat{y} + (1-y) \log (1-\hat{y})\right]$$





Cross-Entropy Loss — Runthrough Example (Part 2)

Recall:

$$P(+|x) = \sigma(\theta^T x) = 0.7$$

$$P(-|x) = 1 - \sigma(\theta^T x) = 0.3$$

Feature	Description	Value	Weight θ_i	$\theta_i x_i$
x_0	Bias *b*	1	0.1	0.1
x_1	Number of positive words	3	2.5	7.5
x_2	Number of negative words	2	-5.0	-10.0
x_3	1 if "no" in text; 0 otherwise	1	-1.2	-1.2
x_4	Number of 1st & 2nd person pronouns	3	0.5	1.5
x_5	1 if "!" in text; 0 otherwise	0	2.0	0
x_6	*ln* of word/token count	4.19	0.7	2.933

$$L_{CE}(\hat{y}, y) = -\left[y \log \hat{y} + (1 - y) \log (1 - \hat{y})\right]$$

Assume the model was right ($y = 1$)

$$L_{CE}(\hat{y}, y) = ???$$

Assume the model was wrong ($y = 0$)

$$L_{CE}(\hat{y}, y) = ???$$

Cross-Entropy Loss — Runthrough Example (Part 2)

$$P(+|x) = \sigma(\theta^T x) = 0.7$$

$$P(-|x) = 1 - \sigma(\theta^T x) = 0.3$$

$$L_{CE}(\hat{y}, y) = -\left[y \log \hat{y} + (1-y) \log (1-\hat{y})\right]$$

Assume the model was right ($y = 1$)

$$\begin{aligned} L_{CE}(\hat{y}, y) &= -[\log \hat{y}] \\ &= -[\log 0.7] \\ &= 0.36 \end{aligned}$$

Assume the model was wrong ($y = 0$)

$$\begin{aligned} L_{CE}(\hat{y}, y) &= -[\log (1-\hat{y})] \\ &= -[\log 0.3] \\ &= 1.2 \end{aligned}$$

Cross-Entropy Loss — Total Loss

- Loss for all training samples (given *m* data samples)

$$
\begin{aligned}
L_{CE} &= \frac{1}{m}\sum_{j=1}^{m} L_{CE}\left(\hat{y}^{(j)}, y^{(j)}\right) \\
&= -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log \hat{y}^{(j)} + \left(1-y^{(j)}\right)\log\left(1-\hat{y}^{(j)}\right)\right] \\
&= -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log \sigma\left(\theta^T x^{(j)}\right) + \left(1-y^{(j)}\right)\log\left(1-\sigma\left(\theta^T x^{(j)}\right)\right)\right] \\
&= -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log \frac{1}{1+e^{-\theta^T x^{(j)}}} + \left(1-y^{(j)}\right)\log\left(1-\frac{1}{1+e^{-\theta^T x^{(j)}}}\right)\right]
\end{aligned}
$$

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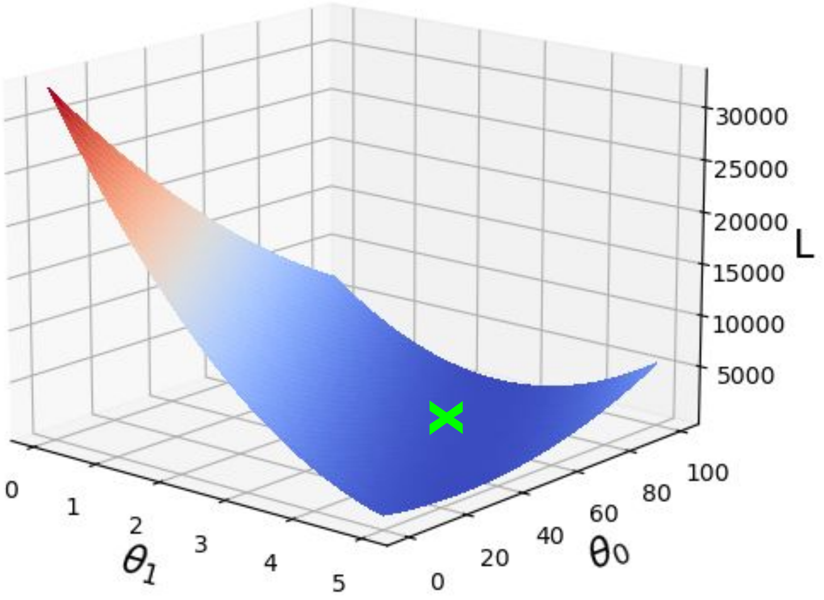
Learning — Minimizing the Loss Function

$$L_{CE} = -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log\frac{1}{1+e^{\theta^T x^{(j)}}} + \left(1-y^{(j)}\right)\log\left(1-\frac{1}{1+e^{\theta^T x^{(j)}}}\right)\right]$$

Visual illustration of loss function

- Just 1 feature θ_1 and bias θ_0
- Good news: L_{CE} for Logistic Regression is a convex function ➜ 1 global minimum



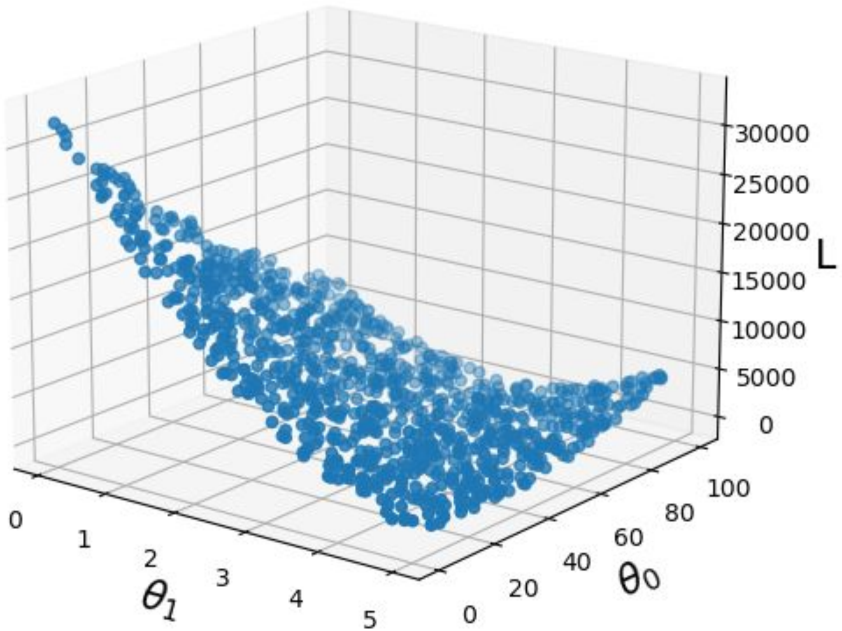
➜ How to find the minimum of L_{CE}?

…this should cause a flashback to your calculus classes :)

Method 1: Random Search (the "stupid" way)

- Repeat "enough" times
  - Select random values for $\theta = \{\theta_0, \theta_1, \theta_2, \ldots, \theta_n\}$
  - Calculate loss *L* for current θ
- Return θ with smallest loss

Plot of 1,000 losses



- Limitation:
  - Not practical beyond toy examples

➜ Don't do that! :)

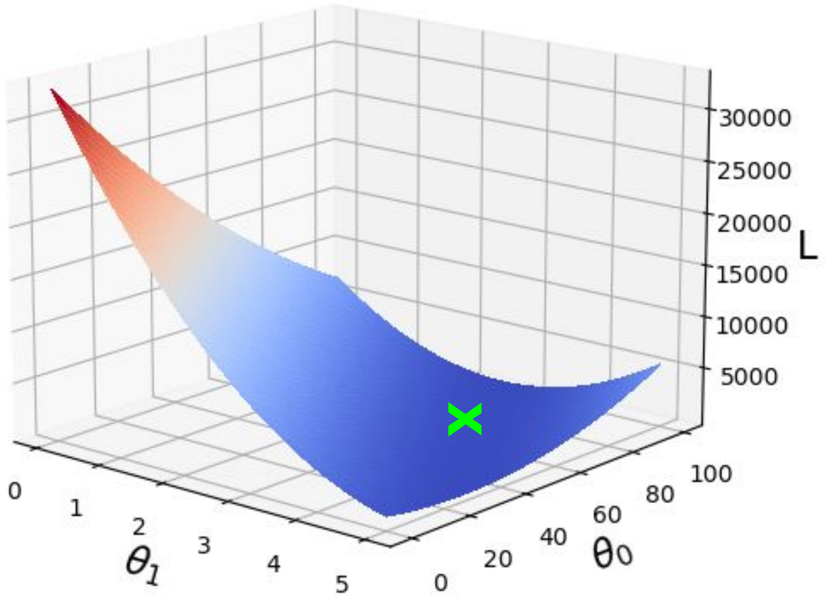
Method 2: Using Calculus (the proper way)

- Minimum of loss function L ➜ Calculus to the rescue!
  - Partial derivatives w.r.t. to all θ_i are 0

$$\frac{\partial L}{\partial \theta_0} = 0, \ \frac{\partial L}{\partial \theta_1} = 0, \ \frac{\partial L}{\partial \theta_2} = 0, \ \dots, \ \frac{\partial L}{\partial \theta_n} = 0$$

  - *n*+1 equations with *n*+1 unknowns
    (➜ 1 unique solution ➜ 1 global minimum)

➜ **What we need:** $\frac{\partial L}{\partial \theta}$



Loss Function — Derivatives

$$L_{CE} = -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log\sigma\left(\theta^T x^{(j)}\right) + \left(1 - y^{(j)}\right)\log\left(1 - \sigma\left(\theta^T x^{(j)}\right)\right)\right]$$

…lots of tedious math here…

$$\frac{\partial L_{CE}}{\partial \theta_i} = \frac{1}{m}\sum_{j=1}^{m}\left[\sigma\left(\theta^T x^{(j)}\right) - y^{(j)}\right] x_i^{(j)}$$

$$\frac{\partial L_{CE}}{\partial \theta} = \frac{1}{m} X^T \left[\sigma\left(X\theta\right) - y\right]$$

Basic approach to find the minimum

(1) Set derivative to 0 ➜ $\frac{1}{m} X^T \left[\sigma\left(X\theta\right) - y\right] \stackrel{!}{=} 0$

(2) Solve for θ

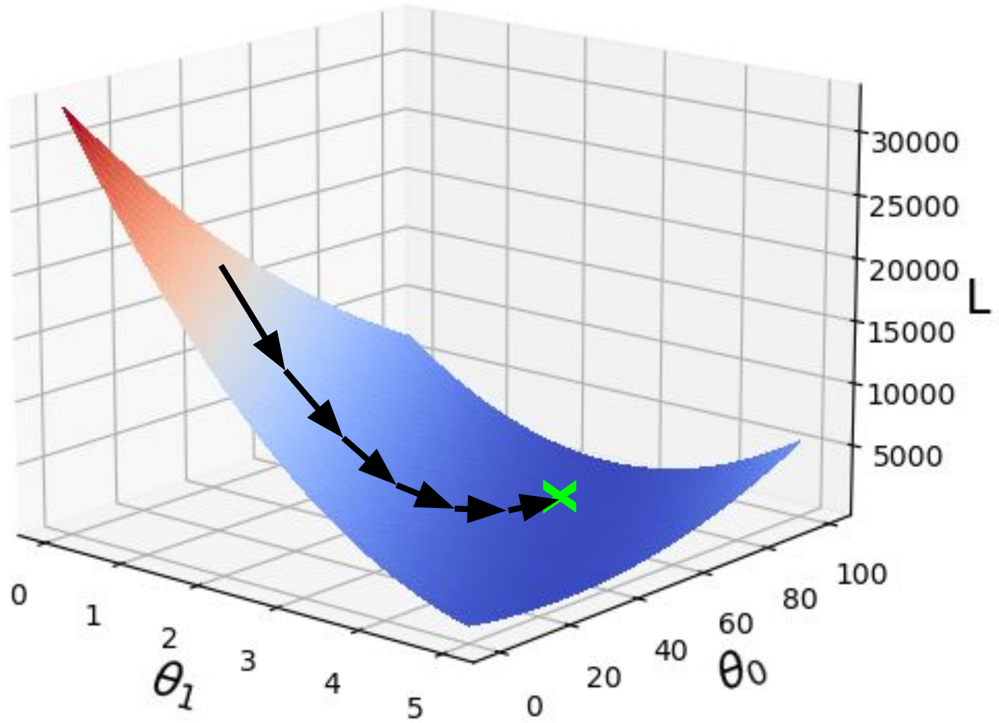
So are we done here?

Gradient Descent

- Problem: $\frac{1}{m} X^T \left[\sigma \left(X\theta \right) - y \right] \stackrel{!}{=} 0$ has no closed-form solution for θ

➜ **Gradient Descent**

- Start with a random setting of θ
- Adjust θ iteratively to minimize L



Gradient — Quick Refresher

- Gradient
  - Vector of partial derivatives of a multivariable function (e.g., θ_0, θ_1, …, θ_n)
  - Partial derivative: slope w.r.t. to a single variable given a current set of values for all θ_0, θ_1, …, θ_n
  - Points in the direction of the steepest ascent

$$\nabla_{\theta} L = \frac{\partial L}{\partial \theta} = \begin{bmatrix} \frac{\partial L}{\partial \theta_0} \\ \frac{\partial L}{\partial \theta_1} \\ \frac{\partial L}{\partial \theta_2} \\ \vdots \\ \frac{\partial L}{\partial \theta_n} \end{bmatrix}$$

Gradients — Runthrough Example (Part 3)

- Calculate Gradients (assuming $y = 1$)

$$\frac{\partial L_{CE}}{\partial \theta} = \frac{1}{m} X^T \left[\sigma\left(X\theta\right) - y\right]$$

Feature	Description	Value	Weight θ_i	$\theta_i x_i$	*Gradients*
x_0	Bias *b*	1	0.1	0.1	**-0.30**
x_1	Number of positive words	3	2.5	7.5	**-0.91**
x_2	Number of negative words	2	-5.0	-10.0	**-0.61**
x_3	1 if "no" in text; 0 otherwise	1	-1.2	-1.2	**-0.30**
x_4	Number of 1st & 2nd person pronouns	3	0.5	1.5	**-0.91**
x_5	1 if "!" in text; 0 otherwise	0	2.0	0	**0.0**
x_6	*ln* of word/token count	4.19	0.7	2.933	**-1.27**

$$\rightarrow \nabla_\theta L_{CE} = \begin{bmatrix} -0.30 \\ -0.91 \\ -0.61 \\ -0.30 \\ -0.91 \\ 0.0 \\ -1.27 \end{bmatrix}$$

Gradients — Runthrough Example (Part 3)

- Interpretation of gradients
  - Negative values: a small <u>increase</u> in, e.g., θ_0 or θ_1 will <u>decrease</u> the loss
  - A small change in θ_1 affects the loss more than the same change in θ_0
    (since the absolute value of θ_1 is larger than the one of θ_0)
  - Absolute values of gradient not a direct indicator of how to update θ

➜ **So how do we adjust θ to decrease the loss?**

$$\nabla_\theta L_{CE} = \begin{bmatrix} -0.30 \\ -0.91 \\ -0.61 \\ -0.30 \\ -0.91 \\ 0.0 \\ -1.27 \end{bmatrix}$$

Gradient Descent Algorithm

- Important concept: learning rate
  - Scaling factor for gradient (typical range: 0.01 - 0.0001)

$$\textbf{Input} : \text{data}\,(X, y),\ \text{loss function}\ L,\ \text{learning rate}\,\eta$$

$$\textbf{Initialization} : \text{Set}\ \theta\ \text{to random values}$$

$$\textbf{while true} :$$

$$\qquad \text{Calculate gradient}\ \nabla_\theta L$$

$$\qquad \theta \leftarrow \theta - (\eta \cdot \nabla_\theta L)$$

In practice: stop loop when θ converges

Gradient Descent — Runthrough Example (Part 4)

- Update weights θ
  - Learning rate: $\eta = 0.1$

$$\theta \leftarrow \theta - (\eta \cdot \nabla_\theta L)$$

Feature	Description	Value	Weight θ_i	$\theta_i x_i$	*Gradients*	New Weight θ_i
x_0	Bias *b*	1	0.1	0.1	-0.30	**0.13**
x_1	Number of positive words	3	2.5	7.5	-0.91	**2.59**
x_2	Number of negative words	2	-5.0	-10.0	-0.61	**-4.94**
x_3	1 if "no" in text; 0 otherwise	1	-1.2	-1.2	-0.30	**-1.17**
x_4	Number of 1st & 2nd person pronouns	3	0.5	1.5	-0.91	**0.59**
x_5	1 if "!" in text; 0 otherwise	0	2.0	0	0.0	**2.0**
x_6	*ln* of word/token count	4.19	0.7	2.933	-1.27	**0.83**

$$L_{CE} = 0.12$$

(down from 0.36)

➜ 1st iteration of Gradient Descent done!

Gradient Descent — Runthrough Example (Part 4)

- Update weights θ
  - Learning rate: $\eta = 0.1$

$$\theta \leftarrow \theta - (\eta \cdot \nabla_\theta L)$$

Feature	Description	Value	Weight θ_i	$\theta_i x_i$	*Gradients*	New Weight θ_i
x_0	Bias *b*	1	0.13	0.13	-0.11	**0.14**
x_1	Number of positive words	3	2.59	7.77	-0.33	**2.62**
x_2	Number of negative words	2	-4.94	-9.88	-0.22	**-4.92**
x_3	1 if "no" in text; 0 otherwise	1	-1.17	-1.17	-0.11	**-1.16**
x_4	Number of 1st & 2nd person pronouns	3	0.59	1.77	-0.33	**0.62**
x_5	1 if "!" in text; 0 otherwise	0	2.0	0	0.0	**2.0**
x_6	*ln* of word/token count	4.19	0.83	3.46	-0.46	**0.87**

$$L_{CE} = 0.075$$

(down from 0.12)

➜ 2nd iteration of Gradient Descent done!

Quick Quiz

What happens if
Logistic Regression gets a
training sample **correct**?

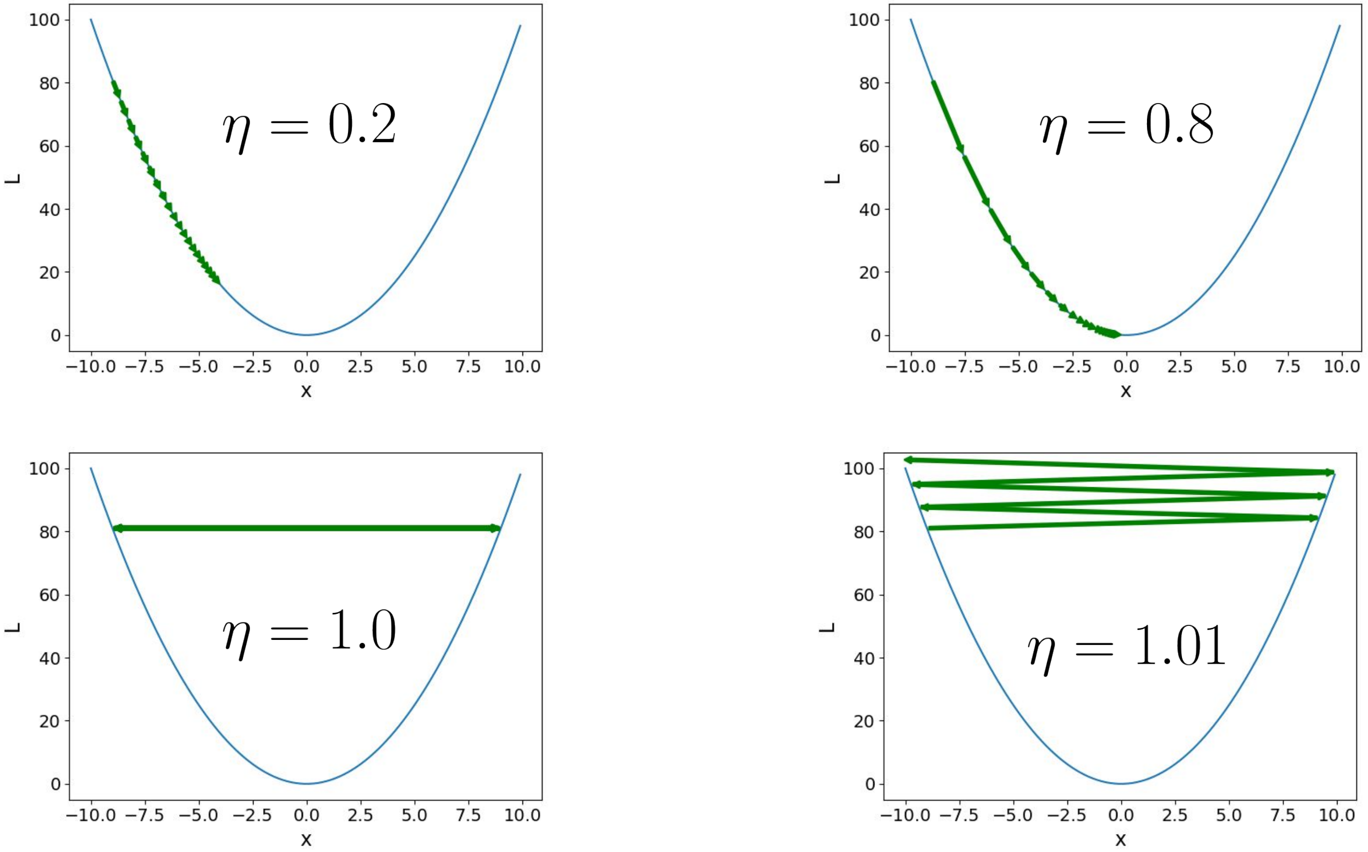
A No loss will be calculated

B The loss will be 0

C The loss will be small

D The loss will be large

Effects of Learning Rate for $L = x^2,\ \frac{\partial L}{\partial x} = 2x,\ 20 \text{ steps}$



Gradient Descent — Variations

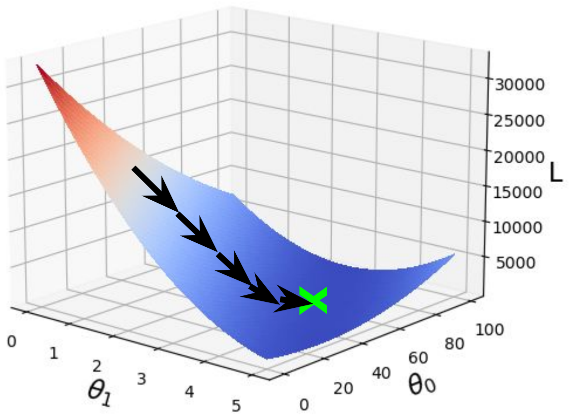
- (Basic) Gradient Descent
  - Calculate gradient und update θ for whole dataset

- Stochastic Gradient Descent (SGD)
  - Calculate gradient und update θ for each data sample

- Mini-batch Gradient Descent
  - Calculate gradient und update θ for batches of sample
  - e.g., batch = 64 data samples
  - In practice often referred to as SGD

Gradient Descent — Variations

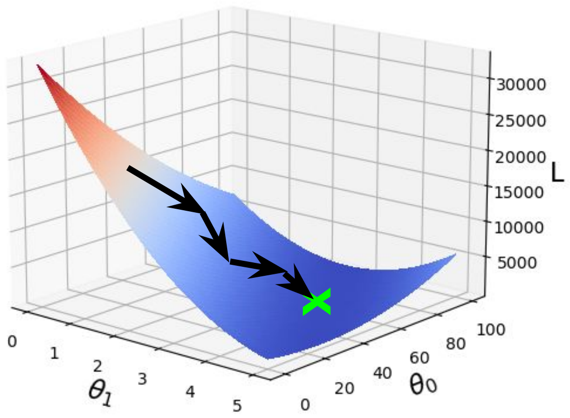
Gradient Descent



Gradient averaged over <u>all</u> data items

- Smooth descent
- Small(er) gradients
- Small(er) update steps

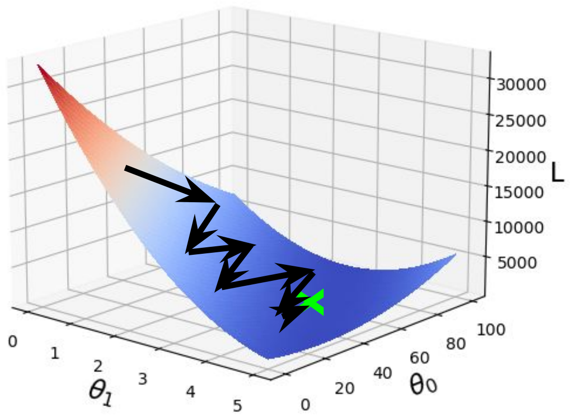
Mini-Batch Gradient Descent



Gradient averaged over <u>some</u> data items

- Well, "somewhere in-between" :)

Stochastic Gradient Descent



Gradient for each data item considered

- Choppy descent
- Large(r) gradients
- Large(r) steps

Gradient Descent — When to Stop?

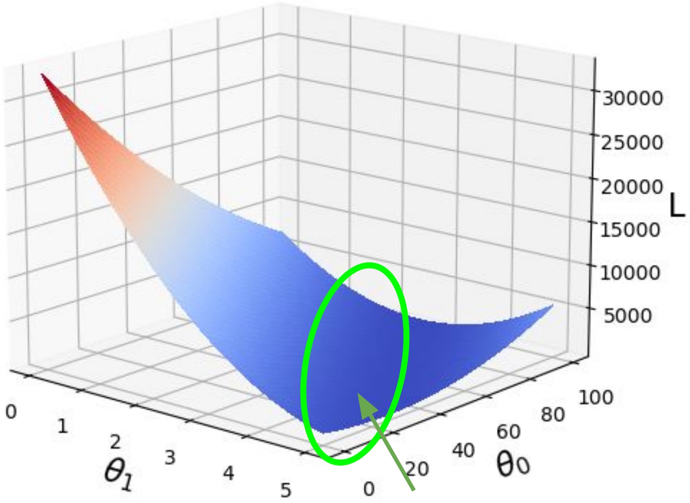
- Intuition: $\nabla_\theta L_{CE} < threshold$

Problem: regions of "near-plateaus":

➜ Gradient $\nabla_\theta L$ very small

➜ Step $\eta \nabla_\theta L$ extremely small

➜ Very slow convergence



Choices of θ with almost(!) equal loss

- Alternative stop conditions:
  - Loss is small (enough)
  - Change in loss is mall enough
  - Max. #iterations reached

Note: This problem is much more pronounced for non-convex loss function with multiple local minima

Outline

- Generative vs. Discriminative Classifiers

- **Logistic Regression**
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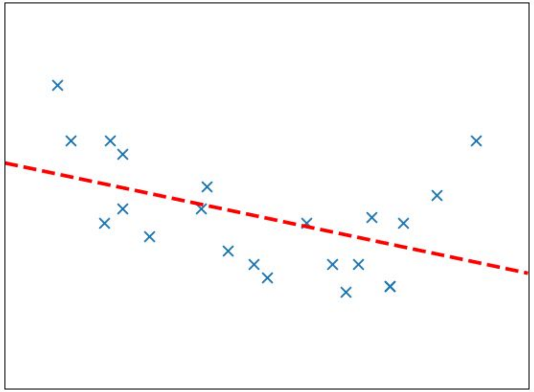
  - Gradient Descent
  - **Overfitting & Regularization**
  - Multiclass Logistic Regression

- Towards Neural Networks
  - Motivation: XOR Problem
  - Basic Neural Network Architecture

Overfitting — Basic Intuition

- Overfitting — Visualized using curve fitting
  - Task: Find a polynomial for degree *p* that best fit the data points

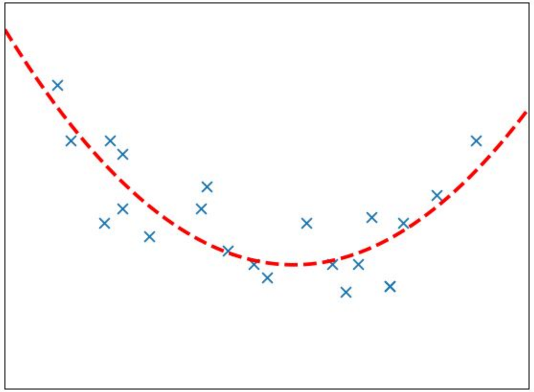
***p* = 1**



Underfitting

- Polynomial of degree 1 just a line
- Not capable to fit non-linear data

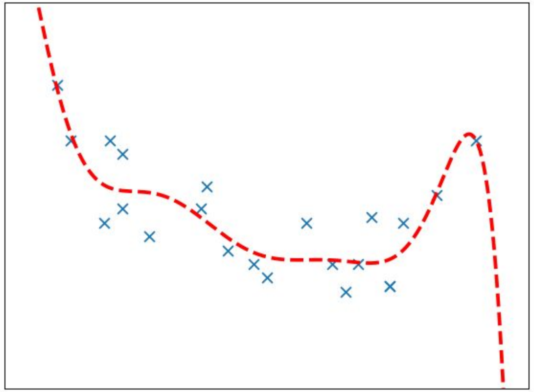
***p* = 2**



Good fit

- Model captures the overall trend
- Probably good fit for unseen data

***p* = 8**



Overfitting

- Model has too much capacity to exactly fit individual data points
- Probably bad fit for unseen data

Overfitting — Intuition (Naive Bayes Classifier)

- Scenario — movie reviews
  - (Very) low number of reviews
  - NB classifier based on 4-grams

This movie drew me in, and it'll do the same to you.	positive
I can't tell you how much I hated this movie. It sucked.	negative
...	...

➜ Effect of Naive Bayes classifier

- Each 4-gram most likely unique and associated with only 1 class
  (e.g., *"tell you how much"* only found in a negative review)
- Unseen positive review x containing "tell you how much" ➜ $P(positive|x) = 0$

Overfitting — Intuition (Logistic Regression Classifier)

- Scenario — movie reviews
  - (Very) low number of reviews
  - Assume the following artifact

    All positive reviews contain many pronouns

    Almost no negative reviews contain pronouns

Feature	Description	Value	Weight θ_i	$\theta_i x_i$
x_0	Bias *b*	1	0.1	0.1
x_1	Number of positive words	3	2.5	7.5
x_2	Number of negative words	2	-5.0	-10.0
x_3	1 if "no" in text; 0 otherwise	1	-1.2	-1.2
x_4	Number of 1st & 2nd person pronouns	3	0.5	1.5
x_5	1 if "!" in text; 0 otherwise	0	2.0	0
x_6	*ln* of word/token count	4.19	0.7	2.933

➜ Effect of Logistic Regression classifier

- Classifiers over-emphasizes the importance of pronouns
  ➜ large value for θ_4 (compared to other θ_i)
- Unseen negative review with many pronouns will most likely be misclassified

Regularization

- Observation
  - Model "too powerful" ⇔ (very) large θ values

➜ **Regularization**: Penalize large θ values

- Extend loss function by penalty term
- For example, for Cross-Entropy loss

λ: Regularization Parameter to control the "strength of the regularization"

$$L = -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log\sigma\left(\theta^T x^{(j)}\right) + \left(1-y^{(j)}\right)\log\left(1-\sigma\left(\theta^T x^{(j)}\right)\right)\right] + \lambda\sum_{i=1}^{n}\theta_i^2$$

L2 Regularization
("Ridge Regression")

$$L = -\frac{1}{m}\sum_{j=1}^{m}\left[y^{(j)}\log\sigma\left(\theta^T x^{(j)}\right) + \left(1-y^{(j)}\right)\log\left(1-\sigma\left(\theta^T x^{(j)}\right)\right)\right] + \lambda\sum_{i=1}^{n}|\theta_i|$$

L1 Regularization
("Lasso Regression")

New Loss ➜ New Gradient

- Since we change L, the gradient $\nabla_\theta L = \dfrac{\partial L}{\partial \theta}$ also changes
  - No big deal, regularization is just an added term
  - For example, for L2 Regularization (Ridge Regression)

$$\frac{\partial L_{CE}}{\partial \theta} = \frac{1}{m} X^T \left[\sigma\left(X\theta\right) - y\right] + \lambda \frac{2}{n} \theta$$

  - No changes to Gradient Descent Algorithms

Quick Quiz

Which of the statements regarding Logistic Regression is **True**?

A It's impossible to overfit given a dataset with only 1 feature

B Scaling the data will change the values for θ

C Gradient Descent can get stuck in local minimum

D Regularization can improve the training loss/error

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Binary LR ➜ Multiclass LR

- Multiclass LR: Classification beyond 2 classes
  - Let's assume we have C classes: c = 1..C
  - Separate weights θ_c for each classes c ➜ C output probabilities

Binary Logistic Regression

$$P(y=1|x) = \sigma(\theta_1^T x)$$

Multiclass Logistic Regression

$$\underbrace{\begin{bmatrix} P(y=1|x) \\ P(y=2|x) \\ \dots \\ P(y=C|x) \end{bmatrix}}_{\text{Probabilities need to sum up to 1}} = f_{mystery}\left(\begin{bmatrix} \theta_1^T x \\ \theta_2^T x \\ \dots \\ \theta_C^T x \end{bmatrix} \right)$$

➜ **How can we ensure that?**

$f_{mystery}$ ➜ Softmax

- Softmax function
  - Converts any vector of scores into a vector of probabilities

$$P(y = c|x) = \frac{\exp\left(\theta_c^T x\right)}{\sum_{i=1}^{C} \exp\left(\theta_i^T x\right)}$$

$$\begin{bmatrix} P(y=1|x) \\ P(y=2|x) \\ \dots \\ P(y=C|x) \end{bmatrix} = \frac{1}{\sum_{i=1}^{C} \exp\left(\theta_i^T x\right)} \begin{bmatrix} \exp\left(\theta_1^T x\right) \\ \exp\left(\theta_2^T x\right) \\ \dots \\ \exp\left(\theta_C^T x\right) \end{bmatrix}$$

Example

- Example with 4 classes and 3 input features

Weight matrix θ $\quad x \quad \theta^T x \quad \hat{y}$

$$\begin{array}{c} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{array} \begin{bmatrix} 0.55 & 0.71 & 0.29 \\ 0.51 & 0.89 & 0.90 \\ 0.13 & 0.21 & 0.05 \\ 0.44 & 0.03 & 0.46 \end{bmatrix} \cdot \begin{bmatrix} -0.4 \\ 0.2 \\ 0.3 \end{bmatrix} = \begin{bmatrix} 0.009 \\ 0.244 \\ 0.005 \\ -0.032 \end{bmatrix} \xrightarrow{\textbf{Softmax}} \begin{bmatrix} 0.238 \\ 0.296 \\ 0.237 \\ 0.229 \end{bmatrix} \begin{array}{c} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \hat{y}_4 \end{array}$$

Cross-Entropy Loss

Cross-Entropy Loss for Binary Logistic Regression

$$L_{CE}(\hat{y}, y) = -\left[y \log \hat{y} + (1 - y) \log (1 - \hat{y})\right]$$

Generalized Cross-Entropy Loss for Multiclass Logistic Regression

probability output after Softmax

$$L_{CE}(\hat{y}, y) = -\sum_{i=1}^{C} y_i \log(\hat{y_i})$$

$y_i = 1$ for correct class, 0 otherwise

New gradient $\nabla_\theta L_{CE}$ but beyond the scope here.

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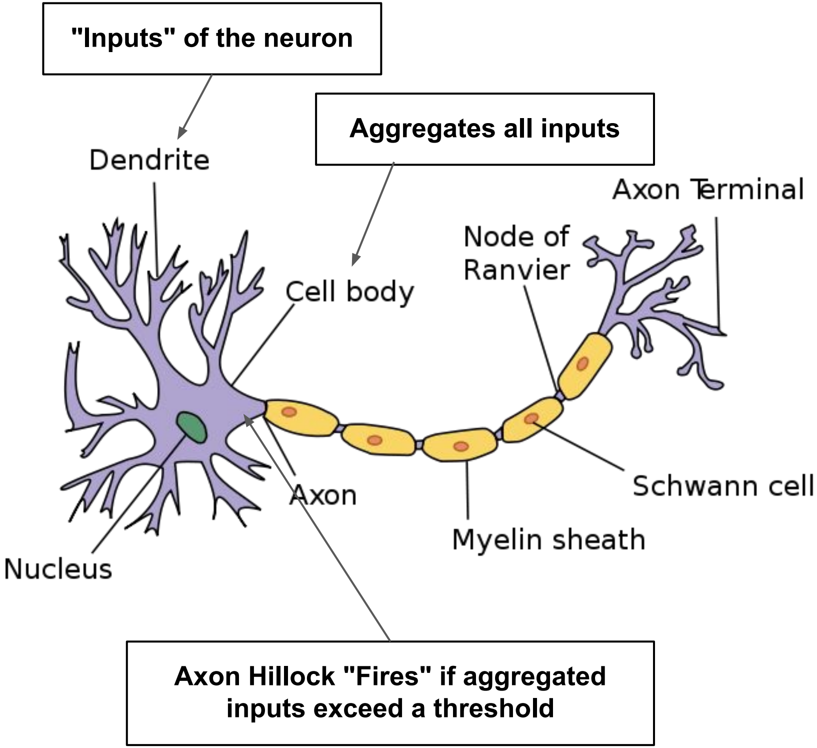
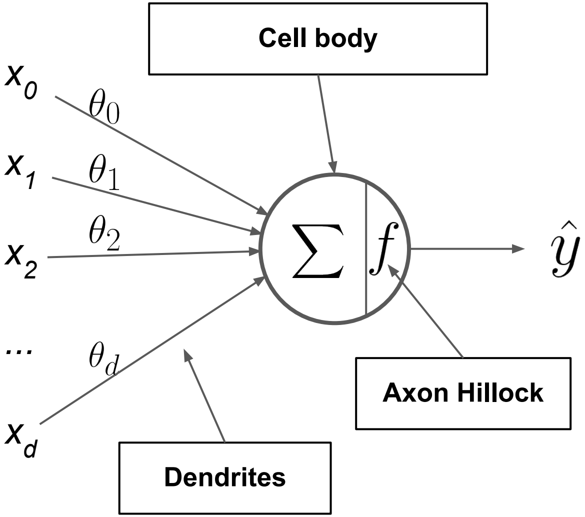
Biological Inspiration — Neuron



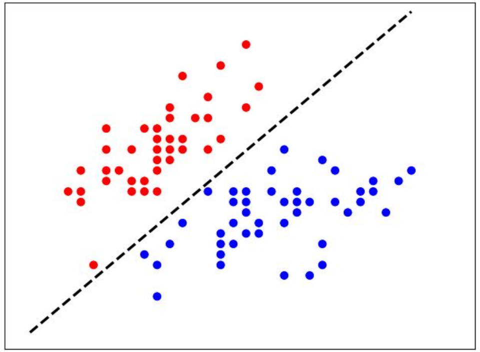


➜ Logistic Regression (crudely) a biological neuron

Source: Wiki Common (CC BY-SA 3.0): neuron

Logistic Regression — Limitations

- Logistic Regression is a linear model
  - Limited to linear combination of features
    (and a non-linear mapping to a probability)
  - Limited to linear decision boundaries
    (i.e., lines, planes, hyperplanes)

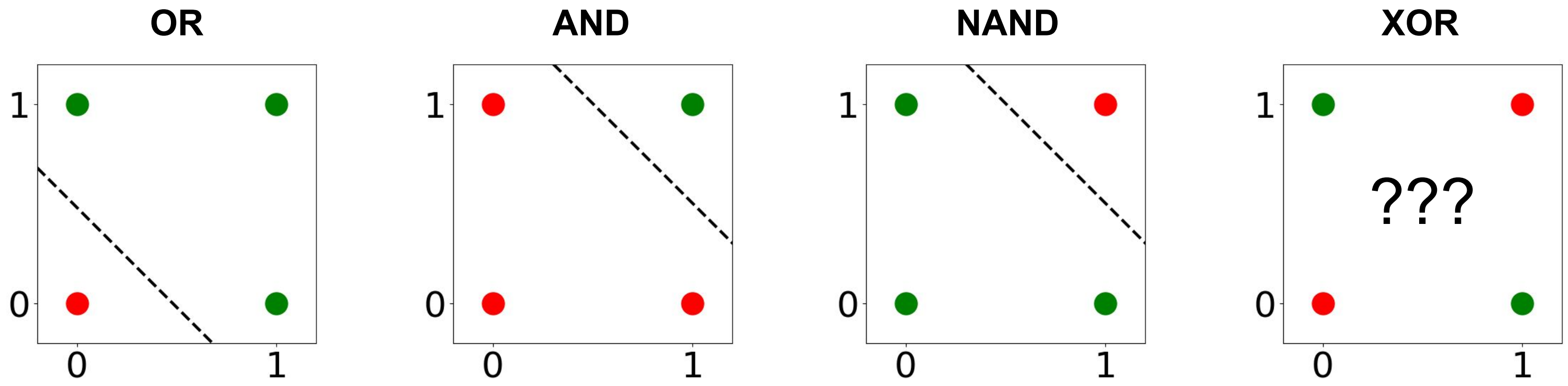


- What if we want or need to represent non-linear relationships between features? We can't!

➜ Scale up: "Stacked" Logistic Regression
  - Feed input into multiple neurons (i.e., LR units)
  - Use output of neurons as input for other neurons

XOR

x_1	x_2	OR	AND	NAND	XOR
0	0	0	0	1	0
0	1	1	0	1	1
1	0	1	0	1	1
1	1	1	1	0	0

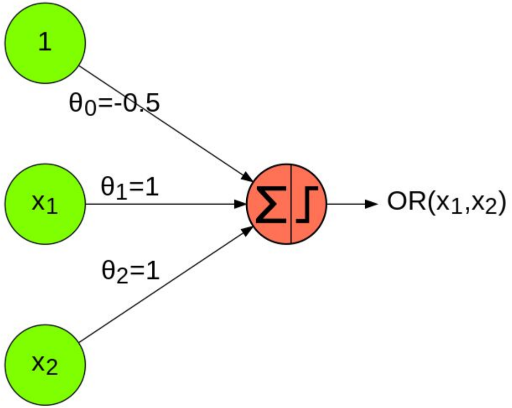


XOR

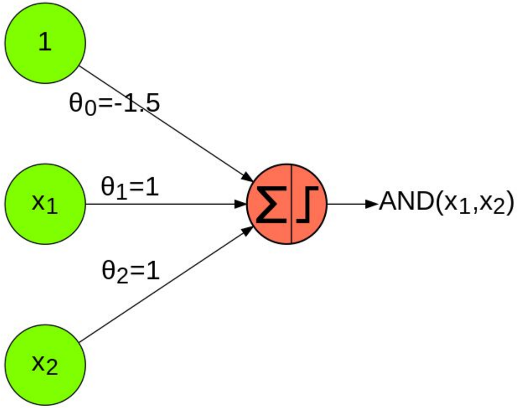
- Learning OR, AND, and NAND
  - Finding correct weights simply by "looking hard"
    (the weights are not unique; there are many ways to set θ)
  - The activation function is the Step Function, not Sigmod
    (strictly speaking, this makes it a Perceptron not a Linear Regression unit)

$$f_{step} = \begin{cases} 1 & \text{, if } \theta^T x > 0 \\ 0 & \text{, otherwise} \end{cases}$$

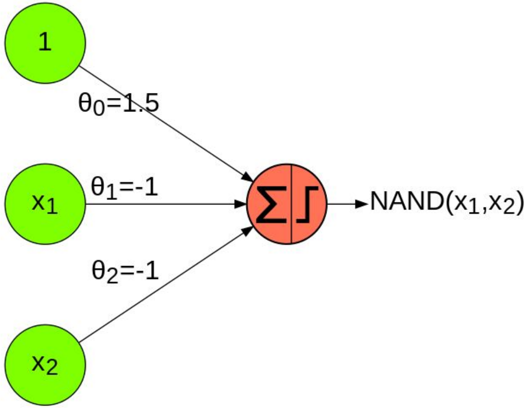
OR



AND



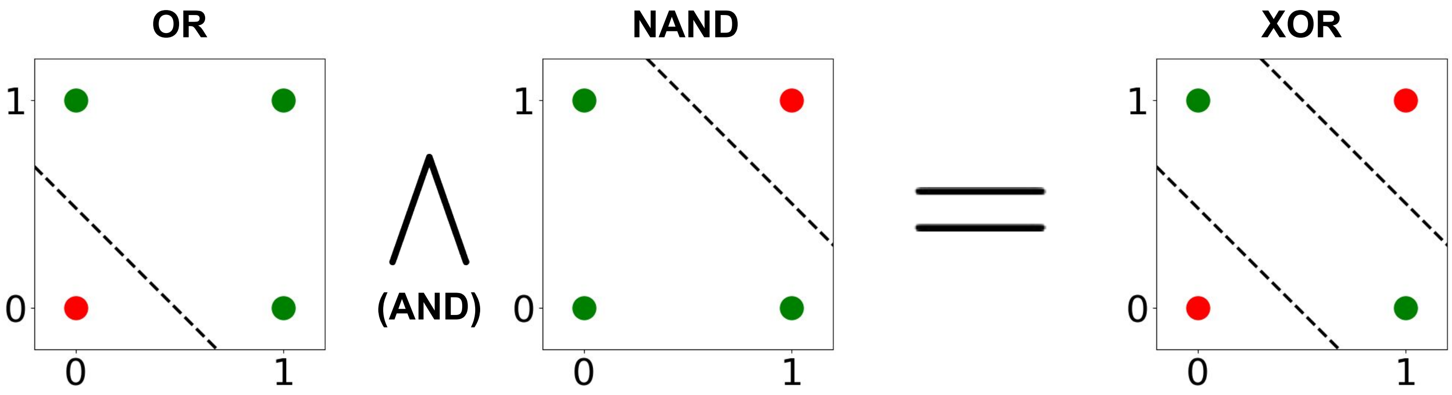
NAND



XOR

x_1	x_2	OR	AND	NAND	XOR
0	0	0	0	1	0
0	1	1	0	1	1
1	0	1	0	1	1
1	1	1	1	0	0

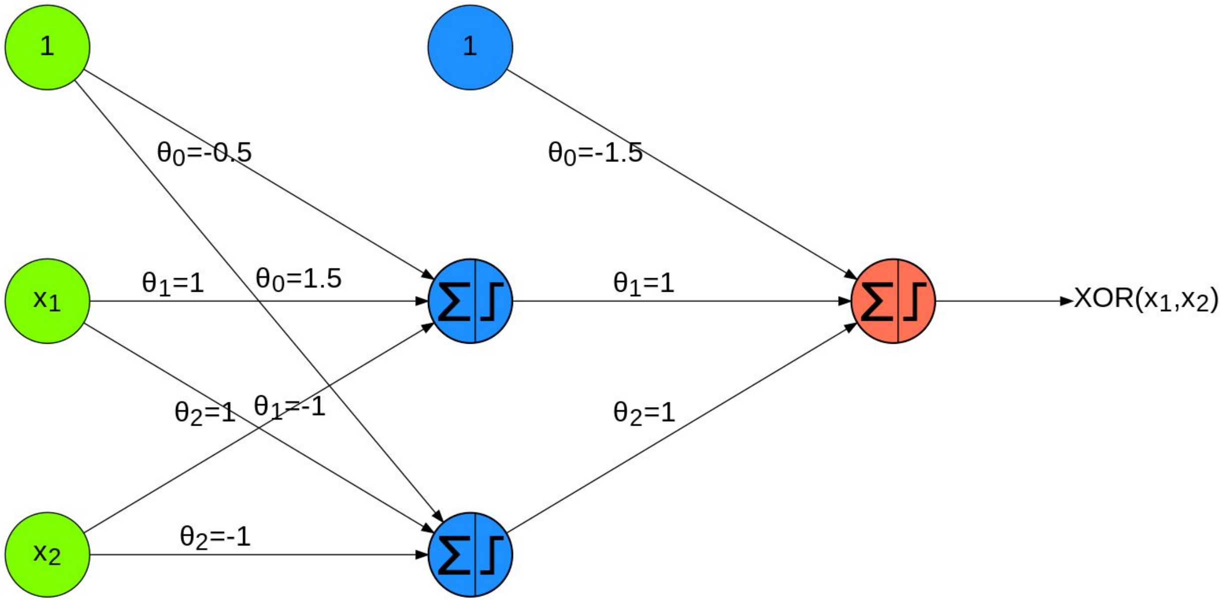
- Deriving XOR from simple classifiers
  - Note: this is not the only way, just convenient



➜ Cool, we know how to do ORs, ANDs and NANDs!

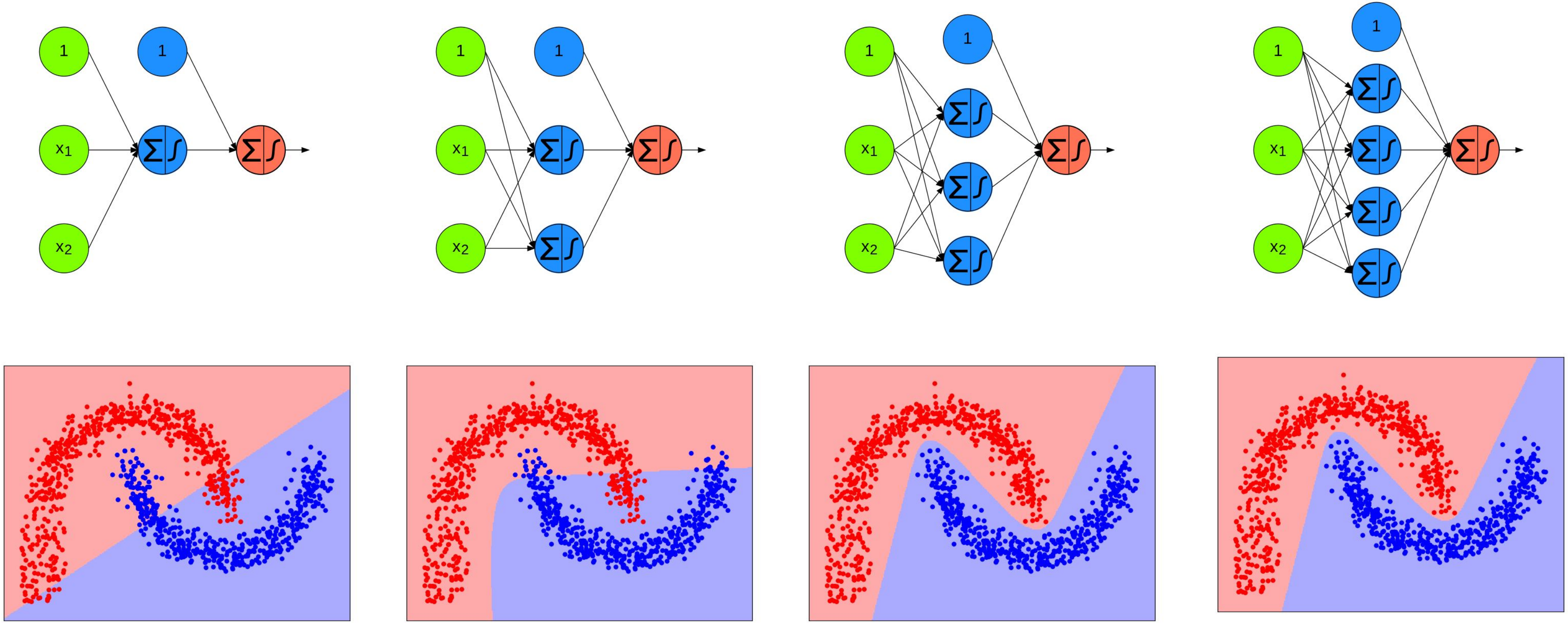
XOR

- Modeling XOR by "stacking" LR units ➜ **Neural Network** (NN)
  - More specifically, a **Feedforward NN** (i.e., network contains no loops)



Network Capacity — Intuition

Quick quiz: Is there any harm to have too many neurons?



Note: The activation function is the Sigmoid, hence the smooth decision boundaries

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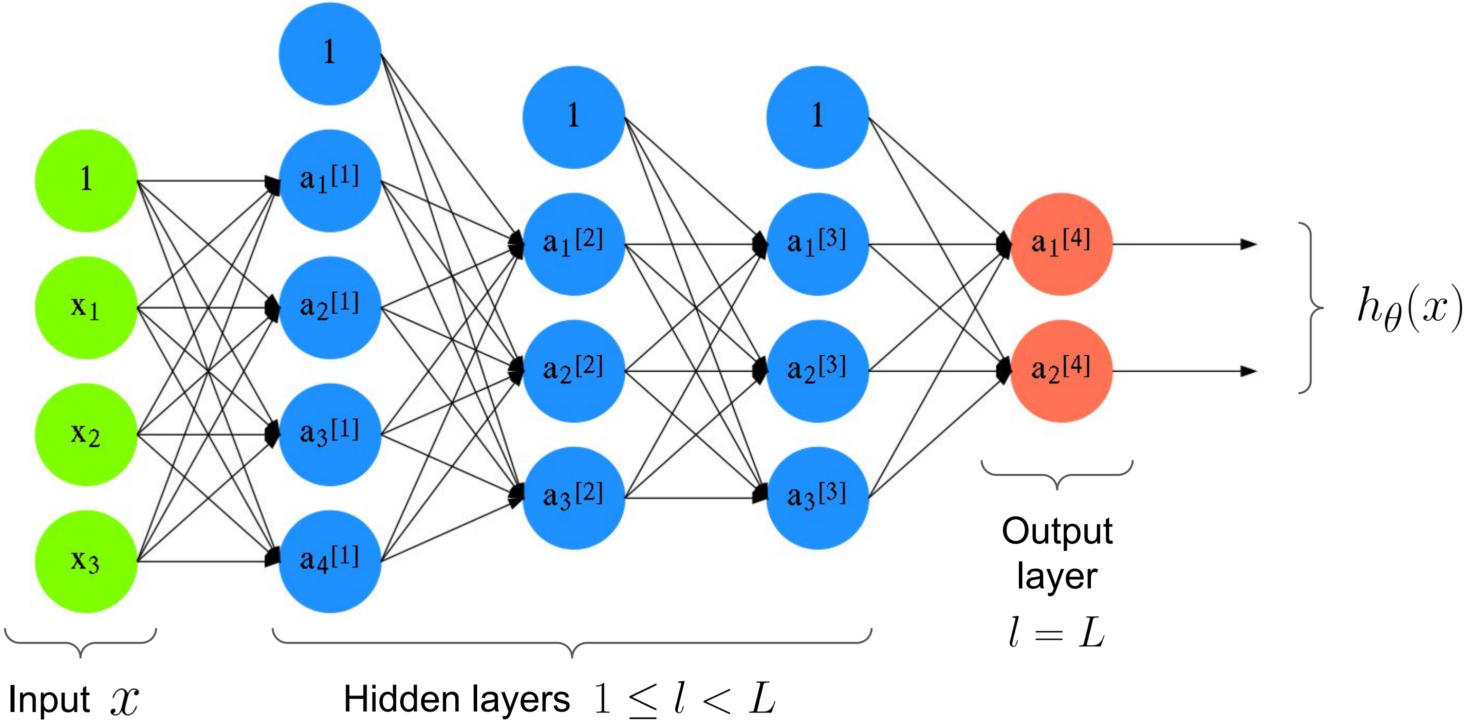
A Neural Network (Feedforward NN)

- Example: *L*-layer Feedforward Neural Network (here: *L* = 4)



Neural Network — Indices

$d^{[l]} =$ #neurons/units in layer l

$\theta^{[l]} = (d^{[l-1]} + 1) \cdot d^{[l]} =$ #weights for layer l

layer l

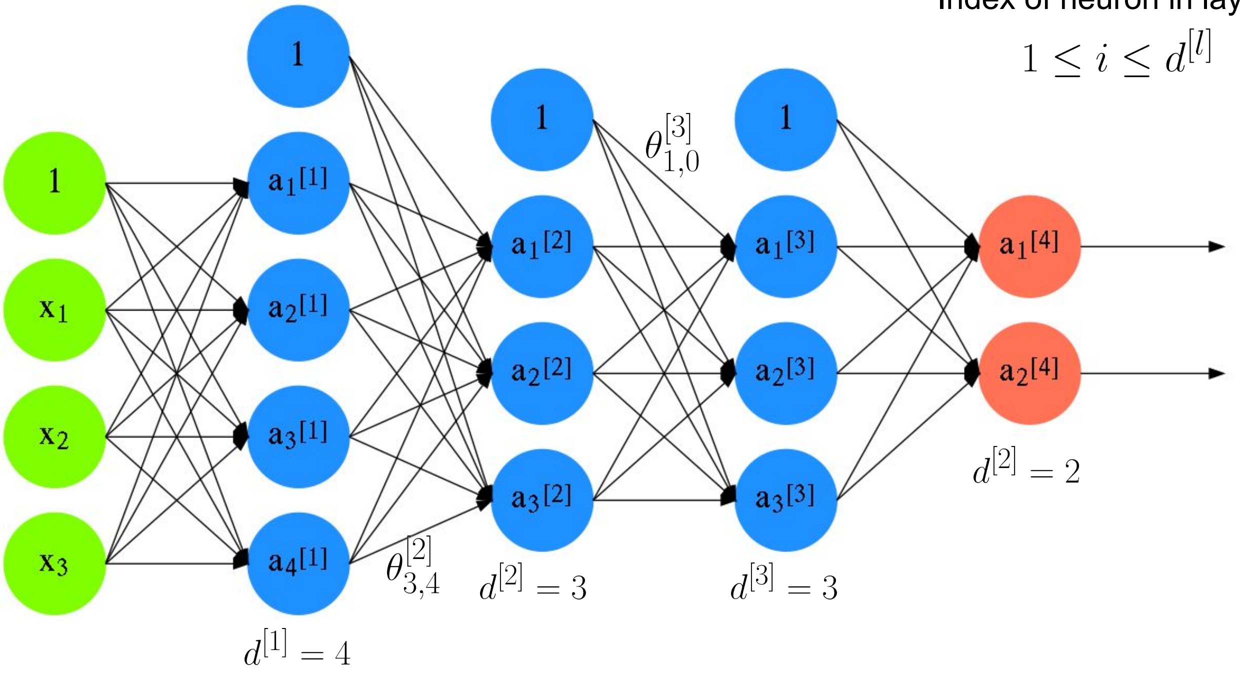
$$\theta^{[l]}_{i,j}$$

Index of neuron in layer l

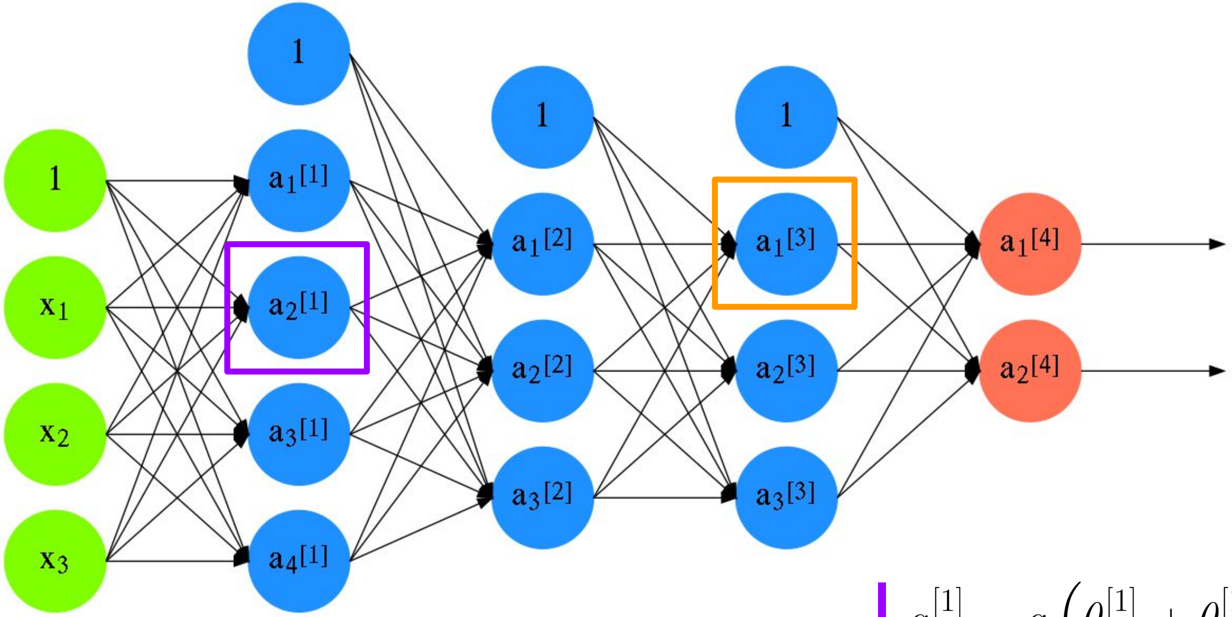
$1 \leq i \leq d^{[l]}$

Index of neuron in layer $l-1$

$0 \leq i \leq d^{[l-1]}$



Neural Network — Activations



$$a_2^{[1]} = g\left(\theta_{2,0}^{[1]} + \theta_{2,1}^{[1]} x_1 + \theta_{2,2}^{[1]} x_2 + \theta_{2,3}^{[1]} x_3\right)$$

$$a_1^{[3]} = g\left(\theta_{3,0}^{[3]} + \theta_{3,1}^{[3]} a_1^{[2]} + \theta_{3,2}^{[3]} a_2^{[2]} + \theta_{3,3}^{[3]} a_3^{[2]}\right)$$

Neural Network — Activations

- Layer-wise computations
  - Let $x^{[l]}$ be the output of layer l
  - $x^{[0]} = x$ — initial input
  - $x^{[L]} = h(x)$ — final output

$$x_i^{[l]} = a_i^{[l]} = g\left(\sum_{j=0}^{d^{[l-1]}} \theta_{i,j}^{[l]} x_j^{[l-1]}\right)$$

$$= g\left(\left[\theta_i^{[l]}\right]^T \cdot x^{[l-1]}\right)$$

Weight vector $\theta_i^{[l]} \in \mathbb{R}^{d^{[l-1]}}$

- Vectorized form
  - Calculate $x^{[l]}$ in practice "in one go"
  - Everything becomes matrix* operations
  - GPUs: hardware-supported processing of matrix operations (+ parallelism)

$$x^{[l]} = a^{[l]} = g\left(\theta^{[l]} x^{[l-1]}\right)$$

Weight matrix $\theta^{[l]} \in \mathbb{R}^{d^{[l]} \times d^{[l-1]}}$

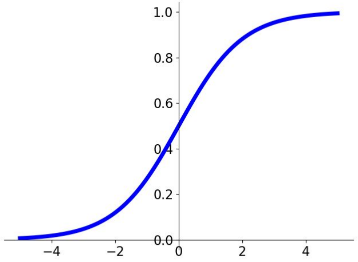
*strictly speaking: tensor operations (tensor ≈ n-dimensional arrays)

Neural Network — Activation Functions

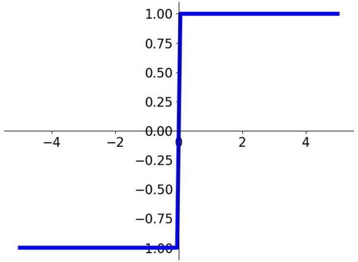
- Wide range of activation functions

- Activations functions for hidden layers
    - Do not need to have a probabilistic interpretation
    - Only requirement: non-linear function!
    - Examples:

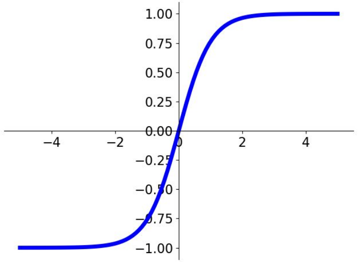
Sigmoid



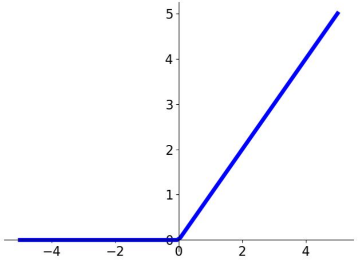
Sign



Tanh

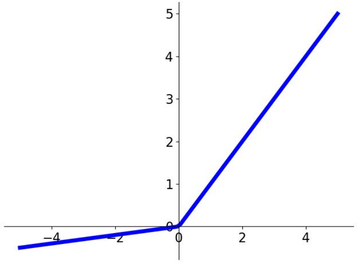


ReLU



ReLU = Rectified Linear Unit

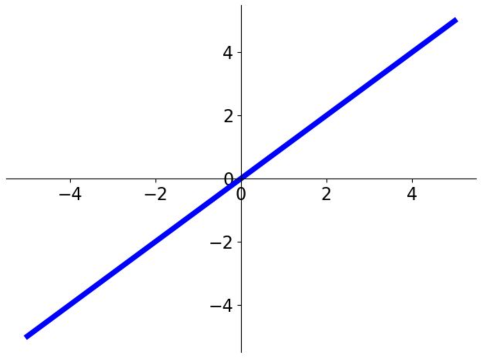
Leaky ReLU



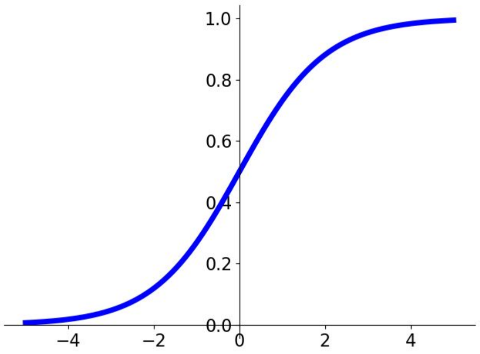
Neural Network — Activation Functions

- Activations functions for output layers
  - Choice of activation function depending on task
    (mainly: classification or regression)
  - Examples:

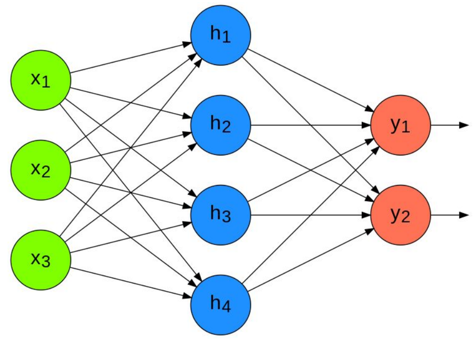
Linear function for regression tasks



Sigmoid function for classification tasks



Example



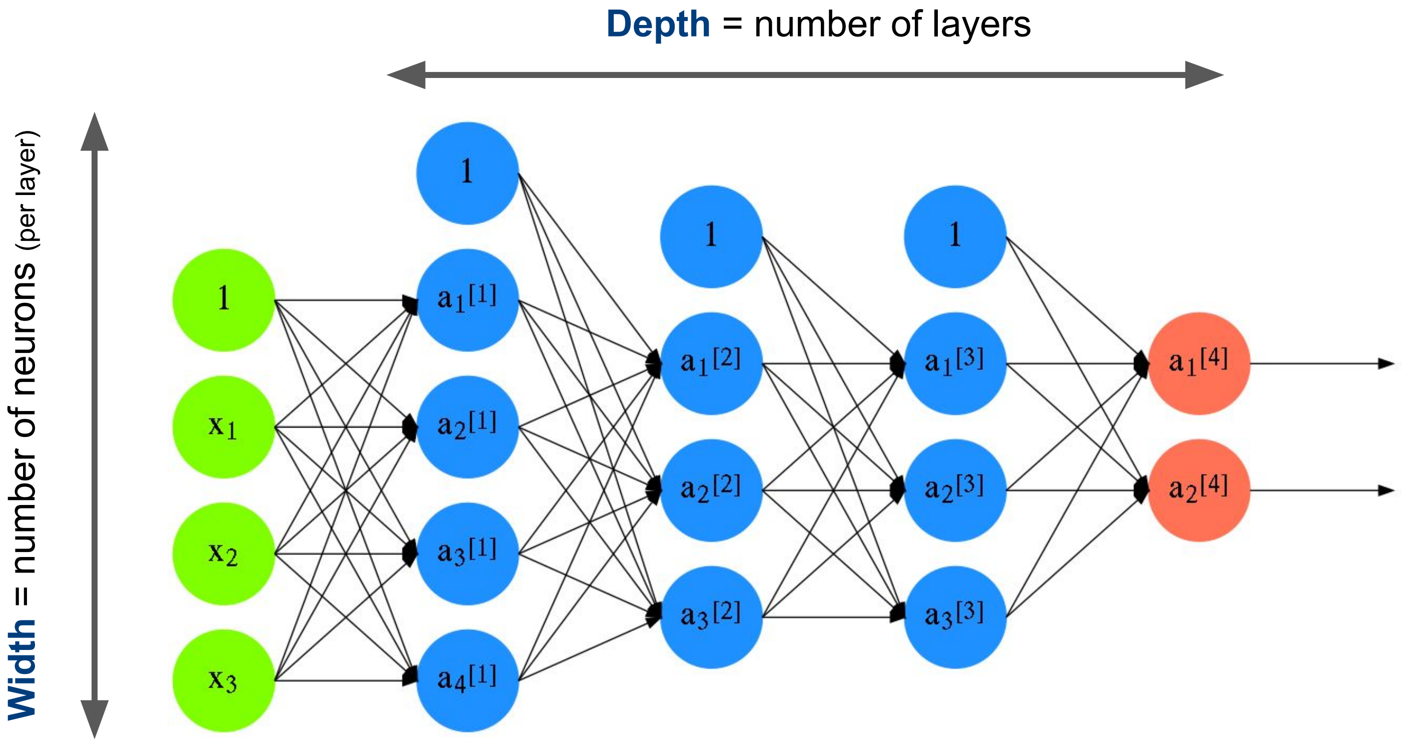
$$h = g_h\left(\theta_h x\right) \ , \text{with } \theta_h \in \mathbb{R}^{4\times 3}$$

$$y = g_y\left(\theta_y h\right) \ , \text{with } \theta_y \in \mathbb{R}^{2\times 4}$$

$g_h, \ g_y$: suitable activation functions

$$\underbrace{\begin{bmatrix} 0.55 & 0.71 & 0.29 \\ 0.51 & 0.89 & 0.90 \\ 0.13 & 0.21 & 0.05 \\ 0.44 & 0.03 & 0.46 \end{bmatrix}}_{\theta_h} \cdot \underbrace{\begin{bmatrix} -0.4 \\ 0.2 \\ 0.3 \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} 0.009 \\ 0.244 \\ 0.005 \\ -0.032 \end{bmatrix}}_{\theta_h x} \Rightarrow ReLU(\theta_h x) = \underbrace{\begin{bmatrix} 0.009 \\ 0.244 \\ 0.005 \\ 0 \end{bmatrix}}_{h} \Rightarrow \underbrace{\begin{bmatrix} 0.65 & 0.28 & 0.68 & 0.59 \\ 0.02 & 0.56 & 0.26 & 0.42 \end{bmatrix}}_{\theta_y} \cdot \underbrace{\begin{bmatrix} 0.009 \\ 0.244 \\ 0.005 \\ 0 \end{bmatrix}}_{h} = \underbrace{\begin{bmatrix} 0.078 \\ 0.138 \end{bmatrix}}_{\theta_y h} \Rightarrow Softmax(\theta_y h) = \underbrace{\begin{bmatrix} 0.48 \\ 0.52 \end{bmatrix}}_{y}$$

Neural Networks



From Logistic Regression to (Deep) Neural Networks

- Fundamentally, nothing new here:
  - A neural network is a function $h_\theta(x)$
  - Define a loss function $L = L(y, \hat{y}) = L(y, h_\theta(x))$
  - Perform Gradient Descent to minimize *L*

- Difference: increased complexity
  - $h_\theta(x)$ and thus $L(y, h_\theta(x))$ are much more complex functions
  - Calculation of $\frac{\partial L}{\partial \theta}$ much more challenging ➜ backpropagation
  - *L* is no longer a convex function ➜ local minima ➜ training more challenging
  - Overfitting becomes a bigger issue ➜ regularization (several different approaches)

Outline

- Generative vs. Discriminative Classifiers

- Logistic Regression
  - Setup as Probabilistic Classifier
  - Cross-Entropy Loss Function
  - Gradient Descent
  - Overfitting & Regularization
  - Multiclass Logistic Regression

- Towards Neural Networks
  - Motivation: XOR Problem
  - Basic Neural Network Architecture

Summary

- Linear model: **Logistic Regression**
  - Very important probabilistic classifier
  - Discriminative classifier ➜ linear decision boundaries
  - Core unit of neural networks

- "Stacked" Logistic Regression ➜ Neural Network
  - Neuron = Linear Regression unit
  - Non-convex loss function ➜ global minimum vs. local minima
  - Higher risk of overfitting ➜ regularization crucial (but also other methods)

Pre-Lecture Activity for Next Week

- Assigned Task
  - Post a 1-2 sentence answer to the following question into the L2 Discussion
    (you will find the Discussion on Canvas)

"What do we mean by sparse or dense vectors?"

"Are documents characterized by tf-idf sparse or dense?"

Side notes:
- This task is meant as a warm-up to provide some context for the next lecture
- No worries if you get lost; we will talk about this in the next lecture
- You can just copy-&-paste others' answers but his won't help you learn better

Solutions to Quick Quizzes

- Slide 43: C
  - The ground truth is 0 or 1, while the prediction will only ever be (very) close to 0 or 1
  - At least with arbitrary mathematical precision, there will always be some loss calculated
- Slide 54: B
  - In case Logistic Regression, scaling does not change the performance of the model
  - However, the values of the coefficients do change
- Slide 67
  - Too many neurons may lead to overfitting
  - Example: the model might try to "learn" an outlier