NUS | Computing
National University of Singapore

CS4248: Natural Language Processing

Lecture 5 — Introduction into Connectionist Machine Learning

Recap of Week 04

Text Classification

- 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)
- Classification task
  - Mapping h from input space X to output space Y $\quad h : X \rightarrow Y$

$h(x) = y$ e.g., $h(\text{“The movie is great.”}) = \text{“positive”}$

"True" mapping which is unknown in practice

Note: A document might be assigned to more than one class ➜ **multilabel classification**

Note 2: Our SLP3 textbook uses d for x and c for y. We'll use both interchangeably.

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Document-Term Matrix with $tf\text{-}idf$ Weights

- Putting it all together

$$w_{t,d} = (1 + \log_{10} tf_{t,d}) \cdot \log_{10} \frac{|D|}{df_t}$$

- Side notes
  - No real theoretic underpinning, but $tf\text{-}idf$ works best in practice
  - Not all definitions of $tf\text{-}idf$ apply a sublinear scaling of $tf_{t,d}$
  - Alternative names: $tf \cdot idf$, $tf \times idf$
  - There are different weighting functions for calculating $tf\text{-}idf$

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Naive Bayes Classifier + BoW — Discussion

- Naive Bayes vs. Language Models
  - Naive Bayes makes a non-contextual decision (unigram model; but can be extended to larger n-grams)
  - Naive Bayes is an LM! It treats each class like a separate language model
- Biggest **pro**: simplicity
  - Easy to understand & implement, fast, not very data hungry, interpretable results
- Biggest **con**: assumption of conditional independence
  - For most types of data, the features are typically not independent
  - For text classification (features = words) it actually often works well in practice (particularly with some additional "tweaking" of the data)

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Classification: Evaluation — Why so Many Measures?

- Observation: FP and FN not always equally problematic

$$Precision = \frac{TP}{TP + FP} \qquad Recall = \frac{TP}{TP + FN}$$

- Example: Suicide prediction (e.g., from social media content posted by users)
  - BAD: misclassifying a high-risk person
  - OK-ish: misclassifying a healthy person

  $\}$ **Recall > Precision**

- Example: News article classification (e.g., for search engines such as Google News)
  - BAD: showing article of wrong category
  - OK: missing a relevant article in result

  $\}$ **Recall < Precision**

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Announcements

- Project Groups Announced
  - There may have been some errors, please 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
  - Live version (best bet) at https://bit.ly/cs4248-2320-iu-template

- Assignment 2 out on Saturday, once Assignment 1 is in
  - Assignment 2 will be a Text Classification competition, restricted to ML algorithms taught (Naive Bayes and Logistic Regression)
  - Emphasis on Natural Language Feature Engineering

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 learning $\hat{h}$ 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

Generative vs. Discriminative Classifiers — Intuition

- Generative classifier
  - Builds 2 models of what zebra and elephant images look like - $\mathcal{R}$

Some abstract internal representation / model of language and the world

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

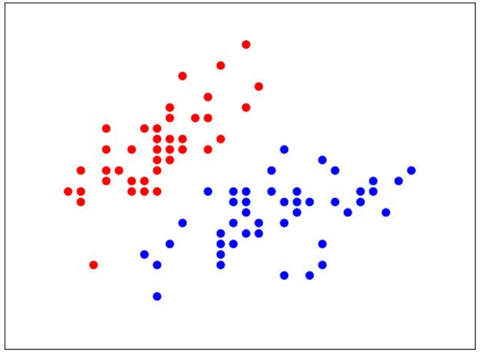
- Discriminative classifier
  - Tries to distinguish zebra and elephant images
  - No model of how zebra and elephant images “look like”

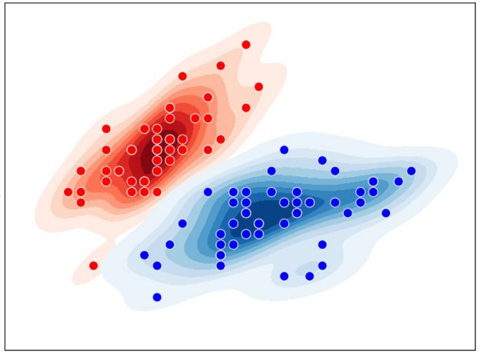
Question: How could we quickly distinguish zebras from elephants?

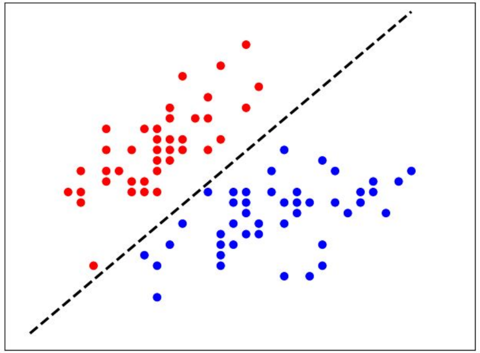
Generative vs. Discriminative Classifiers

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 a 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

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

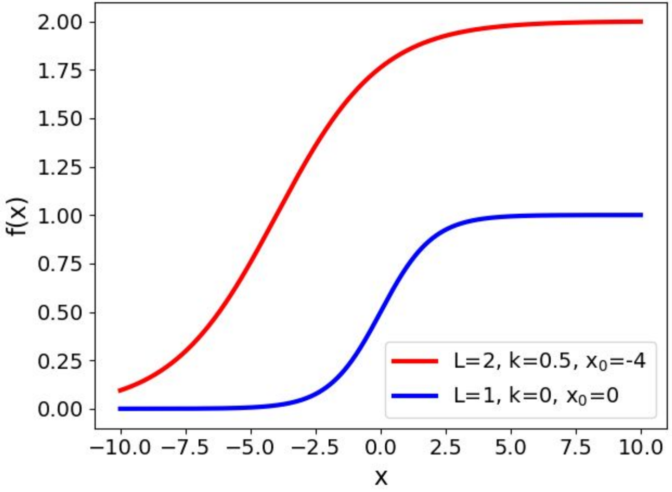
Note: Throughout the rest of the slide, we drop the superscript in $x^{(j)}$ and $y^{(j)}$ if there is no ambiguity.

Map $y \in \mathbb{R}$ to $\sigma \in [0, 1]$

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

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

➜ $\hat{y} = h_\theta(x)$ 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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Sentiment Analysis, redux

Now Showing

Movies – The Omicron Variant

"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."

Photoshopped Fake Vintage Movie Poster image courtesy [Tribune India]

🏃‍♀️🏃🏃‍♂️ What features have positive or negative weights?

Feature	Description	Value	Weight
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		

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	
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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 are often tf-idf weighted vocabulary.

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)

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"

⚠️ **Notation varies**: Weights are also called parameters, sometimes denoted as $\boldsymbol{w}$ (as used in the SLP3 textbook)

Feature	Description	Value	Weight $\boldsymbol{\theta_i}$
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:

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

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

$$\rightarrow \theta^\top x = 0.833$$

Logistic Regression — Runthrough (Part 1)

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

- Step 4: Compute probabilities

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

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

$$\Downarrow$$

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

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 $\hat{y} = \sigma(\theta^\top x)$

  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

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

- 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

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

- Goal: Maximize probability of the correct label $P(y|x)$
  - Find θ that **maximizes**

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

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

$$= y \log \hat{y} + (1-y) \log (1-\hat{y})$$

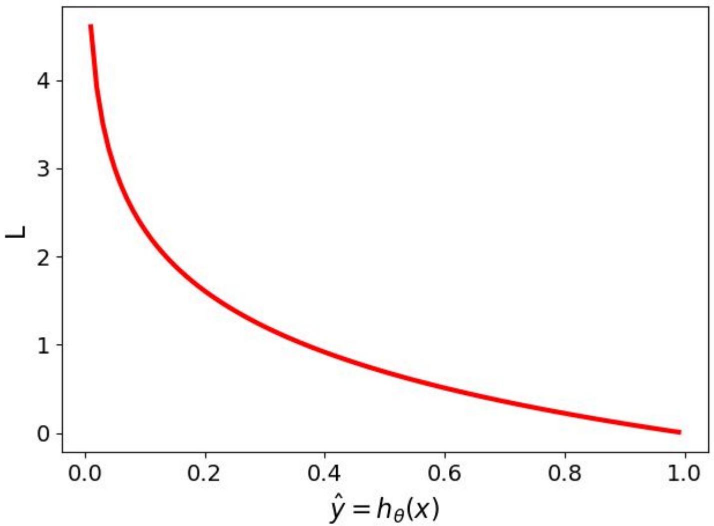
  - Find θ that **minimizes**

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

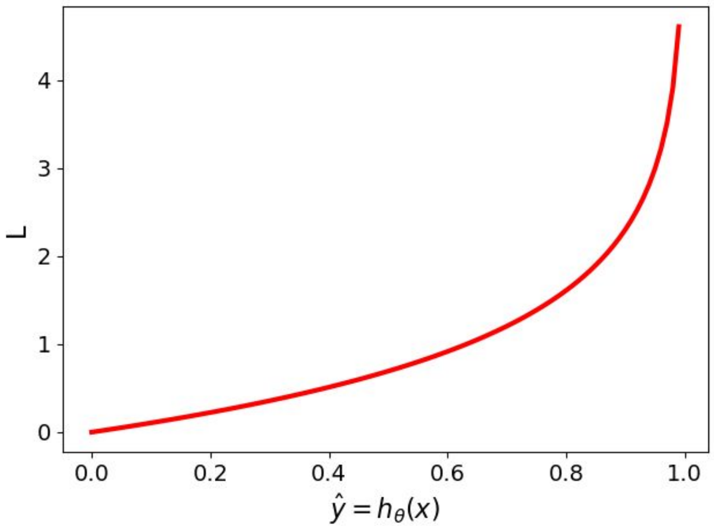
Cross-Entropy Loss — Visualization

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

if $y = 1$



if $y = 0$



Cross-Entropy Loss — Runthrough Example (Part 2)

Recall:

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

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

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
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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)

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

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

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

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)

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

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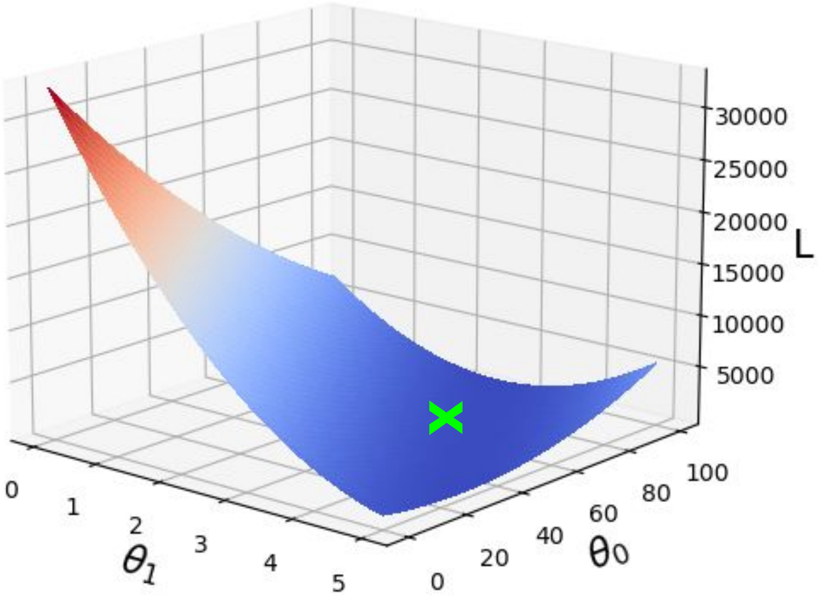
Learning — Minimizing the Loss Function

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

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



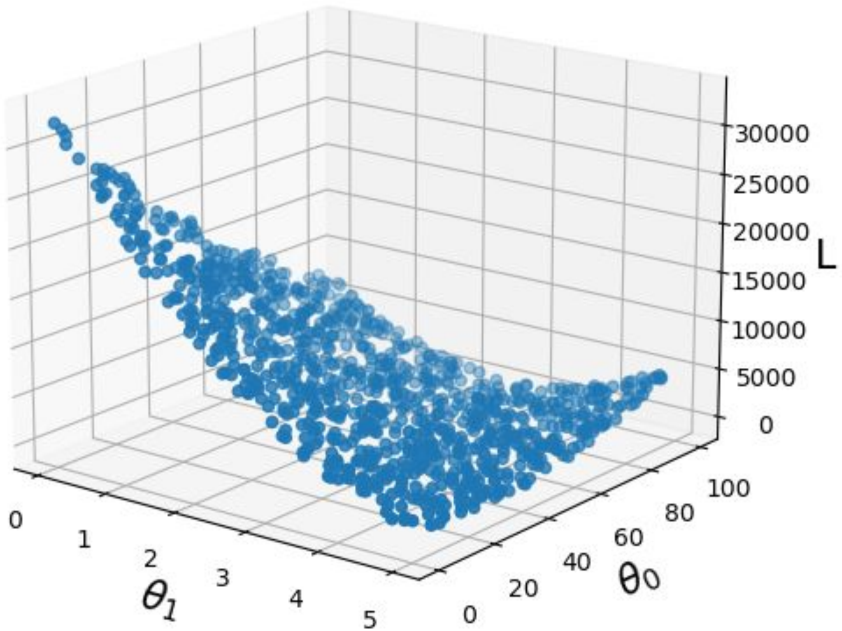
➜ How to find the minimum of L_{CE}?

…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! :)

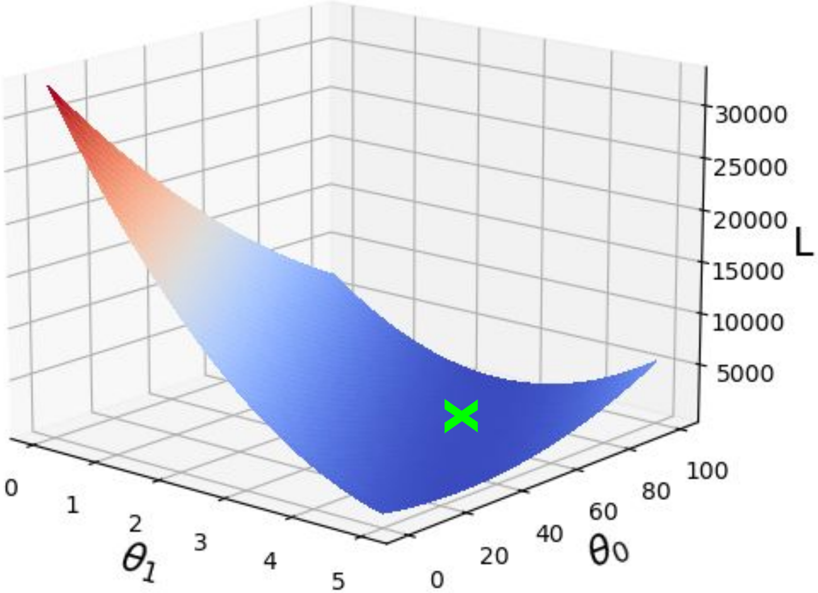
Method 2: Using Calculus (the proper way)

- Minimum of loss function L ➜ Calculus to the rescue!
  - Partial derivatives with respect to to all θ_i are 0

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

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

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



Loss Function — Derivatives

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

$$\Downarrow$$

…lots of tedious math here…

$$\Downarrow$$

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

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

Basic approach to find the minimum

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

(2) Solve for θ

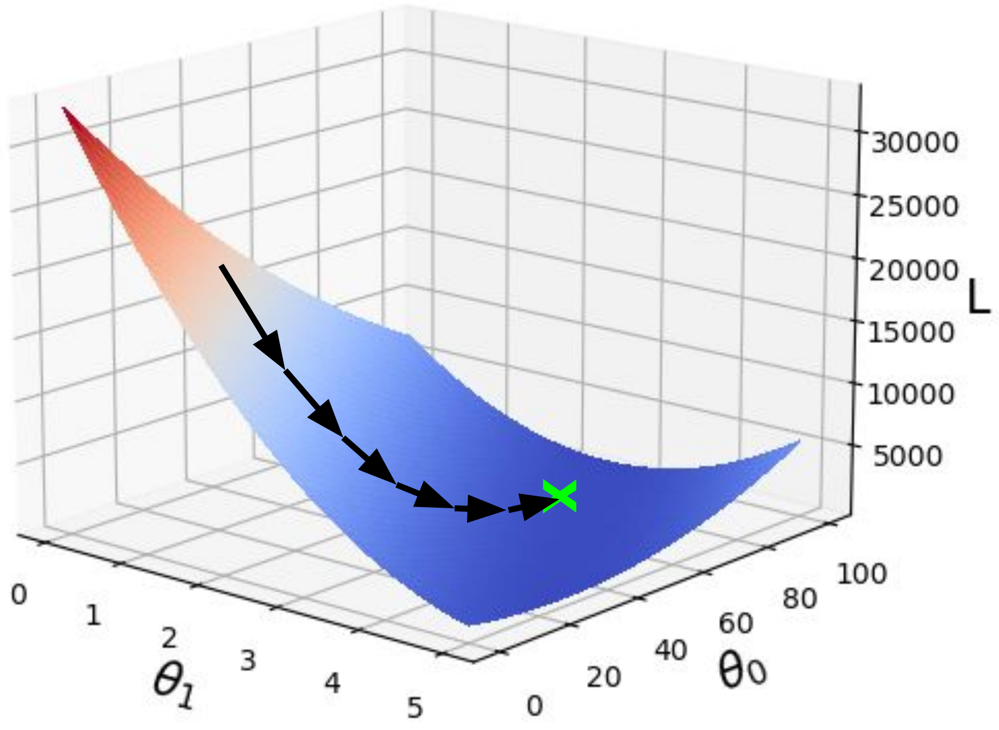
So are we done here?

Gradient Descent

- Problem: $\frac{1}{m}X^\top\left[\sigma\left(X\theta\right)-y\right]\overset{!}{=}0$ 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 with respect 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 $y = 1$)

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

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	$\theta_i x_i$	*Partial derivatives*	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**

➜ **1st iteration of Gradient Descent done!**

$$L_{CE} = 0.12$$

(down from 0.36)

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	$\theta_i x_i$	*Partial derivatives*	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**

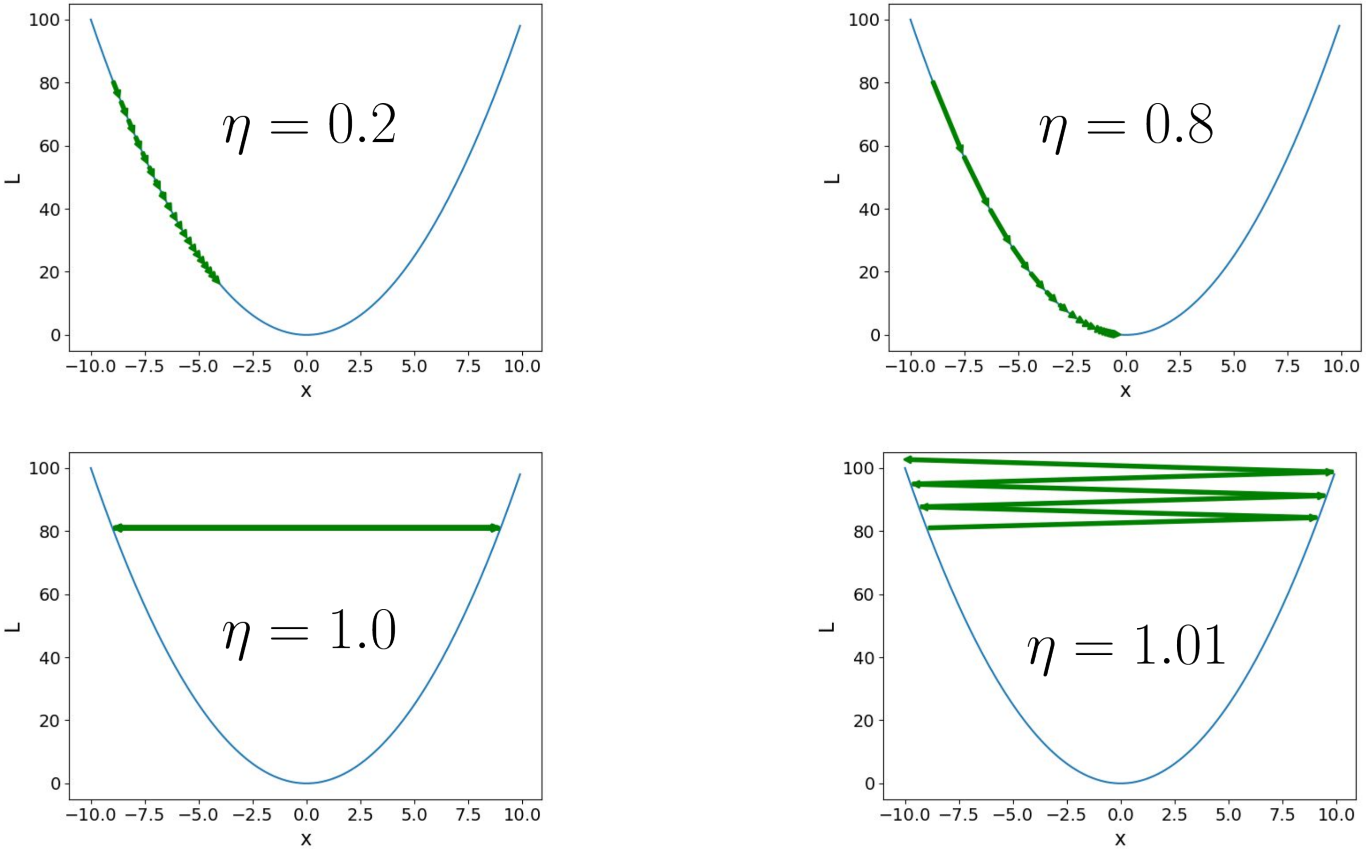
$$L_{CE} = 0.075$$

(down from 0.12)

➜ **2nd iteration of Gradient Descent done!**

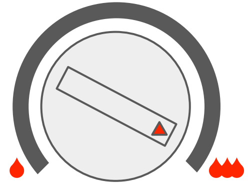
🏃‍♀️🏃🏃‍♂️ Quick Quiz

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

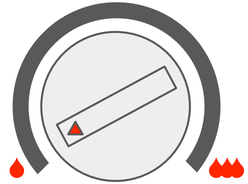


Gradient Descent — Variations

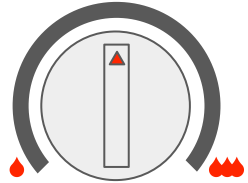
- (Basic) Gradient Descent
  - Calculate gradient und update θ for whole dataset



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

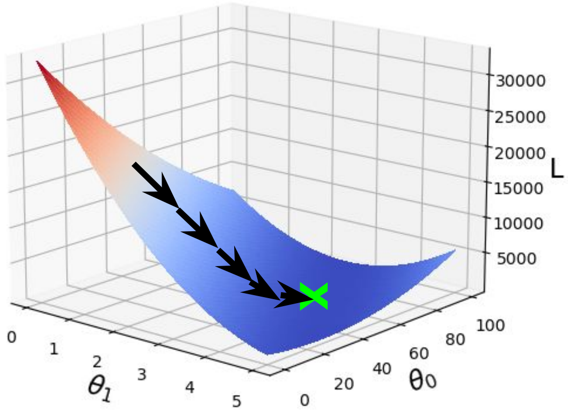


- Mini-batch Gradient Descent
  - Calculate gradient and update θ for batches of sample
  - e.g., batch = 64 data samples
  - In practice, often still referred to as SGD



Gradient Descent — Variations

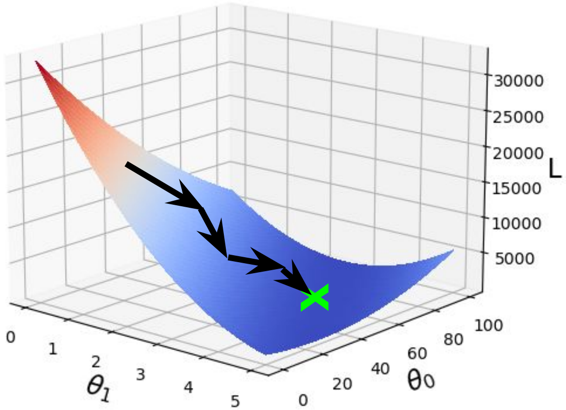
Gradient Descent



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

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

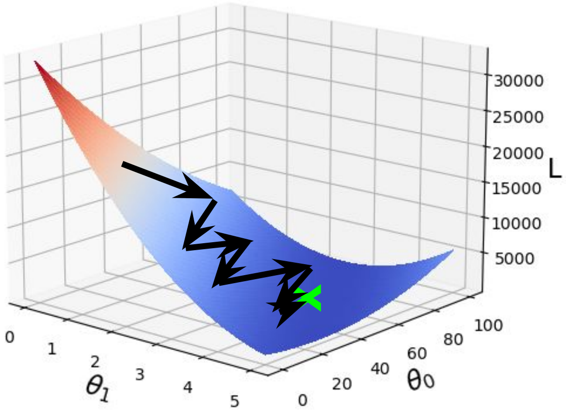
Mini-Batch Gradient Descent



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

Outline

- Generative vs. Discriminative Classifiers

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  - **Overfitting & Regularization**
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  - Basic Neural Network Architecture

Gradient Descent — When to Stop?

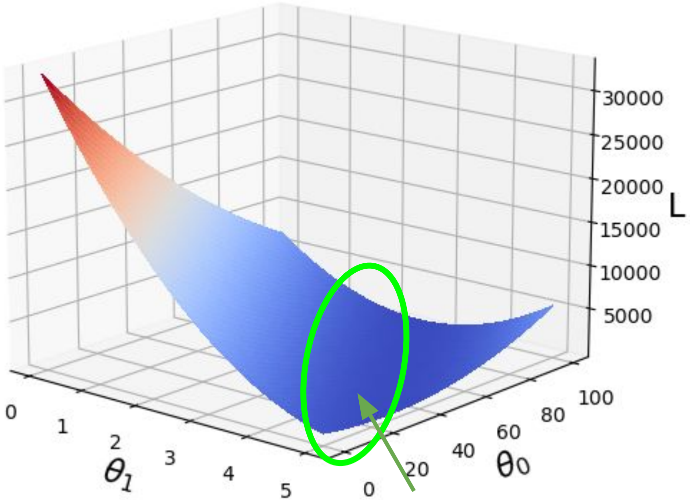
- Intuition: $\nabla_\theta L_{CE} < threshold$

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 small enough
  - Max. # iterations reached

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

🏃‍♀️🏃🏃‍♂️ Overfitting

- A model that perfectly matches the training data often has a problem.

🏃‍♀️🏃🏃‍♂️ Overfitting

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~~ 50	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

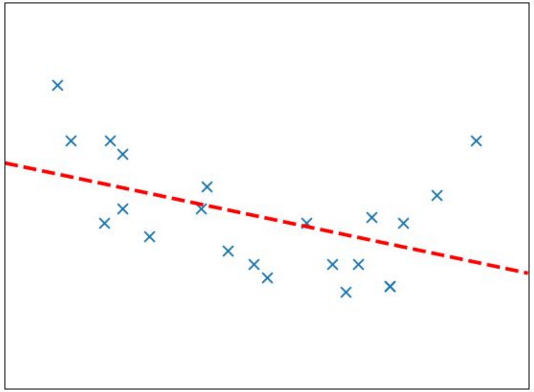
- Classifiers over-emphasizes the importance of pronouns
  ➜ large value for θ_4 (compared to other θ_i)

- Unseen negative review with many pronouns will most likely be misclassified

Overfitting — Basic Intuition

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

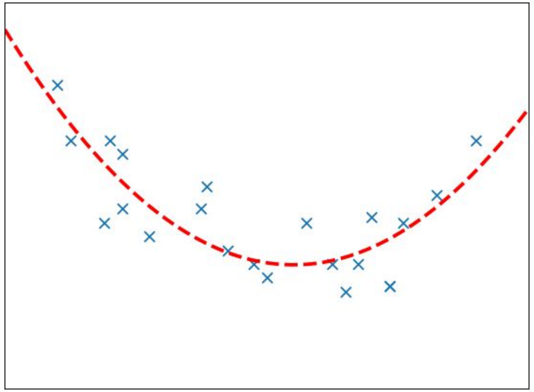
***p* = 1**



Underfitting

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

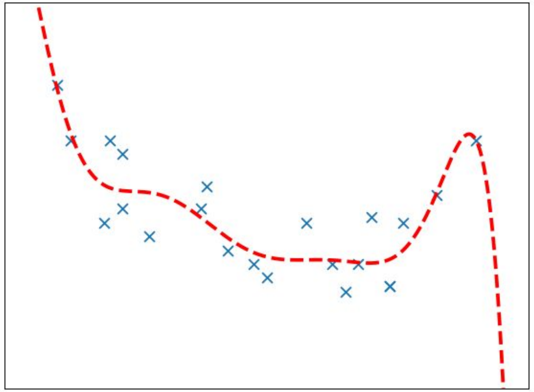
***p* = 2**



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

Regularization

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

⚠️ **Quick Quiz:** What do the indices m and n stand for in the equations here?

➜ **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"

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

L2 Regularization ("Ridge Regression")

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

L1 Regularization ("Lasso Regression")

New Loss ➜ New Gradient

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

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

  - No changes to Gradient Descent Algorithms

🏃‍♀️ 🏃 🏃‍♂️ Quick Quiz

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

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

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

⇒

Multiclass Logistic Regression

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

➜ **How can we ensure that?**

$f_{mystery}$ → Softmax

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

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

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

Example

- Example with 4 classes and 3 input features

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

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

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.

Break

Outline

- Generative vs. Discriminative Classifiers

- Logistic Regression
  - Setup as Probabilistic Classifier
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  - Gradient Descent
  - Overfitting & Regularization
  - Multiclass Logistic Regression

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

Pre-Lecture Activity from Last Week

- Assigned Task
  - Post a 1–2 sentence answer to the following question into your Tutorial Group's discussions
    (you will find the thread on Canvas > Discussions)

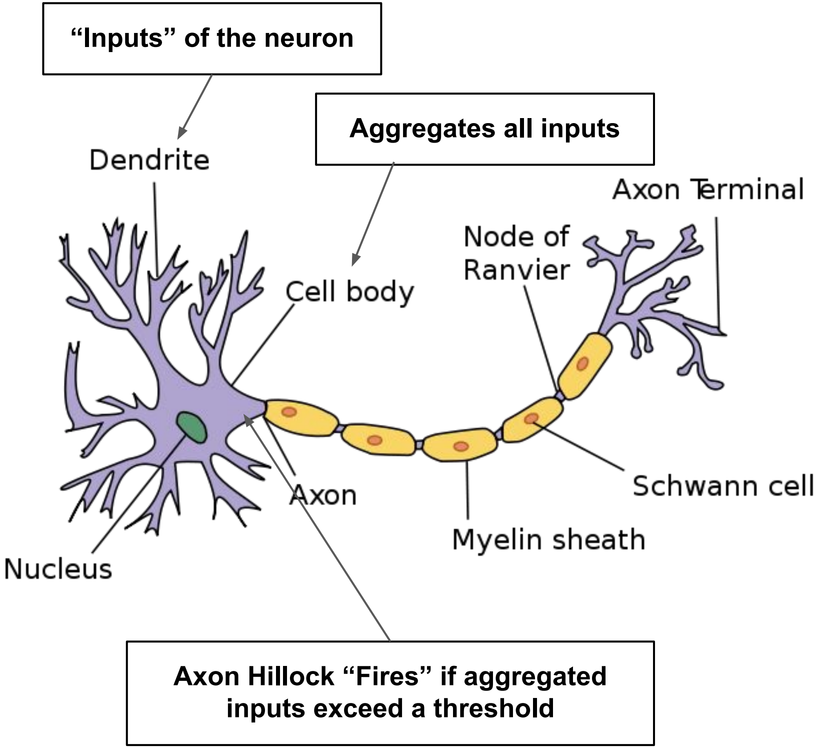
"What is a common myth about neural networks?"

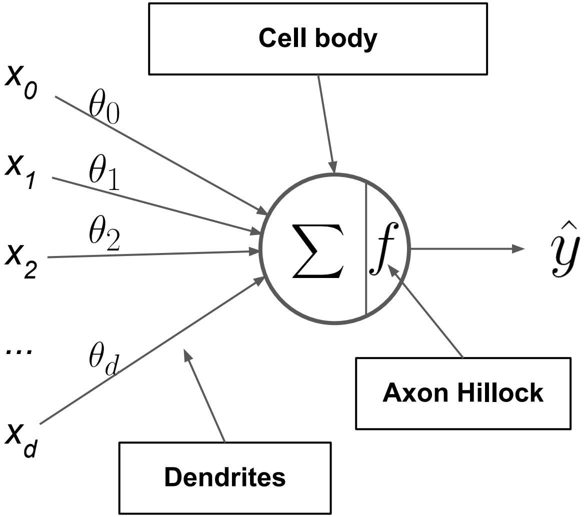
Side notes:

- 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

brain works. Moreover, as the field of ML progressed over the years, and

Biological Inspiration — Neuron



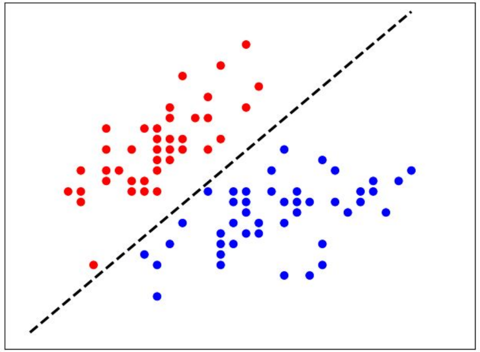


➜ Logistic Regression (crudely) a biological neuron

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)



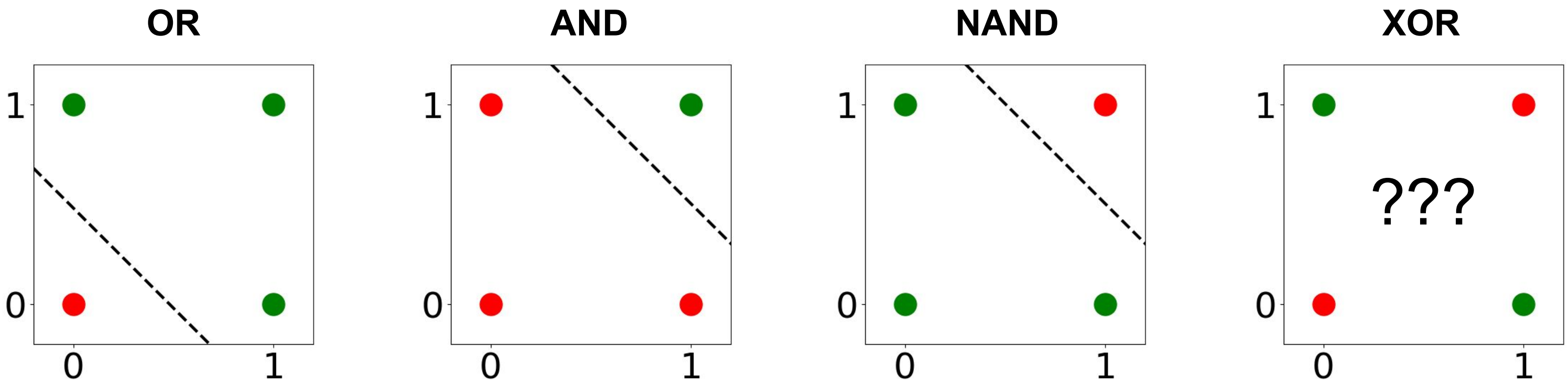
- What if we want or need to represent non-linear relationships between features? We can't!

➜ 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

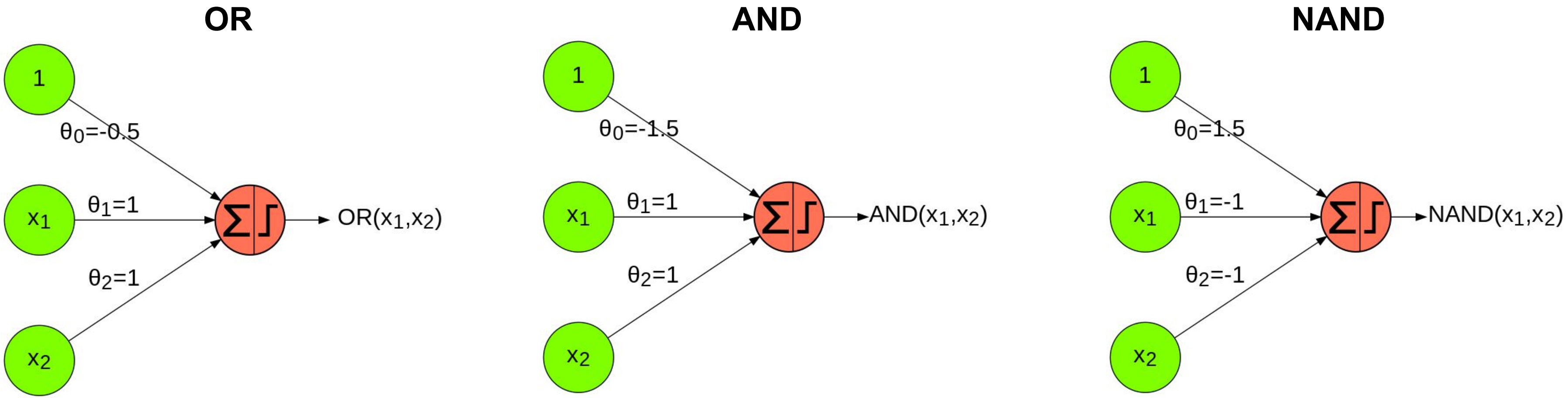
Follow along yourself!
https://www.desmos.com/calculator/waert4utde



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 Sigmoid
    (strictly speaking, this makes it a Perceptron not a Linear Regression unit)

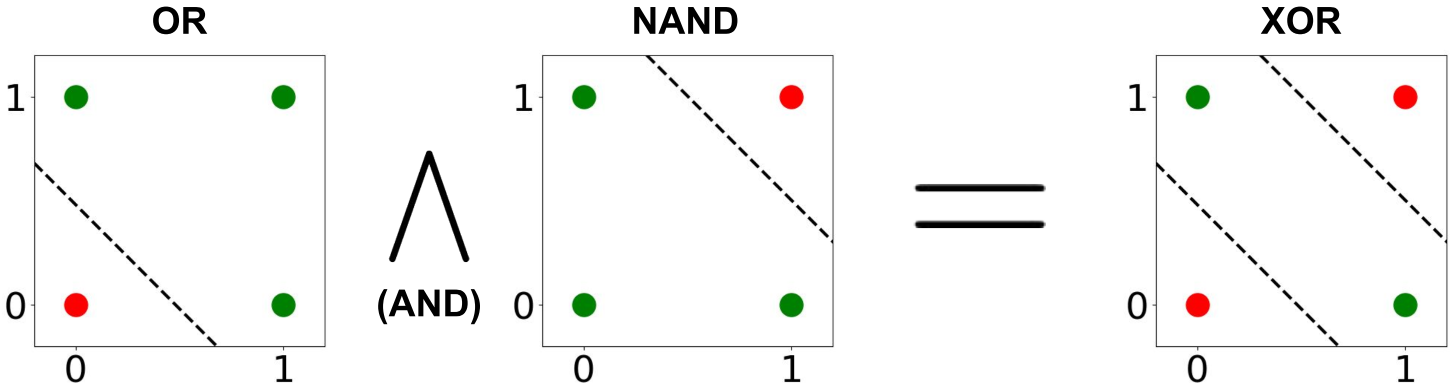
$$f_{step} = \begin{cases} 1 & , \text{if } \theta^\top x > 0 \\ 0 & , \text{otherwise} \end{cases}$$



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

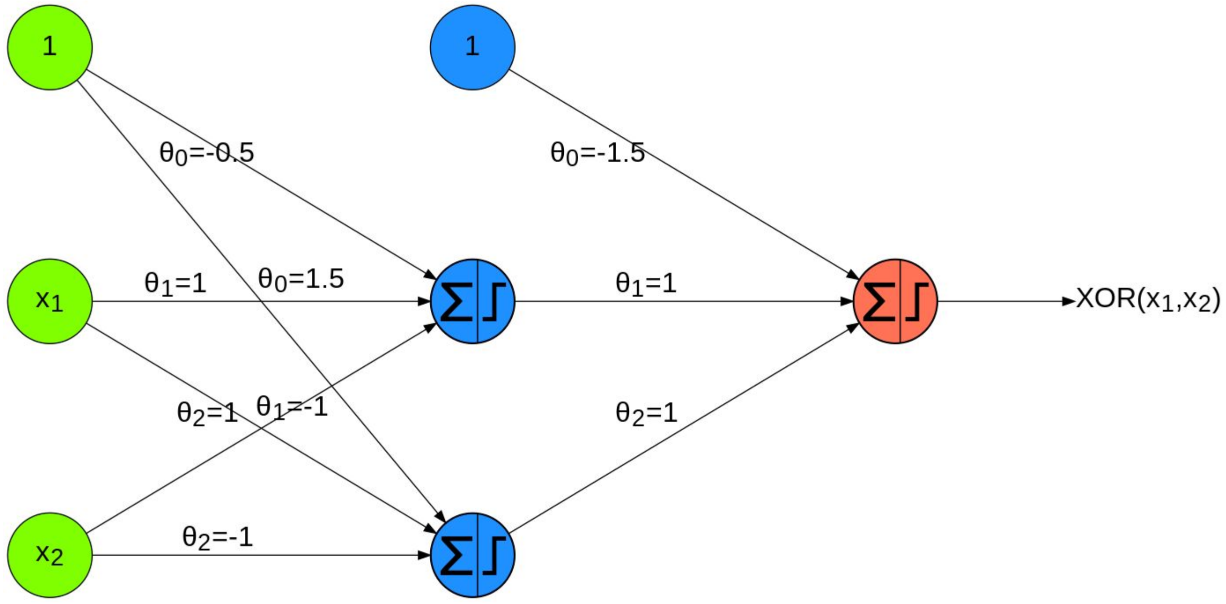
- Deriving XOR from simple classifiers
    - Note: this is not only way to do it, just convenient



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

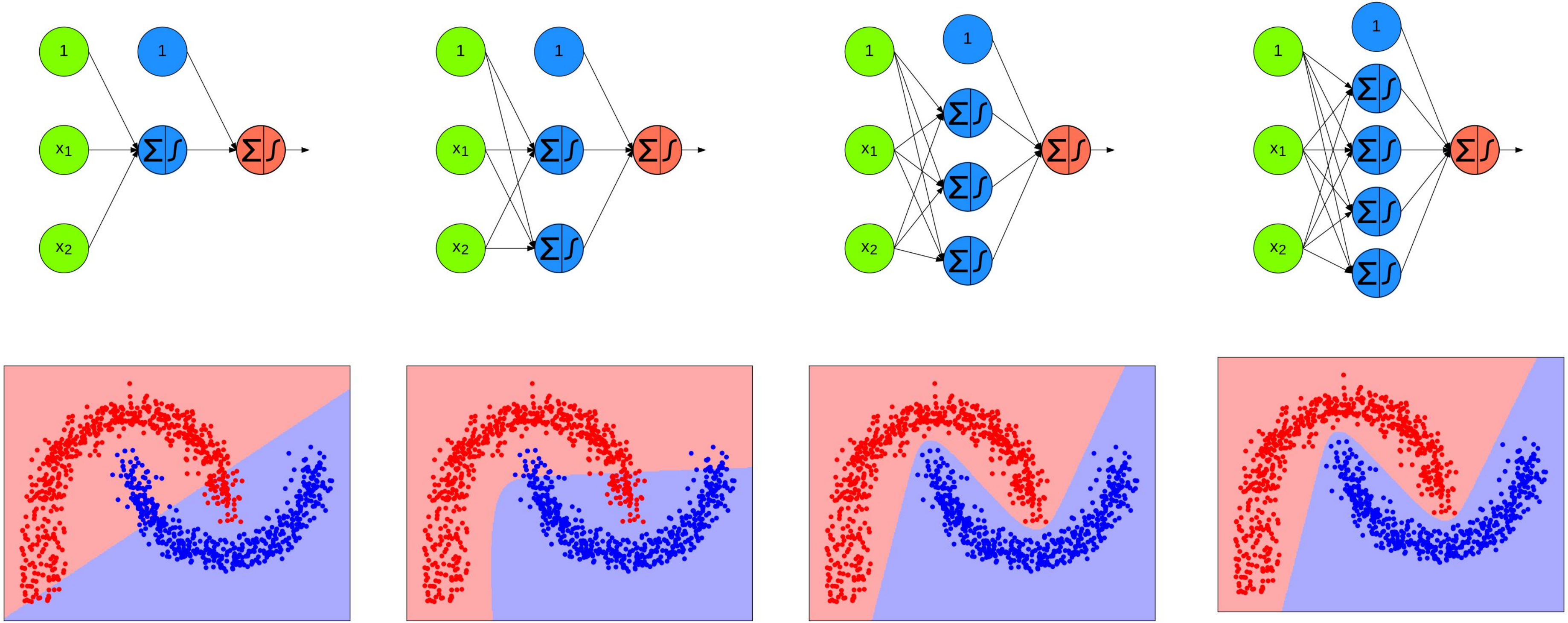
XOR

- 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 in having too many neurons?



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

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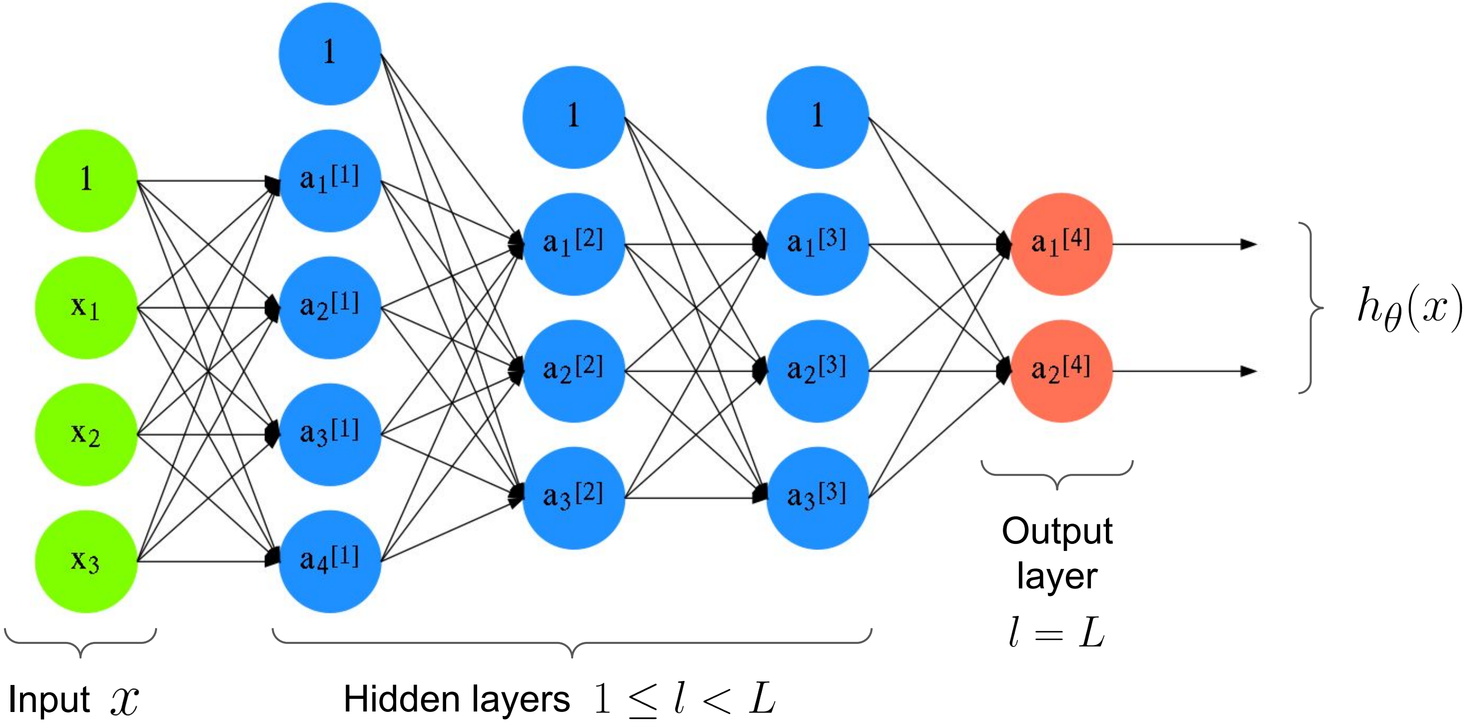
A Neural Network (Feedforward NN)

- 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

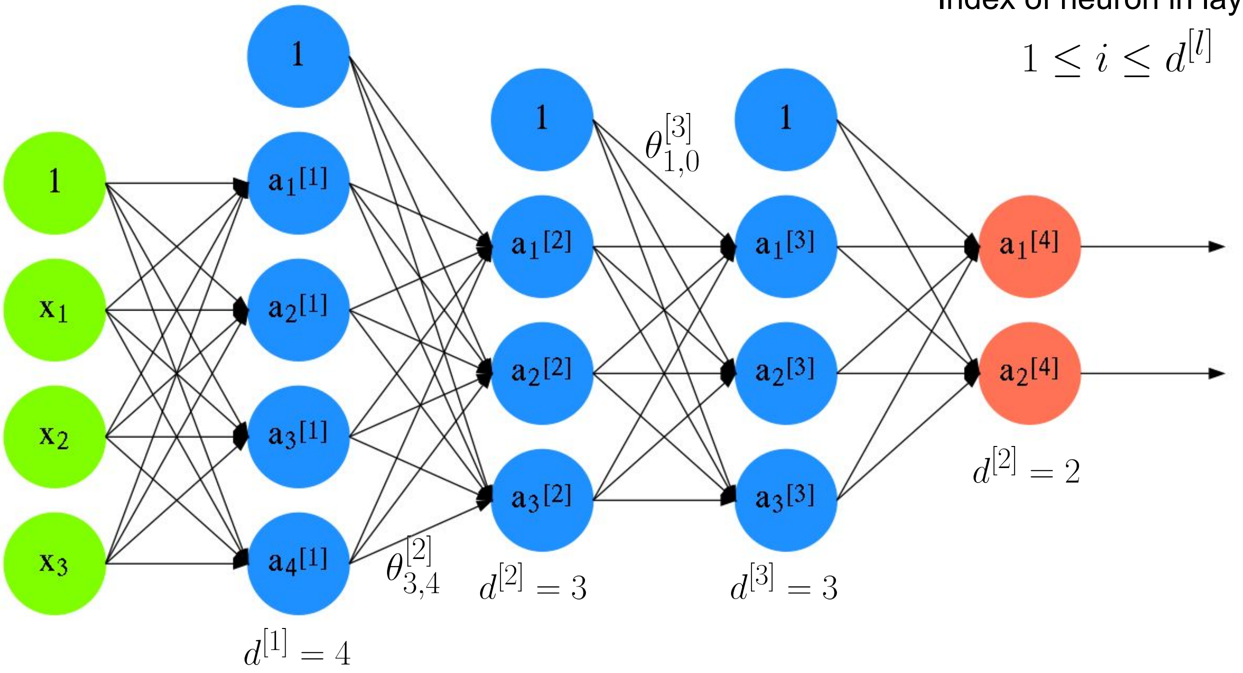
$$\theta^{[l]}_{i,j}$$

Index of neuron in layer l

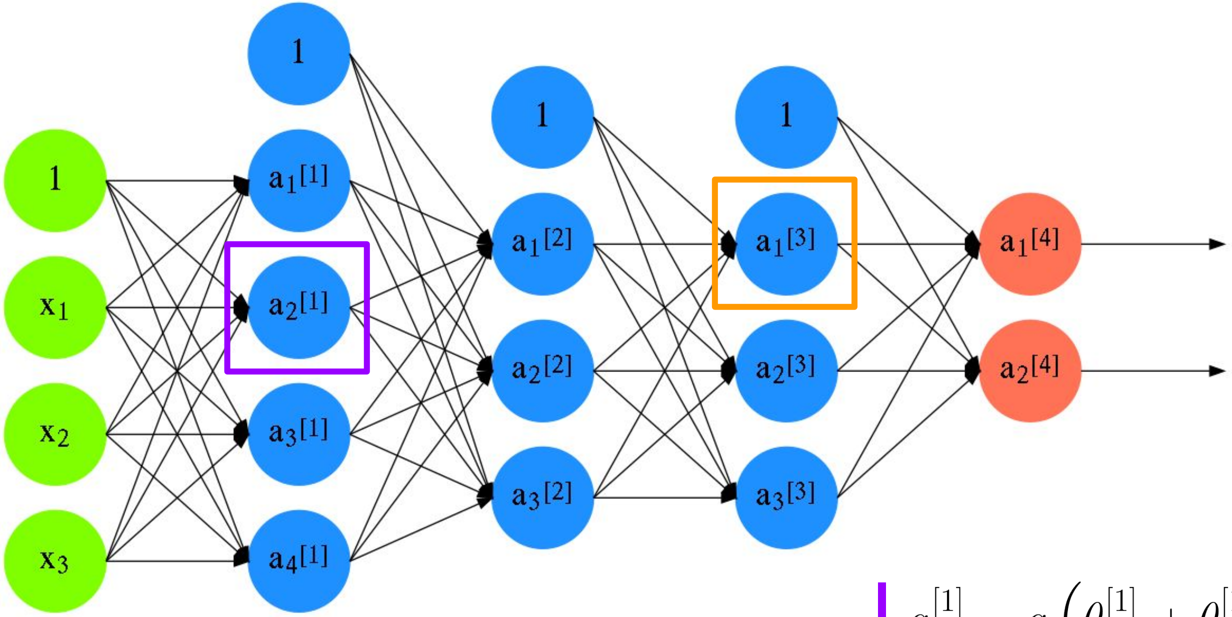
$1 \leq i \leq d^{[l]}$

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

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

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

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)

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

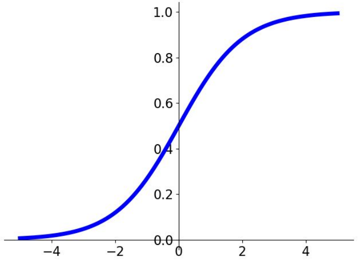
Weight matrix $\theta^{[l]} \in \mathbb{R}^{d^{[l]} \times d^{[l-1]}}$

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

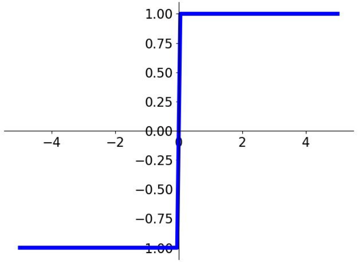
Neural Network — Activation Functions

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

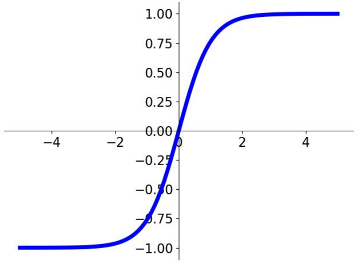
Sigmoid



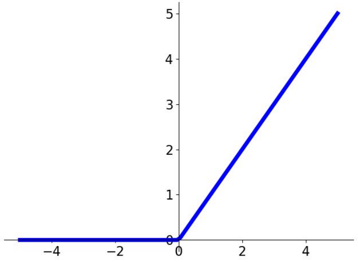
Sign



Tanh

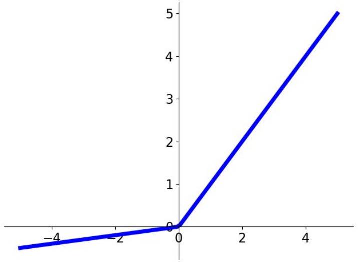


ReLU



ReLU = Rectified Linear Unit

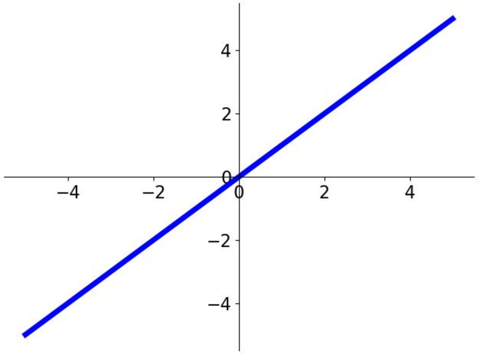
Leaky ReLU



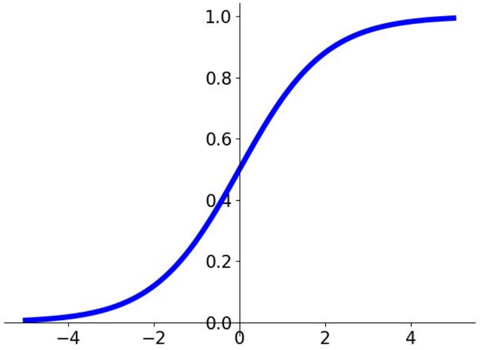
Neural Network — Activation Functions

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

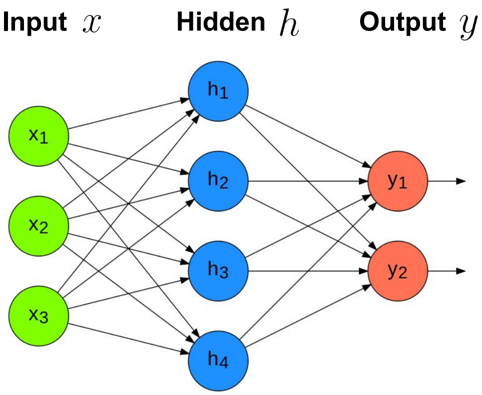
Linear function for regression tasks



Sigmoid function for classification tasks



Example



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

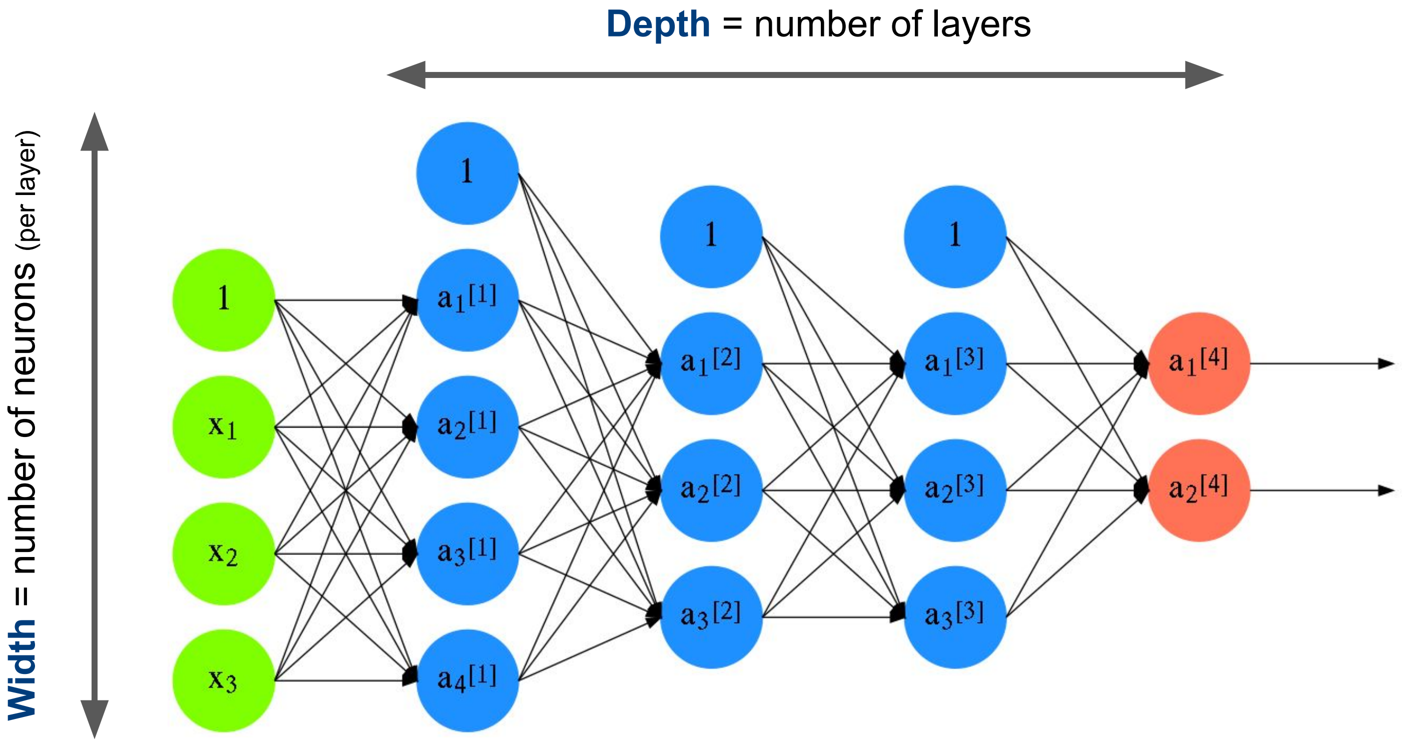
$$y = g_y\left(\theta_y h\right) \quad \text{, with } \theta_y \in \mathbb{R}^{2\times 4}$$

$g_h,\ g_y$: 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

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)

Outlook for Next Week: Embeddings and Ethics

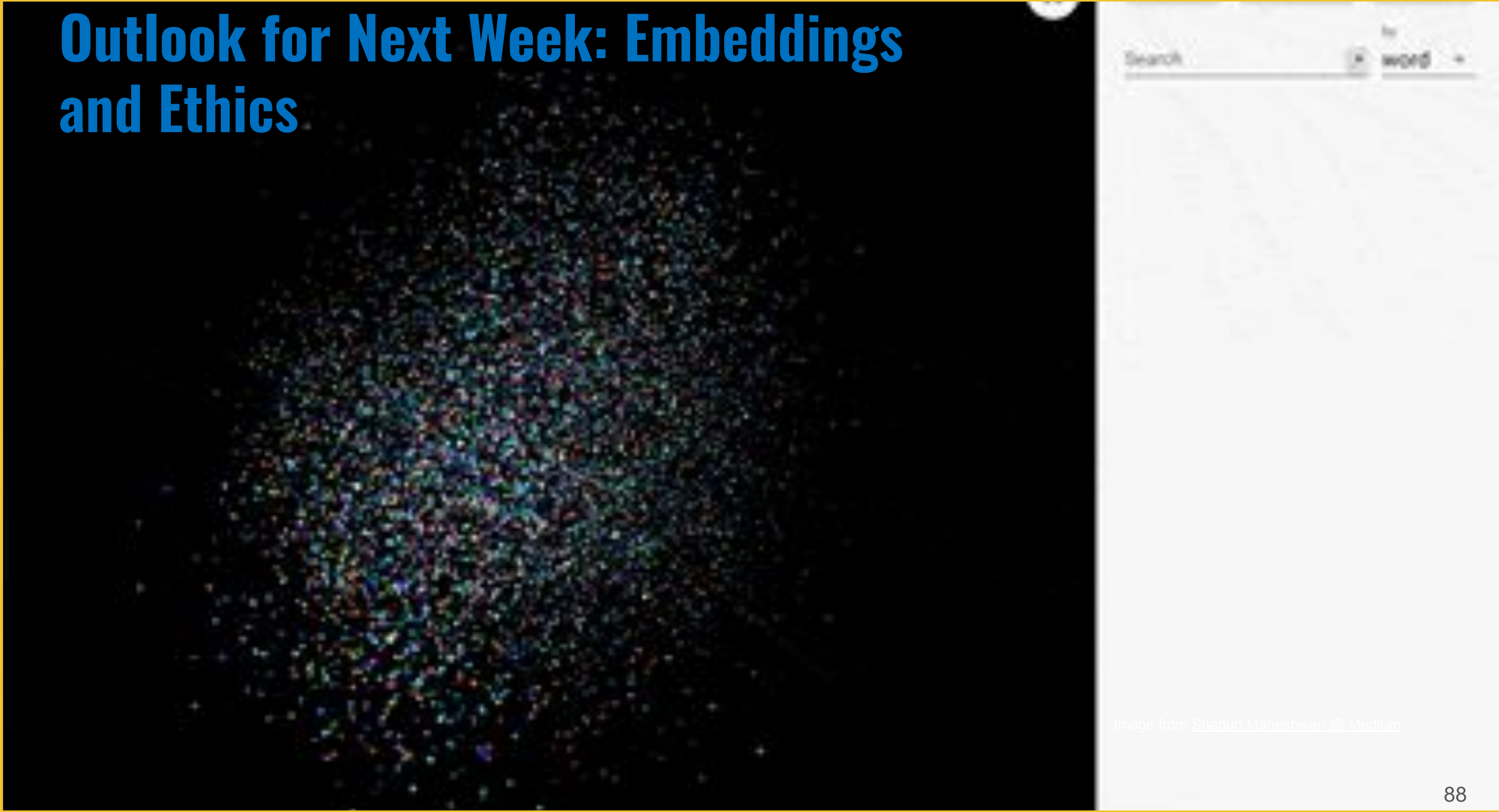


Image from Shagun Maheshwari @ Medium

Pre-Lecture Activity for Next Week

- Assigned Task (due before Feb 23)
    - Post a 1-2 sentence answer to the following question in your Tutorial Group's discussion
      (you will find the thread on Canvas > Discussions)

"What do we mean by sparse or dense vectors?
Are documents characterised by tf-idf sparse or dense?"

Read some blog posts or online articles, and cite them with the links in your answer

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 this won't help you learn better