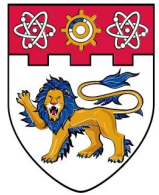


NANYANG TECHNOLOGICAL UNIVERSITY
SINGAPORE

Natural Language Processing

SC4002 / CE4045 / CZ4045

by Wang Wenya

Email: wangwy@ntu.edu.sg

Contents adapted from Dr. Joty Shafiq's notes

Click here for Lecture 1

Outline for today

01 Course Logistics

02 What is NLP (a quick recap)

03 Plan for the second half

04 Introduction to ML & DL

01 Course Logistics

Time

- Lecture: Wednesday 9:30 - 11:30 (LT27)
- Tutorial: Wednesday 11:30 - 12:30 (LT27)

Materials: will be uploaded before each lecture

Pre-requisites

- Basic probability and statistics
- Multivariate Calculus, linear algebra
- Fundamentals of machine learning

01 Course Logistics

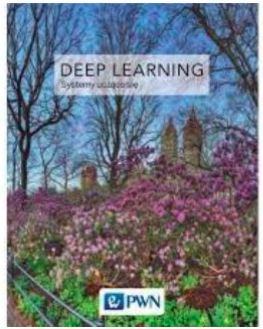
Objectives

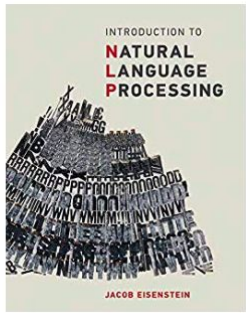
- Understand deep learning methods in NLP
- Be familiar with typical NLP applications
- Be able to build simple deep learning systems to solve NLP problems
- Be aware of and adapt to emerging trends of NLP
- Understand key challenges for current techniques

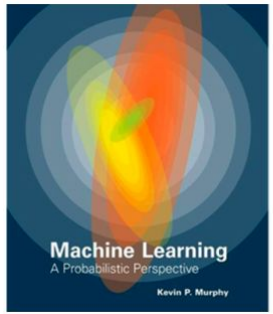
01 Course Logistics

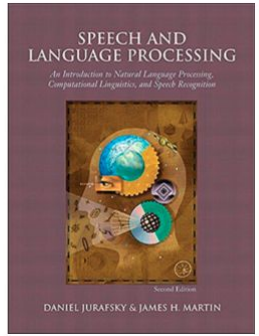
Optional Textbooks

- Deep Learning by Goodfellow, Bengio, and Courville
- Machine Learning – A Probabilistic Perspective by Kevin Murphy
- Natural Language Processing by Jacob Eisenstein
- Speech and Language Processing by Dan Jurafsky and James H. Martin









01 Course Logistics

Evaluation

- 15% midterm quiz (for 1st half, week 8 tutorial)
- 35% group assignment (released)
- 50% final exam

Outline for today

01 Course Logistics

02 What is NLP (a quick recap)

03 Plan for the second half

04 Introduction to ML & DL

02

What is NLP?

"We study formalisms, models and algorithms to allow computers to perform useful tasks involving knowledge about human languages."

Useful Tasks

Text classification

sentiment analysis, spam detection, topic classification

Information extraction

entity and relation recognition, event extraction

Structured prediction

dependency parsing, semantic role labeling

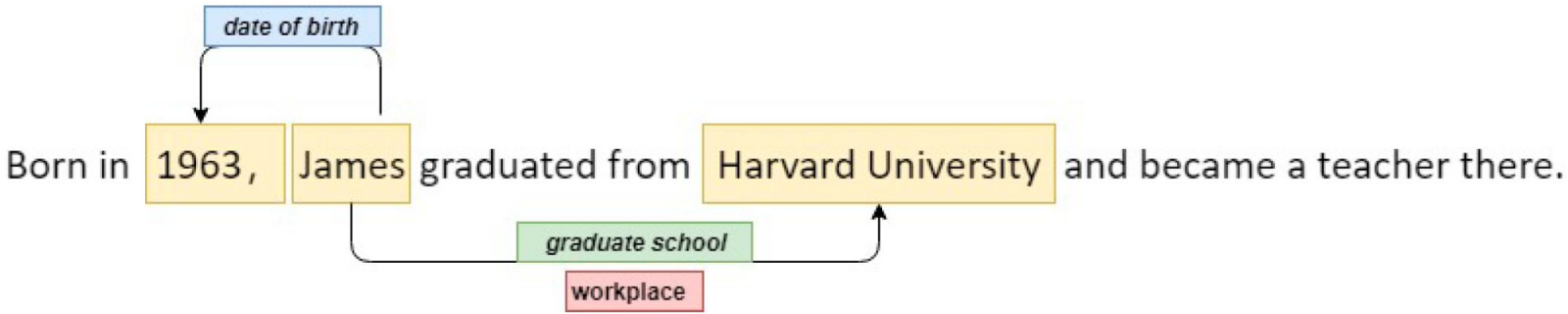
Text generation

summarization, conversation

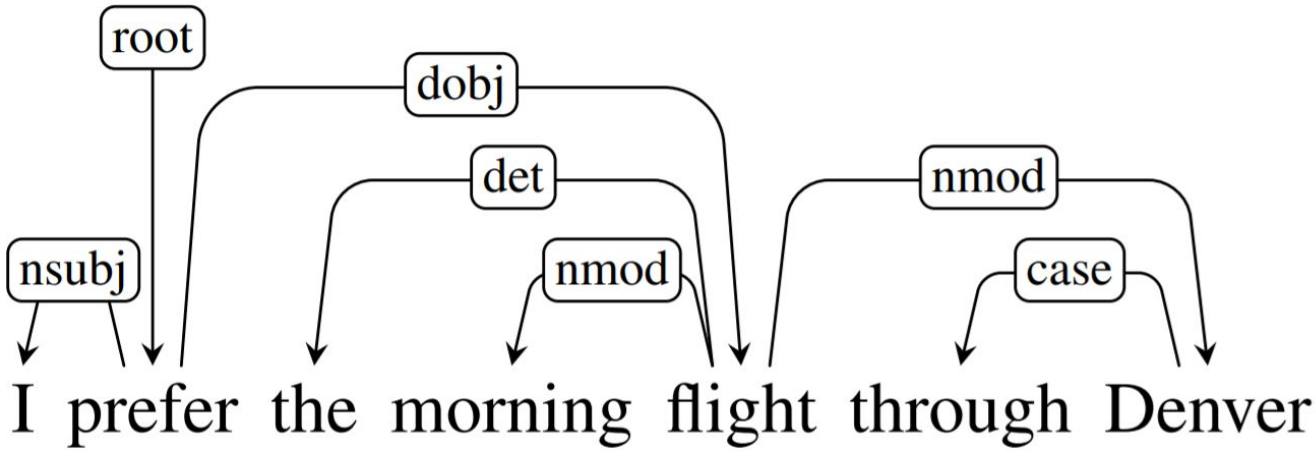
Text Classification - Sentiment

The dessert is excellent.	★★★★☆
Service was quite slow.	★★☆☆☆
Good for a quick meal, but nothing special.	★★★☆☆
Completely lacking in good taste, good service, and good ambience.	★☆☆☆☆

Information Extraction



Structured Prediction - Parsing



Text Generation - Summarization

(a) Extractive Summarization

Source Text: Peter and Elizabeth took a taxi to attend the night party in the city.

While in the party, Elizabeth collapsed and was rushed to the hospital.

Summary: Peter and Elizabeth attend party city. Elizabeth rushed hospital.

(b) Abstractive Summarization

Source Text: Peter and Elizabeth took a taxi to attend the night party in the city.

While in the party, Elizabeth collapsed and was rushed to the hospital.

Summary: Elizabeth was hospitalized after attending a party with Peter.

Useful Tasks

Question answering

Reading comprehension, open-domain

Multimodal

Image-to-text, text-to-speech synthesis

Machine translation

Source language to target language

Knowledge graph

KG construction, link prediction

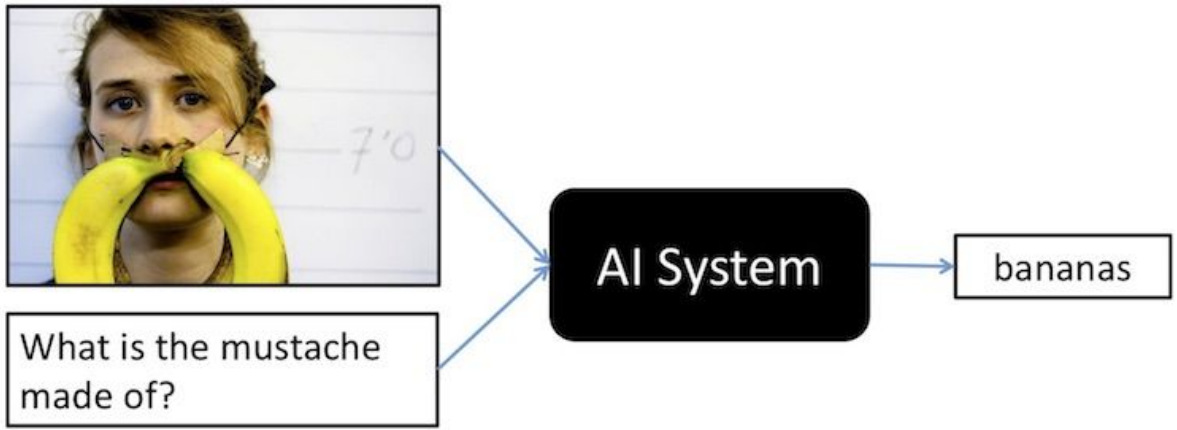
Reading Comprehension

Passage:
The two halves of the city were actually founded and plotted as separate cities, but soon grew together. The north side is characterized by very diverse and fashionable urban neighborhoods near the city center and sprawling suburbs further north. South Oklahoma City is generally more blue collar working class and significantly more industrial, having grown up around the Stockyards and meat packing plants at the turn of the century, and is currently the center of the city's rapidly growing Latino community.

Question:
Which side is more urban and fashionable?

Gold Answer: North Oklahoma City

Multimodal - VQA

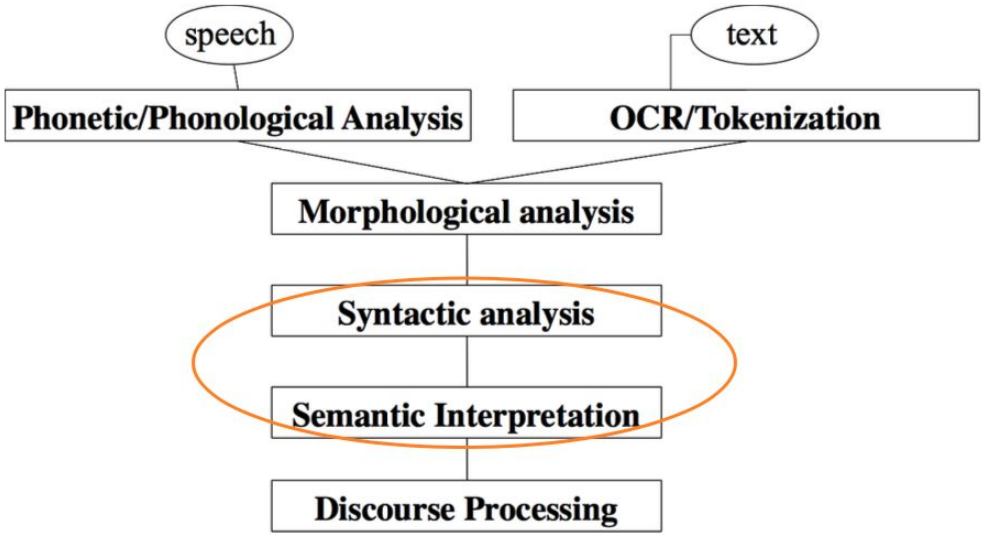


02

What is NLP?

"We study formalisms, models and algorithms to allow computers to perform useful tasks involving knowledge about human languages."

Knowledge about Languages



Mainly covered in the first half, not this one

02

What is NLP?

"We study formalisms, models and algorithms to allow computers to perform useful tasks involving knowledge about human languages."

Outline for today

01 Course Logistics

02 What is NLP (a quick recap)

03 Plan for the second half

04 Introduction to ML & DL

Modules we will cover

ML & DL
Introduction to machine/deep learning

Word
Word vectors, language modeling

Transformer
Attention mechanism, encoder/decoder

Sequence
Sequence modeling, seq2seq learning

Pretraining
Masking, natural language generation

Prompting
Prompts, in-context learning

Outline for today

01 Course Logistics

02 What is NLP (a quick recap)

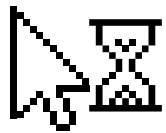
03 Plan for the second half

04 Introduction to ML & DL

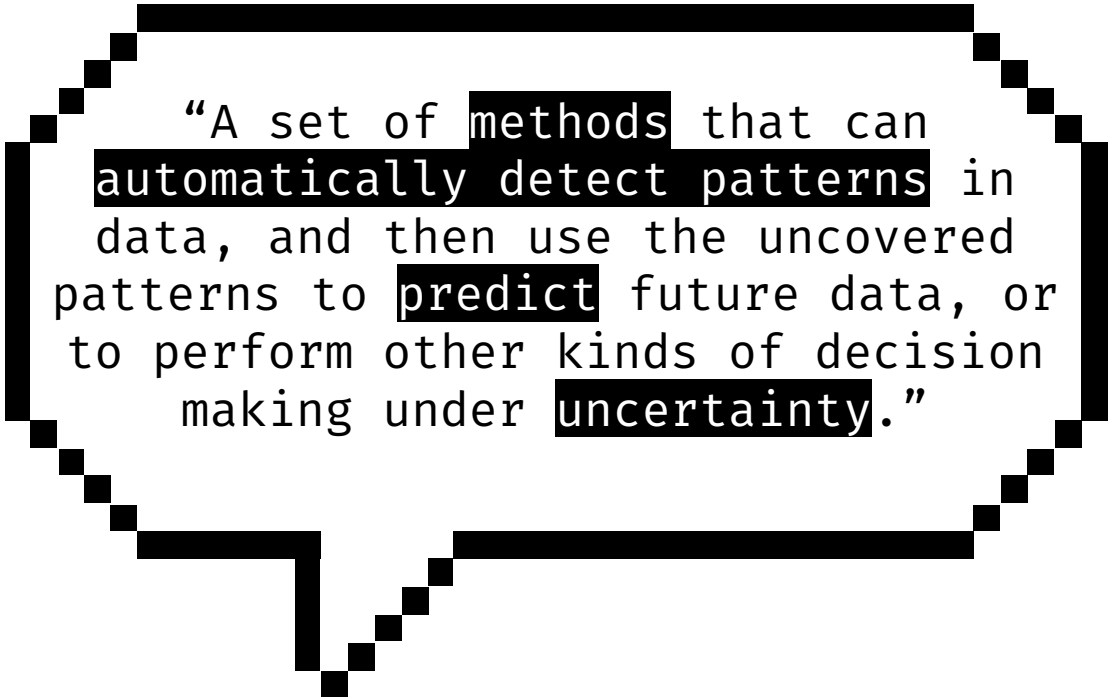
Introduction to ML & DL

Machine Learning

- Definition
- Paradigms of machine learning
- Machine learning pipeline
- Typical algorithms
  - Linear regression
  - Logistic regression
- Optimization – gradient descent



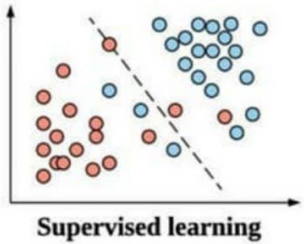
What is Machine Learning?



Paradigms of Machine Learning

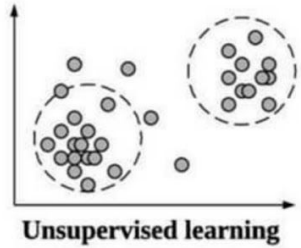
Supervised Learning

Learning a function that maps input data to output data, based on labeled examples.



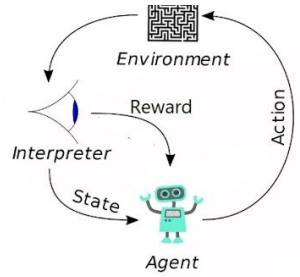
Unsupervised Learning

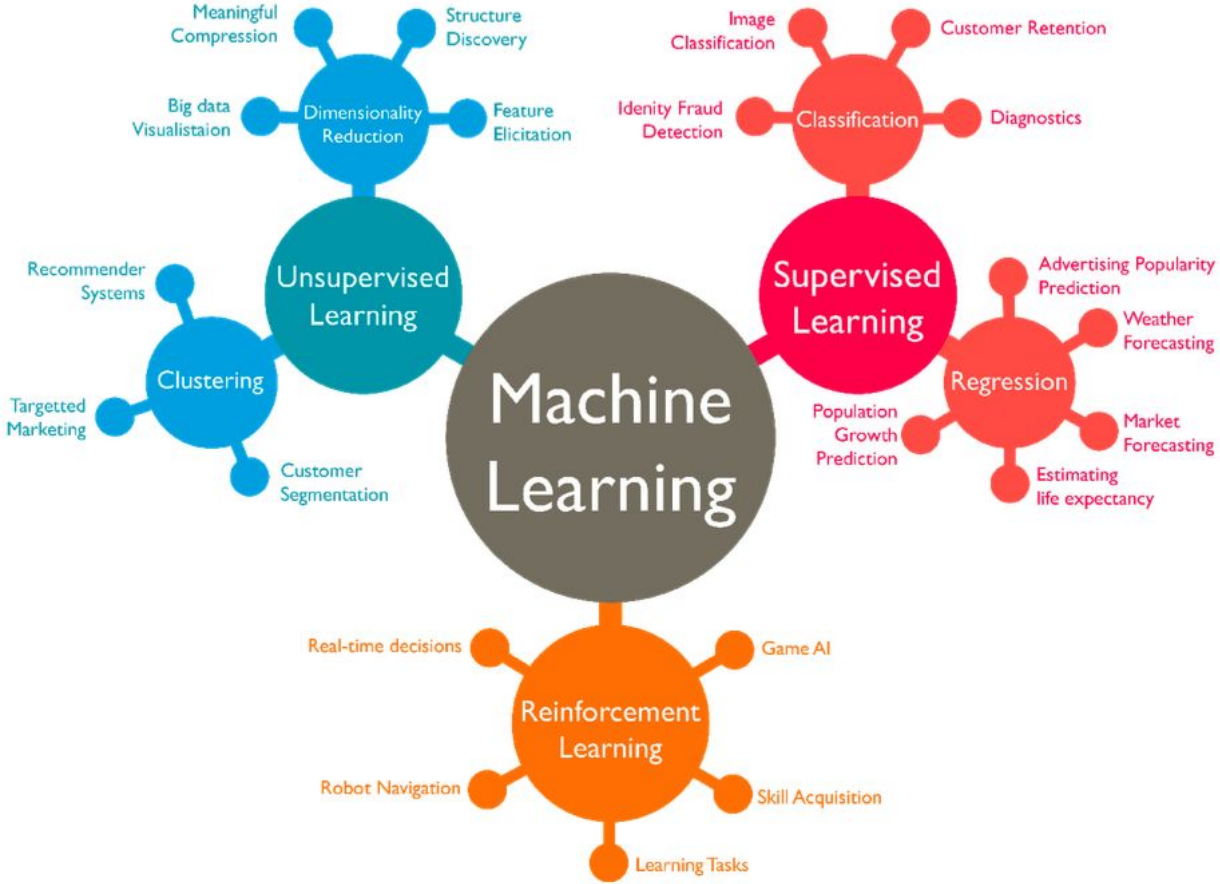
Finding hidden patterns or intrinsic structures in unlabeled data.



Reinforcement Learning

learning how to act or behave when given occasional reward or punishment signals




Machine Learning
Unsupervised Learning
Dimensionality Reduction
Meaningful Compression
Structure Discovery
Big data Visualistaion
Feature Elicitation
Clustering
Recommender Systems
Targetted Marketing
Customer Segmentation
Supervised Learning
Classification
Image Classification
Customer Retention
Idenity Fraud Detection
Diagnostics
Regression
Advertising Popularity Prediction
Weather Forecasting
Population Growth Prediction
Market Forecasting
Estimating life expectancy
Reinforcement Learning
Real-time decisions
Game AI
Robot Navigation
Skill Acquisition
Learning Tasks

Supervised Learning

Classification: To learn a mapping from inputs x to outputs y, where $y \in \{1, \ldots, C\}$, with C being the number of classes, which means y is categorical.

- If C = 2, this is called binary classification (in which case we often assume $y \in \{0, 1\}$
- If C > 2, this is called multiclass classification.

Examples

(1) Document classification and email spam filtering

(2) Sentiment classification

(3) Image classification and handwriting recognition

(4) Face detection and recognition

Supervised Learning

Regression: To learn a mapping from inputs x to outputs y, where y is real-valued.

Examples

1. Predict tomorrows stock market price given current market conditions and other possible side information.
2. Predict the age of a viewer watching a given video on YouTube.
3. Predict the location in 3d space of a robot arm end effector, given control signals (torques) sent to its various motors.
4. Predict the temperature at any location inside a building using weather data, time, door sensors.

Unsupervised Learning

We are just given input data, without any outputs. The goal is to discover interesting structure in the data; this is sometimes called knowledge discovery.

1. Discovering clusters: To cluster data into groups and estimate which cluster each data sample belongs to.
2. Discovering latent factors: To project the data to a lower dimensional subspace which captures the essence of the data. It is also called "Dimension Reduction". (eg, PCA)
3. Discovering graph structure.

Machine Learning Pipeline

Model Assumption

Inductive bias:
linear? non-linear?

Model training

Learn the model approximating input-output mapping

Model testing

Evaluate the model on test data

Linear Regression

Problem Setup

Training Data is represented by:

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$$ Supervised

Here,
$\mathcal{D}$ is called the training set.
N is the number of training example.
$\mathbf{x}_i$ is a d-dimensional vector of features (also called attributes or covariates) i.e. #features is d.
y_i is called output or response variable.

For regression: y_i is real-valued i.e. $y_i \in \mathbb{R}$

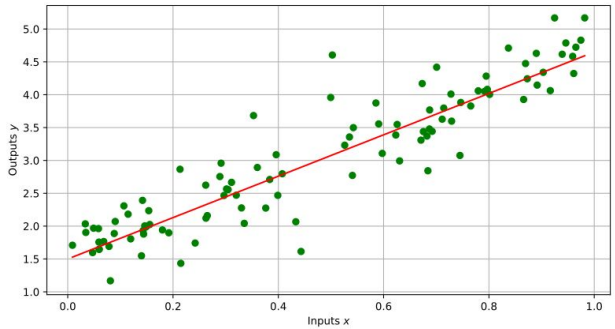
Linear Regression

What is it?

The basic idea behind regression is that, you want to model the relationship between a real valued outcome variable y, and a vector of explanatory variables $\mathbf{x} = (x_1, x_2, \ldots, x_n)$.

A linear regression relates y to a linear predictor function of $\mathbf{x}$.
For a given data point i, the linear function is of the form:

$$\hat{y}_i = w_0 + w_1 x_{i1} + \ldots + w_d x_{id}$$



Linear Regression

Least Square Formulation of the Loss

In this formulation, the least squares fit is the line that **minimizes** the sum of the squared distances between observed data and predicted values, i.e. it minimizes the **Residual Sum of Squares** (*RSS*):

$$\arg\min_{\mathbf{w}} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Predicted output

Linear Regression

Least Square Formulation

So our **objective function** is:

$$J(\theta) = \arg\min_{\theta} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

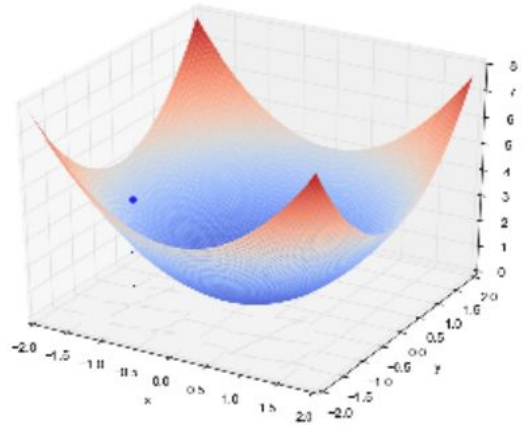
$$= \sum_{i=0}^{N} (y_i - \mathbf{x}_i^\intercal \mathbf{w})^2 = (y - \mathbf{X}\mathbf{w})^\intercal (y - \mathbf{X}\mathbf{w})$$

Vector notation

Linear Regression

Least Square Formulation

Notice that, we want to minimize $J(\theta)$.
We see that $J(\theta)$ is **Quadratic**. Hence it will be Bowl Shaped.



Linear Regression (Optional)

Least Square Formulation

$$J(\theta) = (y - \mathbf{X}\mathbf{w})^\top (y - \mathbf{X}\mathbf{w}) = (y^\top - \mathbf{w}^\top \mathbf{X}^\top)(y - \mathbf{X}\mathbf{w})$$
$$= y^\top y - y^\top \mathbf{X}\mathbf{w} - \mathbf{w}^\top \mathbf{X}^\top y + \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w}$$

Taking partial derivative with respect to $\mathbf{w}$:

$$\frac{\partial}{\partial \mathbf{w}} J(\theta) = \frac{\partial}{\partial \mathbf{w}} (y^\top y - y^\top \mathbf{X}\mathbf{w} - \mathbf{w}^\top \mathbf{X}^\top y + \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w})$$
$$= 0 - 2\mathbf{X}^\top y + 2\mathbf{X}^\top \mathbf{X}\mathbf{w}$$

Equqating $\frac{\partial}{\partial \mathbf{w}} J(\theta)$ to 0 we get,

$$\frac{\partial}{\partial \mathbf{w}} J(\theta) = 0 = -2\mathbf{X}^\top y + 2\mathbf{X}^\top \mathbf{X}\mathbf{w}$$
$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top y$$

Closed form Solution

Linear Regression

Probabilistic Formulation

If we ever want to understand linear regression from a **Bayesian perspective** we need to start thinking probabilistically.

We need to *flip things over* and instead of thinking about the line minimizing the cost, think about it as maximizing the likelihood of the observed data.

As we will see, this amounts to the **exact same thing** - *mathematically speaking* - it's just a different way of looking at it.

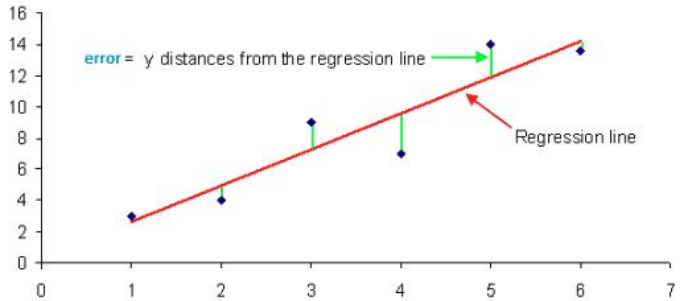
Linear Regression

Least Square Formulation

We can write the actual value of the i^{th} observation as:

$$y_i = w_0 + w_1 x_i + \epsilon_i$$

where ϵ_i is the residual, or error, we get for the i^{th} observation, i.e. the difference between our linear predictions and the true response.



Linear Regression

Probabilistic Formulation

If we ever want to understand linear regression from a **Bayesian perspective** we need to start thinking probabilistically.

We have seen previously:

$$y_i = \mathbf{w}^\intercal \mathbf{x}_i + \epsilon_i$$

We often assume that ϵ_i normally distributed with a mean of 0 i.e.

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

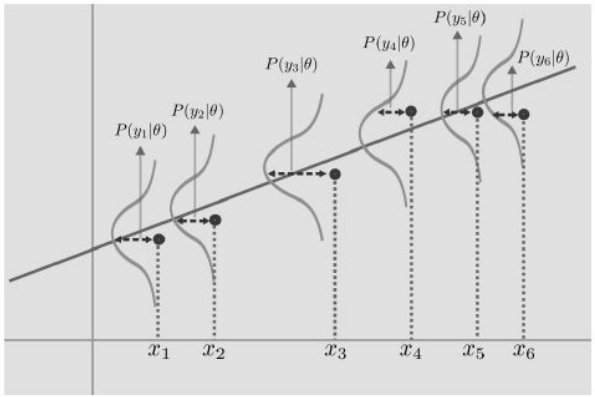
So, From the above equation we can say that:

$$y_i \sim \mathcal{N}(\mathbf{w}^\intercal \mathbf{x}_i, \sigma^2)$$

Linear Regression

Probabilistic Formulation

It is common to assume the training examples are Independent and Identically Distributed, commonly abbreviated to **IID**.
So, we assume all our training examples are Normally distributed with mean $\mathbf{w}^\top \mathbf{x}_i$ and variance σ^2.



Linear Regression

Maximum Likelihood Estimation

We can write Linear regression as a model of the form:

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\mathbf{w}^\intercal \mathbf{x}, \sigma^2)$$

Maximum likelihood Estimation

A common way to estimate the parameters of a statistical model is to compute the Maximum likelihood Estimation(MLE), which is defined as:

$$\hat{\boldsymbol{\theta}} \triangleq \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p(\mathcal{D}|\boldsymbol{\theta})$$

Linear Regression

Maximum Likelihood Estimation

$$\ell(\boldsymbol{\theta}) \triangleq \log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \boldsymbol{\theta})$$

$$= \sum_{i=1}^{N} \log \left[\left(\frac{1}{2\pi\sigma^2} \right)^{\frac{1}{2}} \exp \left(-\frac{1}{2\sigma^2}(y_i - \mathbf{w}^\mathsf{T}\mathbf{x}_i)^2 \right) \right]$$

$$= \frac{-1}{2\sigma^2} RSS(\mathbf{w}) - \frac{N}{2} \log(2\pi\sigma^2)$$

RSS stands for Residual Sum of Squares $\quad RSS(\mathbf{w}) \triangleq \sum_{i=1}^{N} (y_i - \mathbf{w}^\mathsf{T}\mathbf{x}_i)^2$

Linear Regression

Maximum Likelihood Estimation

$$\ell(\boldsymbol{\theta}) \triangleq \log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \boldsymbol{\theta})$$

$$= \sum_{i=1}^{N} \log \left[\left(\frac{1}{2\pi\sigma^2} \right)^{\frac{1}{2}} \exp \left(-\frac{1}{2\sigma^2}(y_i - \mathbf{w}^\mathsf{T}\mathbf{x}_i)^2 \right) \right]$$

$$= \frac{-1}{2\sigma^2} RSS(\mathbf{w}) - \frac{N}{2} \log(2\pi\sigma^2)$$

Least Square Formulation

RSS stands for Residual Sum of Squares

$$RSS(\mathbf{w}) \triangleq \sum_{i=1}^{N} (y_i - \mathbf{w}^\mathsf{T}\mathbf{x}_i)^2$$

Logistic Regression

Classification in NLP

- News stories: politics? sports? business? technology?
- Reviews of films, restaurants, products: positive? negative?
- Email, arXiv submissions: spam? Not spam?
- Will a piece of proposed legislation pass?
- What dialect is a text written in?
- Does the text contain content that will likely offend end people?

Logistic Regression

Problem Setup

Training Data is represented by

$$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$$ Supervised

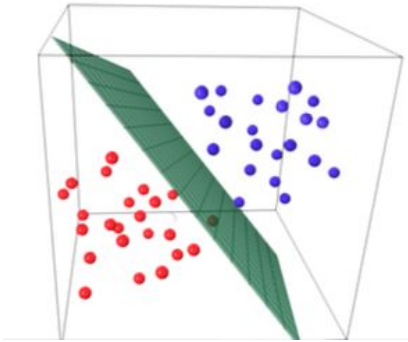
Here
$\mathcal{D}$ is called the training set.
N is the number of training examples.
x_i is a d-dimensional vector of features (also called attributes or covariates) i.e. #features is d.
y_i is called output or response variable.

For classification: y_i is categorial i.e. $y_i \in \{1, .. C\}$

Logistic Regression

y_i is categorial i.e. $y_i \in \{1, .., C\}$

First, we will consider the case of **binary response variable** that is, where it can take only two values, "0" and "1".
Cases where the response variable has more than two outcome categories may be analyzed in **Multinomial Logistic Regression**.



Logistic Regression

Linear regression for binary outcomes? No!

- The relationship between x and y is not linear.
- The response y is not normally distributed.
- Linear models cannot constrain y to be 0 or 1.

What do we need?

- We are interested in $p(y_i = 1|\mathbf{x}_i, \mathbf{w}) \in [0, 1]$
- Replace normal distribution with Bernoulli distribution, imaging we are tossing a coin, p=probability of success.

$$y \sim Bernoulli(p) \in \{0, 1\}$$

Logistic Regression

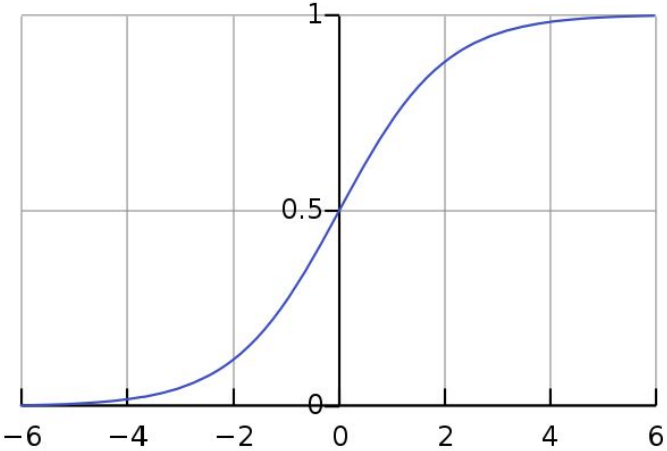
Ensure outputs to be probabilities $p(y_i = 1|\mathbf{x}_i, \mathbf{w}) \in [0, 1]$

Sigmoid Function

Sigmoid is a squashing function.
It maps the whole real line to [0,1].
It is also known as *logistic* or *logit* function
The term "sigmoid" means S-shaped. This is defined as:

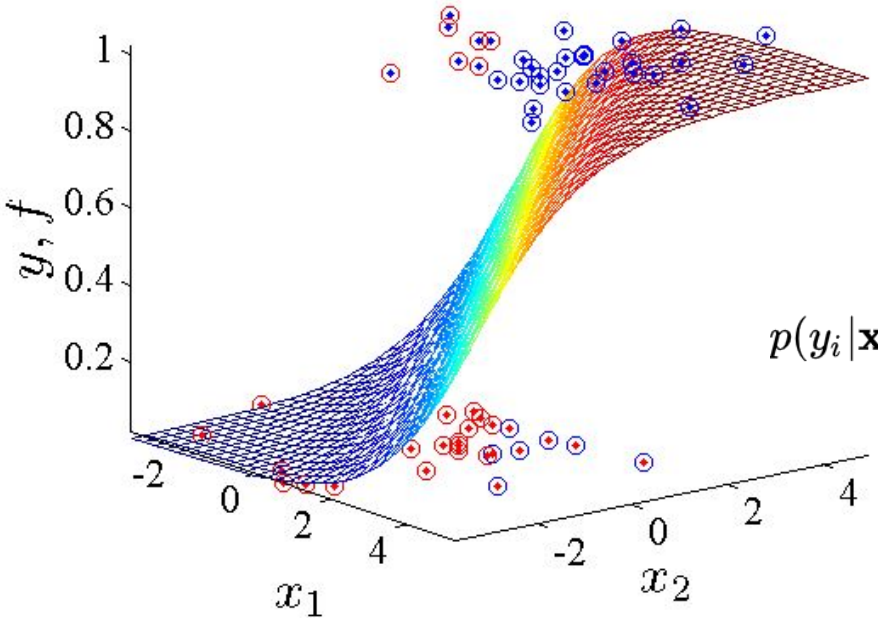
$$sigm(\eta) \triangleq \frac{1}{1 + \exp(-\eta)} = \frac{e^{\eta}}{e^{\eta} + 1}$$

$\sigma(\eta)$



Logistic Regression

Combine sigmoid function with Bernoulli distribution



$$\mathcal{P}(y|\mathbf{x},\mathbf{w}) = Bernoulli(y|sigm(\mathbf{w}^\top \mathbf{x}))$$

$$p(y_i = 1|\mathbf{x}_i,\mathbf{w}) = sigm(\mathbf{w}^\top \mathbf{x}_i)$$

$$p(y_i = 0|\mathbf{x}_i,\mathbf{w}) = 1 - sigm(\mathbf{w}^\top \mathbf{x}_i)$$

$$p(y_i|\mathbf{x}_i,\mathbf{w}) = sigm(\mathbf{w}^\top \mathbf{x}_i)^{y_i} \cdot (1 - sigm(\mathbf{w}^\top \mathbf{x}_i))^{1-y_i}$$

Logistic Regression

Maximum Likelihood Estimation

$$\begin{aligned}
\mathbf{w}^* &= \text{argmax}_{\mathbf{w}} \log p(\mathcal{D}|\mathbf{w}) \\
&= \text{argmax}_{\mathbf{w}} \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \mathbf{w}) \qquad \boxed{\mu_i = sigm(\mathbf{w}^\top \mathbf{x}_i)} \\
&= \text{argmax}_{\mathbf{w}} \sum_{i=1}^{N} \log(\mu_i^{y_i} \cdot (1-\mu_i)^{1-y_i}) \\
&= \text{argmin}_{\mathbf{w}} - \sum_{i=1}^{N} (y_i \log \mu_i + (1-y_i) \log(1-\mu_i))
\end{aligned}$$

Negative Log Likelihood (NLL)

This is also called the Cross Entropy Error Function.

Logistic Regression (Optional)

Unlike linear regression, we can no longer write down the MLE in closed form. Instead, we need to use an **optimization algorithm** to compute it.

For this, we need to derive the gradient and Hessian.

$$\mathbf{g} = \frac{d}{d\mathbf{w}} f(\mathbf{w}) = -\sum_i (\mu_i - y_i)\mathbf{x}_i = \mathbf{X}^\intercal(\mu - \mathrm{y})$$

$$\mathbf{H} = \frac{d}{d\mathbf{w}} \mathbf{g}(\mathbf{w})^\intercal = -\sum_i (\nabla_{\mathbf{w}} \mu_i \mathbf{x}_i^\intercal = -\sum_i \mu_i(1-\mu_i)\mathbf{x}_i\mathbf{x}_i^\intercal = \mathbf{X}^\intercal \mathbf{S}\mathbf{X}$$

where $\mathrm{S} \triangleq diag(\mu_i(1-\mu_i))$

One can also show that **H** is positive definite.
Hence the *NLL* is convex and has a unique global minimum.

Multiclass Logistic Regression

Logistic regression can be extended to handle more than two classes. This is called **Multi-class logistic regression**.

Also called **Multinomial logistic regression**.

In this case, the response variable $y_i \in \{1, 2, \ldots, C\}$

Different from binary logistic regression, we model the probability using **Softmax** as

$$\mathcal{P}(y_i = c|\mathbf{x}_i, \mathbf{W}) = \mu_{ic} = \frac{\exp(\mathbf{w}_c^\top \mathbf{x}_i)}{\sum_{c'=1}^{C} \exp(\mathbf{w}_{c'}^\top \mathbf{x}_i)}$$

$$\mathcal{P}(y_i|\mathbf{x}_i, \mathbf{W}) = \prod_{c=1}^{C} \mu_{ic}^{y_{ic}}$$

Multiclass Logistic Regression

Maximum Likelihood Estimation

$$
\begin{aligned}
\mathbf{W}^* &= \text{argmax}_{\mathbf{W}} \log p(\mathcal{D}|\mathbf{W}) \\
&= \text{argmax}_{\mathbf{W}} \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \mathbf{W}) \\
&= \text{argmax}_{\mathbf{W}} \sum_{i=1}^{N} \log \prod_{c=1}^{C} \mu_{ic}^{y_{ic}} \\
&= \text{argmax}_{\mathbf{W}} \sum_{i=1}^{N} \sum_{c=1}^{C} y_{ic} \log \mu_{ic} \\
&= \text{argmax}_{\mathbf{W}} \sum_{i=1}^{N} \left[\left(\sum_{c=1}^{C} y_{ic} \mathbf{w}_c^\top \mathbf{x}_i \right) - \log \left(\sum_{c'=1}^{C} \exp(\mathbf{w}_{c'}^\top \mathbf{x}_i) \right) \right]
\end{aligned}
$$

$$\mathbf{W} = [\mathbf{w}_1; \ldots; \mathbf{w}_C]$$

$$y_{ic} = \mathbb{I}(y_i = c)$$

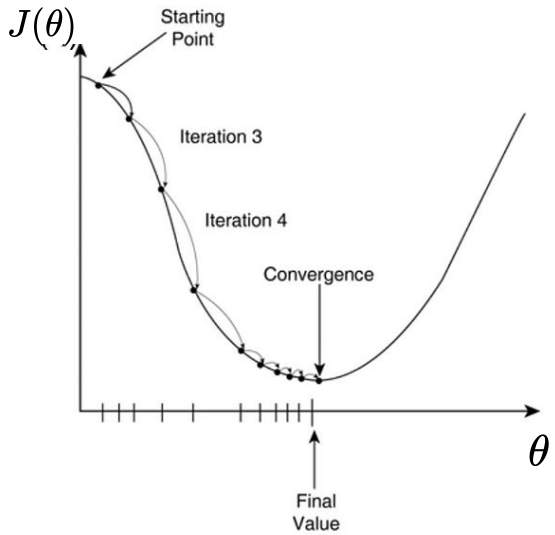
"hope" "fear"

Gradient Descent

The most commonly used method for unconstrained optimization

Goal: minimize $J(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$

$$\theta_{k+1} = \theta_k - \eta_k g_k$$



Gradient Descent

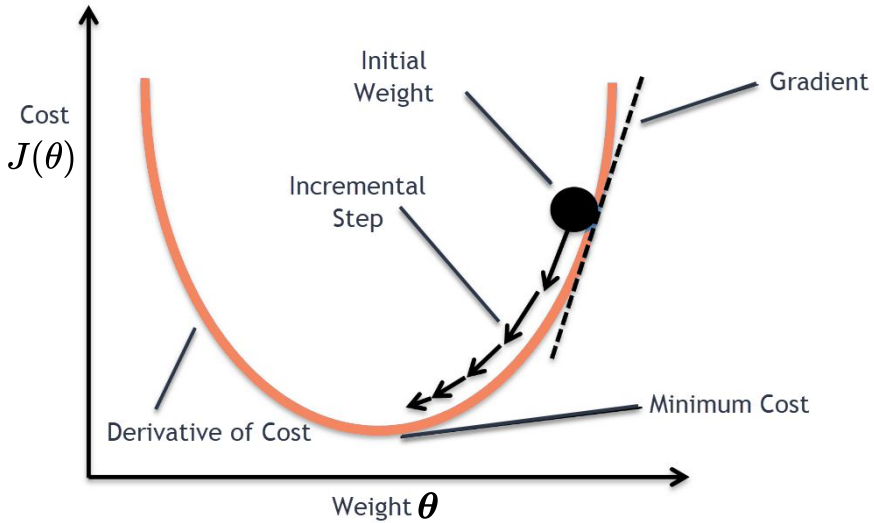
The most commonly used method for unconstrained optimization

Goal: minimize $J(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$

$$\theta_{k+1} = \theta_k - \eta_k g_k$$

g_k: gradient

η_k: step size / learning rate

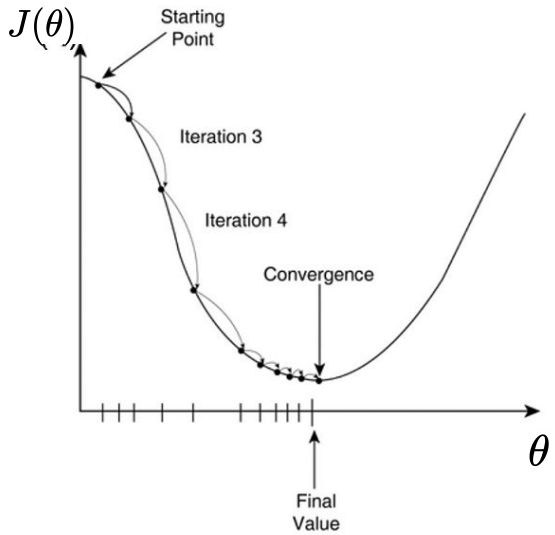


Gradient Descent

The most commonly used method for unconstrained optimization

Goal: minimize $\sum_{i=1}^{N} J_i(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$

$J_i(\theta)$ is the loss for the ith data



Gradient Descent

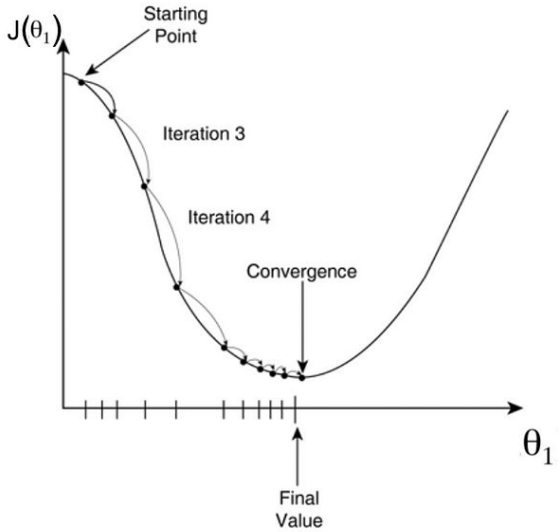
Batch Gradient Descent uses the entire dataset to compute the a single gradient update

For $t \in \{1, \ldots, T\}$:

Epoch index

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \cdot \nabla_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^{N} J_i$$

Output: $\boldsymbol{\theta}$



Gradient Descent

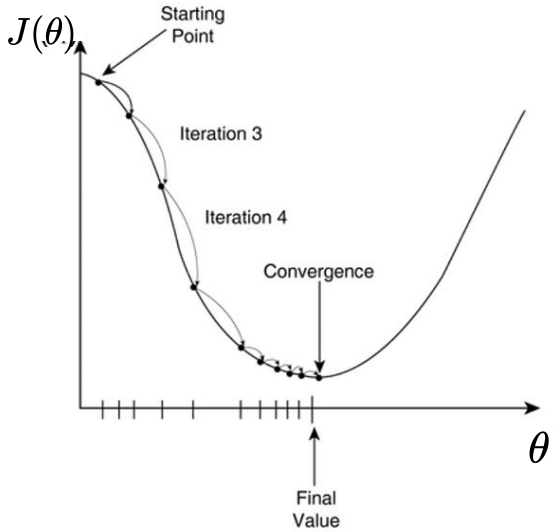
Stochastic Gradient Descent (SGD) updates parameters after every single data point.

For $t \in \{1, \ldots, T\}$:

- Choose a random permutation π of $\{1, \ldots, N\}$
- For $i \in \{1, \ldots, N\}$:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \cdot \nabla_{\boldsymbol{\theta}} J_{\pi(i)}$$

Output: $\boldsymbol{\theta}$



Gradient Descent

Mini-batch Gradient Descent updates parameters after every batch of data points.

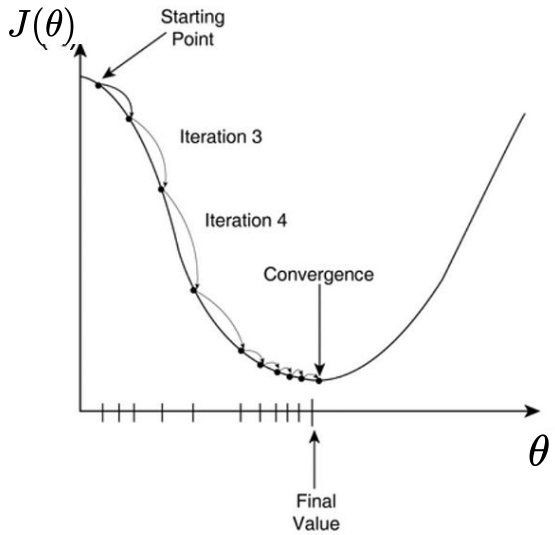
For $t \in \{1, \ldots, T\}$:

For each batch $\{b_1, \ldots, b_S\} \subset \{1, \ldots, N\}$

- Choose a batch of size S $\{x_{b_1}, \ldots, x_{b_S}\}$
- Do batch gradient descent on this batch

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \cdot \nabla_{\boldsymbol{\theta}} \frac{1}{S} \sum_{i=b_1}^{b_S} J_i$$

Output: $\boldsymbol{\theta}$



Comparison

Method	Accuracy	Update Speed	Memory Usage	Online Learning
Batch gradient descent	Good	Slow	High	No
Stochastic gradient descent	Good (with annealing)	High	Low	Yes
Mini-batch gradient descent	Good	Medium	Medium	Yes

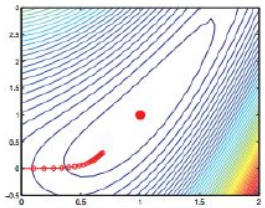
Table: Comparison of trade-offs of gradient descent variants

Gradient Descent

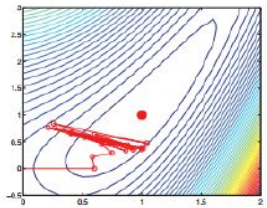
The main issue in gradient descent is:

How should we set the step size?

This turns out to be quite tricky. If we use a constant learning rate, but make it **too small**, convergence will be very slow, but if we make it **too large**, the method can fail to converge at all.



(a)



(b)

Gradient Descent Variants

Several ways to remedy this.

- Choose the optimal step size η by line-search.
- Add a momentum term to the updates.
- Use methods such as Conjugate Gradient
- Use second-order methods (e.g., Newtons method) to exploit the **curvature of the objective function**. This requires the Hessian matrix.

Use Adaptive Methods with Stochastic Gradient Descent

Gradient Descent Variants

1. Momentum
2. Nesterov accelerated gradient
3. Adagrad
4. Adadelta
5. RMSprop
6. Adam
7. Adam extensions

See https://ruder.io/optimizing-gradient-descent/

Example

Let's consider how to compute MLE for linear regression

The stochastic gradient at iteration k is given by

$$l(\theta) = \sum_{i=1}^{N} (y_i - \theta^\top \mathbf{x}_i)^2$$

$$g_k = 2\mathbf{x}_k(\theta_k^\top \mathbf{x}_k - y_k)$$

Assuming k is the training example to use at iteration k.

After computing the gradient, we take a step along it as follows:

$$\theta_{k+1} = \theta_k - \eta_k g_k$$

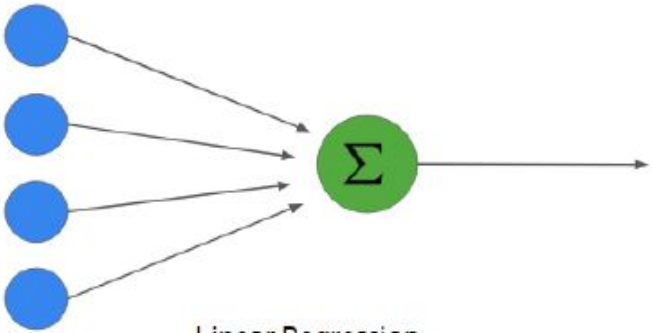
Example

After computing the gradient, we take a step along it as follows:

$$\theta_{k+1} = \theta_k - \eta_k g_k \qquad g_k = 2\mathbf{x}_k(\theta_k^\top \mathbf{x}_k - y_k)$$

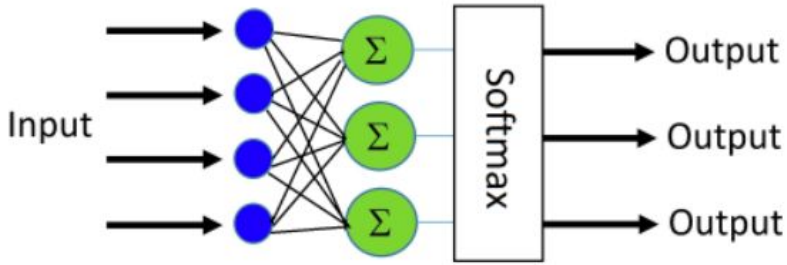
Interpretation: it is the feature vector $\mathbf{x}_k$ weighted by the difference between what we predicted, $\hat{y_k} = \theta_k^\mathsf{T}\mathbf{x}_k$, and the true response, y_k; hence the gradient acts like an **error signal**.

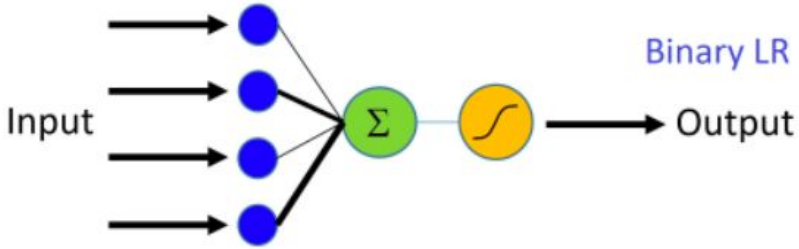
Summary



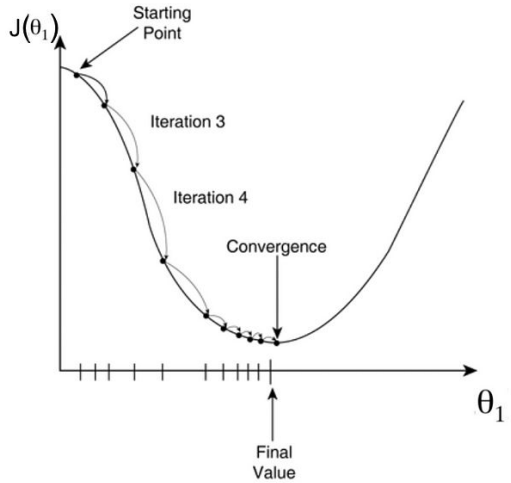
Linear Regression

Multiclass LR





Binary LR

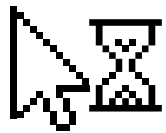


GD

Introduction to ML & DL

Deep Learning

- What is Deep Learning and why
- From Logistic/Linear Regression to Neural Networks
- Non-linearity of Neural Networks
- How to train Neural Networks
- Regularisation (dropout, gradient clipping)



What is Deep Learning and Why

- **Deep learning** is a subfield of **machine learning.**
- Most machine learning methods work well because of **human-designed representations/input features.**
- Machine learning becomes just optimizing feature weights to make a good prediction.

Feature	NER
Current Word	✓
Previous Word	✓
Next Word	✓
Current Word Character n-gram	all
Current POS Tag	✓
Surrounding POS Tag Sequence	✓
Current Word Shape	✓
Surrounding Word Shape Sequence	✓
Presence of Word in Left Window	size 4
Presence of Word in Right Window	size 4

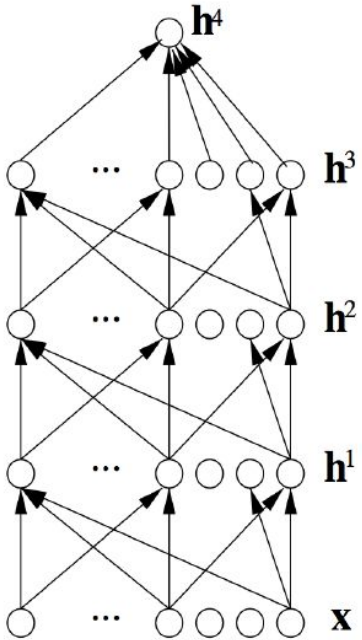
Features for NER (Finkel et al., 2010)

Figure 1: An example of NER application on an example text

What is Deep Learning and Why

Source: stanford 224n

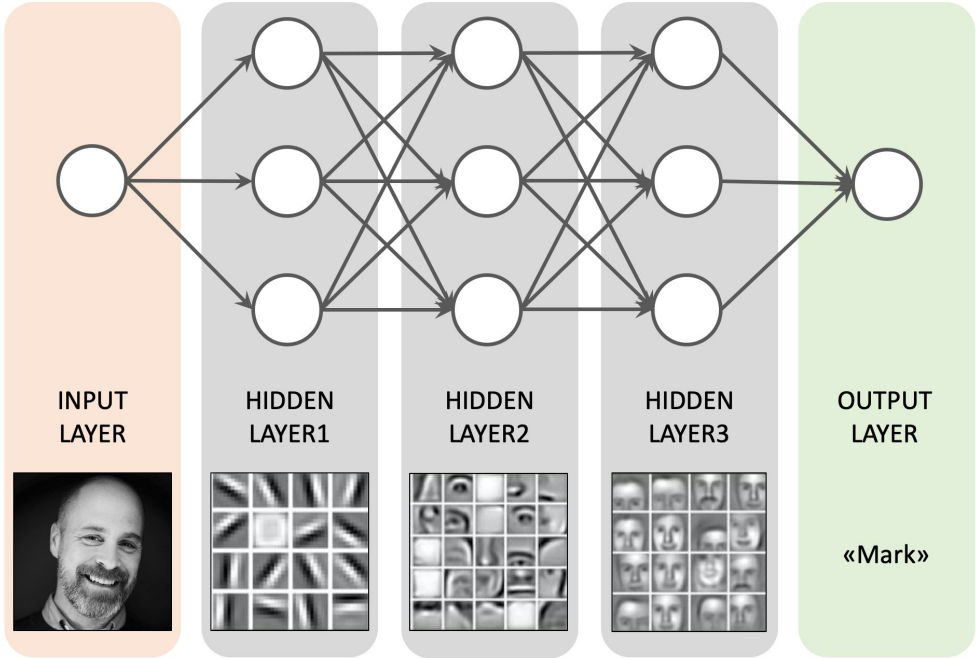
- Representation learning attempts to automatically learn good features or representations
- Deep learning algorithms attempt to learn (multiple levels of) representations (here: h^1,h^2,h^3) and an output (h^4)
- From "raw" inputs **x** (e.g. sound, pixels, characters, or words)



Deep Learning

Multiple hidden layers learn different abstractions of the input:

- Lower layers capture lower-level features, e.g., edges, parts
- Higher layers capture higher-level features, e.g., faces



What is Deep Learning and Why

Source: stanford 224n

- Manually designed features are often over-specified, incomplete and take a long time to design and validate
- **Learned Features** are easy to adapt, fast to learn
- Deep learning provides a very flexible, learnable framework for **representing** world, visual and linguistic information.
- Deep learning can learn in **unsupervised** (from raw text) and **supervised** (with specific labels like positive/negative) settings

What is Deep Learning and Why NLP

Source: stanford 224n

Combine NLP knowledge with representation learning and deep learning

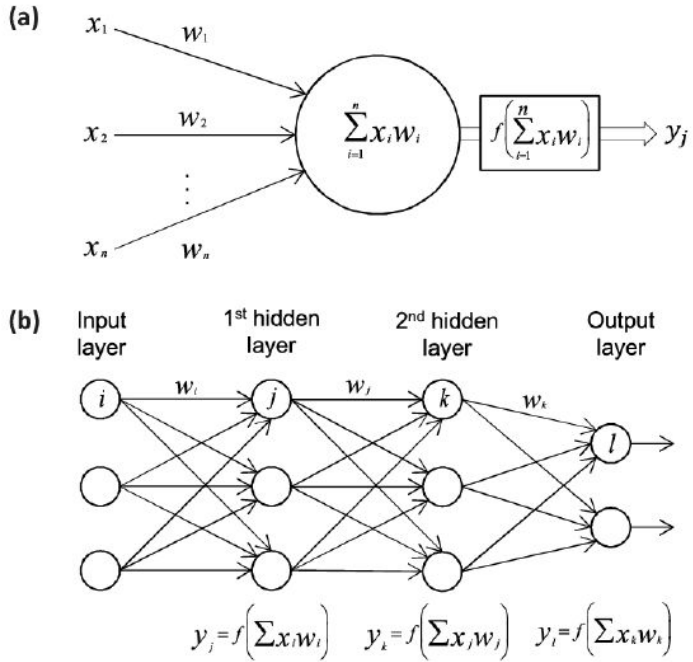
Improvements in recent years in all levels

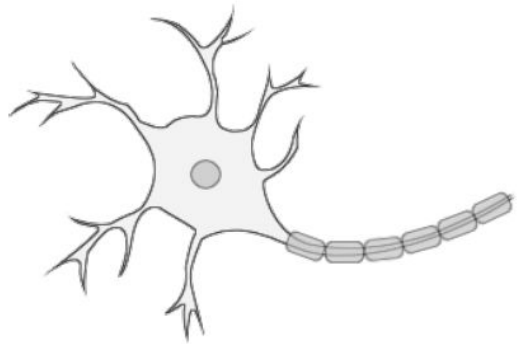
- **Linguistic levels**: speech, words, syntax, semantics, discourse
- **Full applications**: sentiment analysis, question answering, dialogue agents, machine translation

Neuron

if you understand how logistic regression works

Then **you already understand** the operation of a basic neural network neuron!



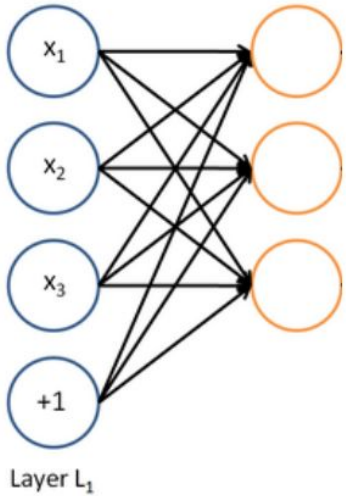


From LR to NN

A neural network = running several logistic regressions at the same time

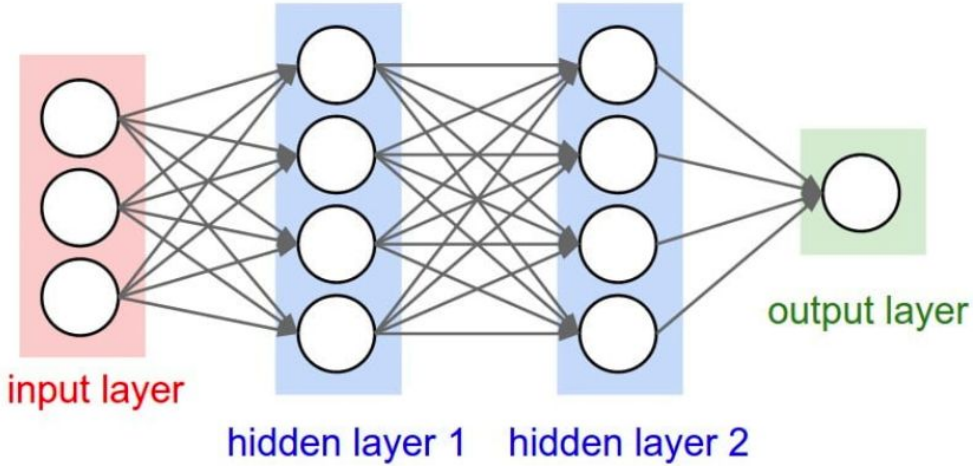
If we feed a vector of inputs through a bunch of logistic regression functions, then we get a vector of outputs …

But these are not random variables



From LR to NN

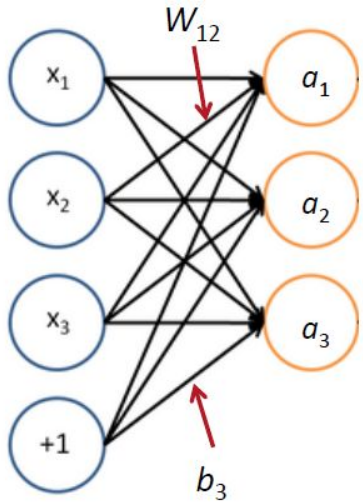
... which we can feed into another logistic regression function



Output layer can be a classification layer or a regression layer

From LR to NN

$$a_1 = f(W_{11}x_1 + W_{12}x_2 + W_{13}x_3 + b_1)$$
$$a_2 = f(W_{21}x_1 + W_{22}x_2 + W_{23}x_3 + b_2)$$
.....



In Matrix Notation $z = Wx + b$

$a = f(z)$

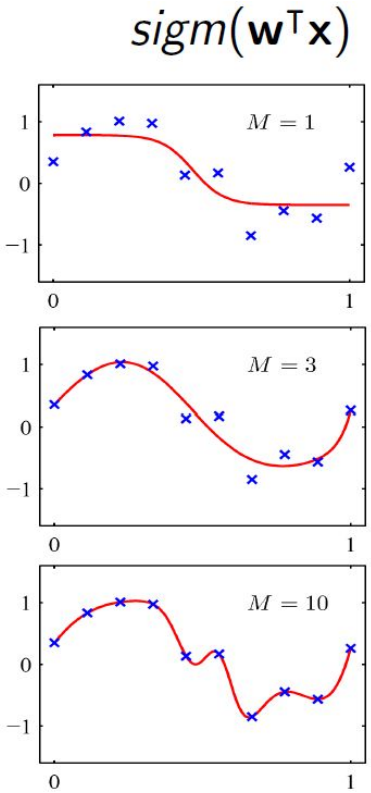
Where f() is applied element-wise

$$f([z_1, z_2, z_3]) = [f(z_1), f(z_2), f(z_3)]$$

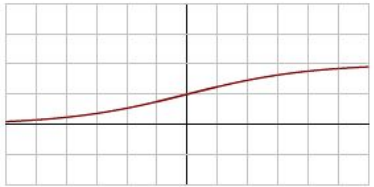
Activation function

Why non-linearity

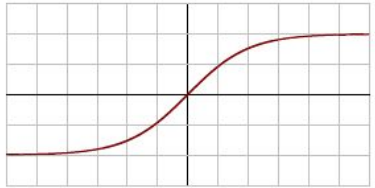
- For logistic regression: map to probabilities
- For NN: function approximation, e.g., regression or classification
  - Without non-linearities, NNs can't do anything more than a linear transform
  - Extra layers could just be compiled down into a single linear transform W(Wx) = Vx



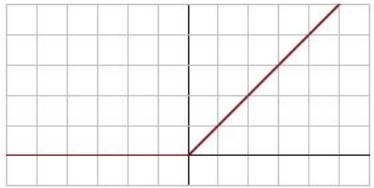
Activation functions



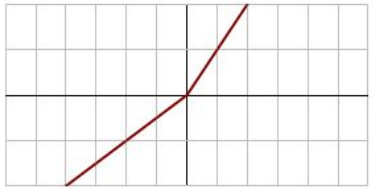
(a) Sigmoid



(b) tanh



(c) ReLU



(d) Leaky ReLU

- Sigmoid

$$\sigma(x) = \frac{1}{1+\exp^{-x}}$$

- Hyperbolic Tangent:

$$\tanh(x) = \frac{\exp^{x} - \exp^{-x}}{\exp^{x} + \exp^{-x}}$$

- Rectified Linear Unit (ReLU):

$$f(x) = \max(0, x)$$

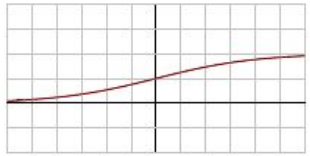
- Leaky ReLU:

$$f(x) = \begin{cases} \alpha x & x < 0 \\ x & x \geq 0 \end{cases}$$

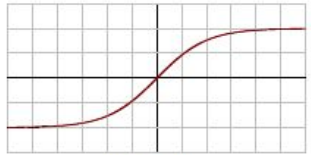
, where α is small constant

Activation functions

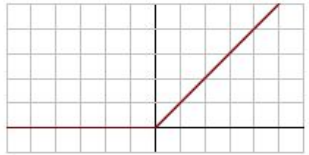
- Sigmoid
  - Biological analogy. Very popular before DL era.
  - Range: $[0, 1]$
  - Gradient vanishing $\rightarrow$ losing popularity in DL era, but still used a lot e.g., LSTM
- Hyperbolic Tangent
  - Centered at 0
  - Gradient vanishing (slightly better than sigmoid function)
- Rectified Linear Unit (ReLU)
  - Alleviate gradient vanishing problem. Safe choice in general.
  - Piece-wise linear
- Leaky ReLU: variant of ReLU



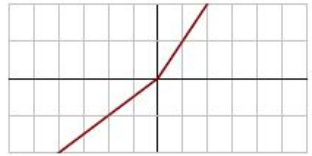
(a) Sigmoid



(b) tanh



(c) ReLU



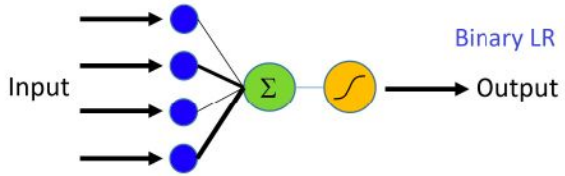
(d) Leaky ReLU

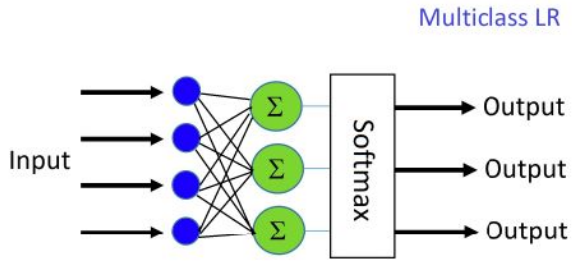
How to Train Neural Networks

If we have only one layer (linear)

It is same as Linear/Logistic Regression

- Use Gradient Descent
- Or L-BFGS (2nd order)
- Or SGD





See the first part of the slides for details.

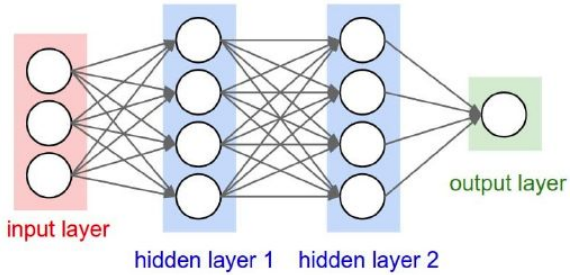
How to Train Neural Networks

But we have internal (hidden) layers in a multi-layer NN

This makes the loss/objective function non-convex

- But, we can still use the same ideas/algorithms (just without guarantees)
- Use SGD or its variants

- We "backpropagate" error derivatives through the model



Algorithm 2 Stochastic Gradient Descent Algorithm

initialize θ, η
repeat
  Randomly permute data
  for $i = 1 : N$ **do**
    $\mathbf{g} = \nabla f(\theta, \mathbf{z}_i)$
    $\theta \leftarrow proj_{\Theta}(\theta - \eta \mathbf{g})$
    Update η
  end for
until *converged*

How to Train Neural Networks

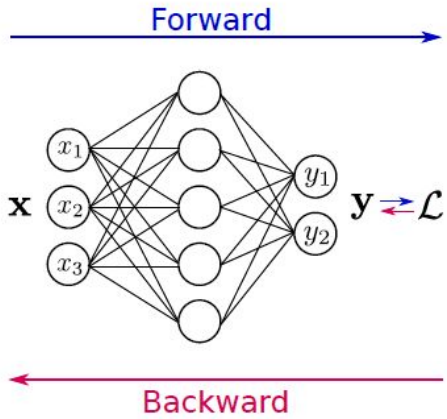
Two information flow directions:

Forward propagation

- NN accepts an input **x** and produces an output **y**
- During training, it continues onward until it produces a scalar cost **L**

Back-propagation

- Information (**gradients** with respect to the parameters) from the cost flows backward through the network

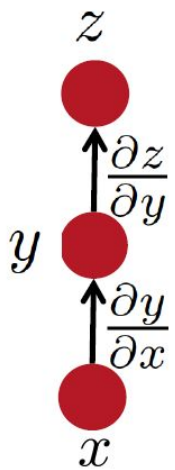


Chain Rule of Derivatives

Compute gradient of example-wise loss wrt parameters

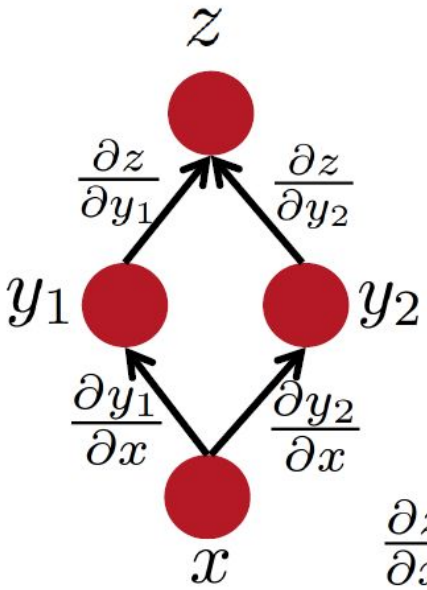
- Simply apply the chain rule of derivative

$$z = f(y) \quad y = g(x) \quad \frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$



Chain Rule of Derivatives

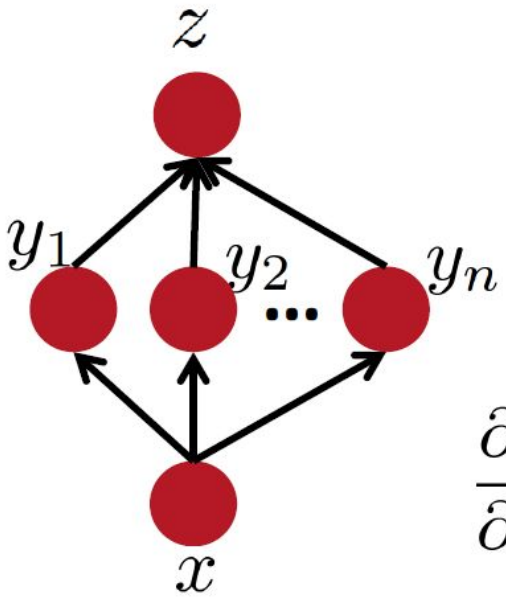
- Multiple-path chain rule



$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

Chain Rule of Derivatives

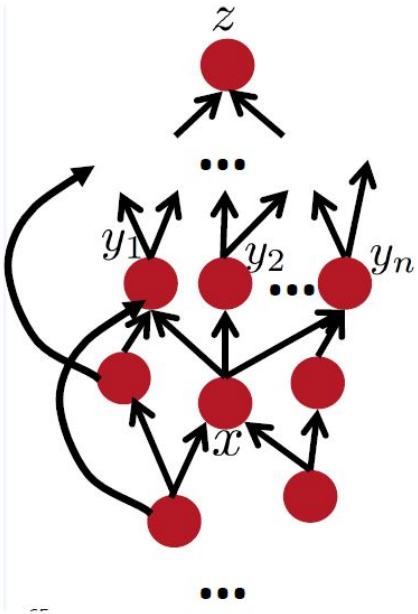
- Multiple-path chain rule (general)



$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Chain Rule of Derivatives

- Chain rule in computational graph



Flow graph: any directed acyclic graph
node = computation result
arc = computation dependency

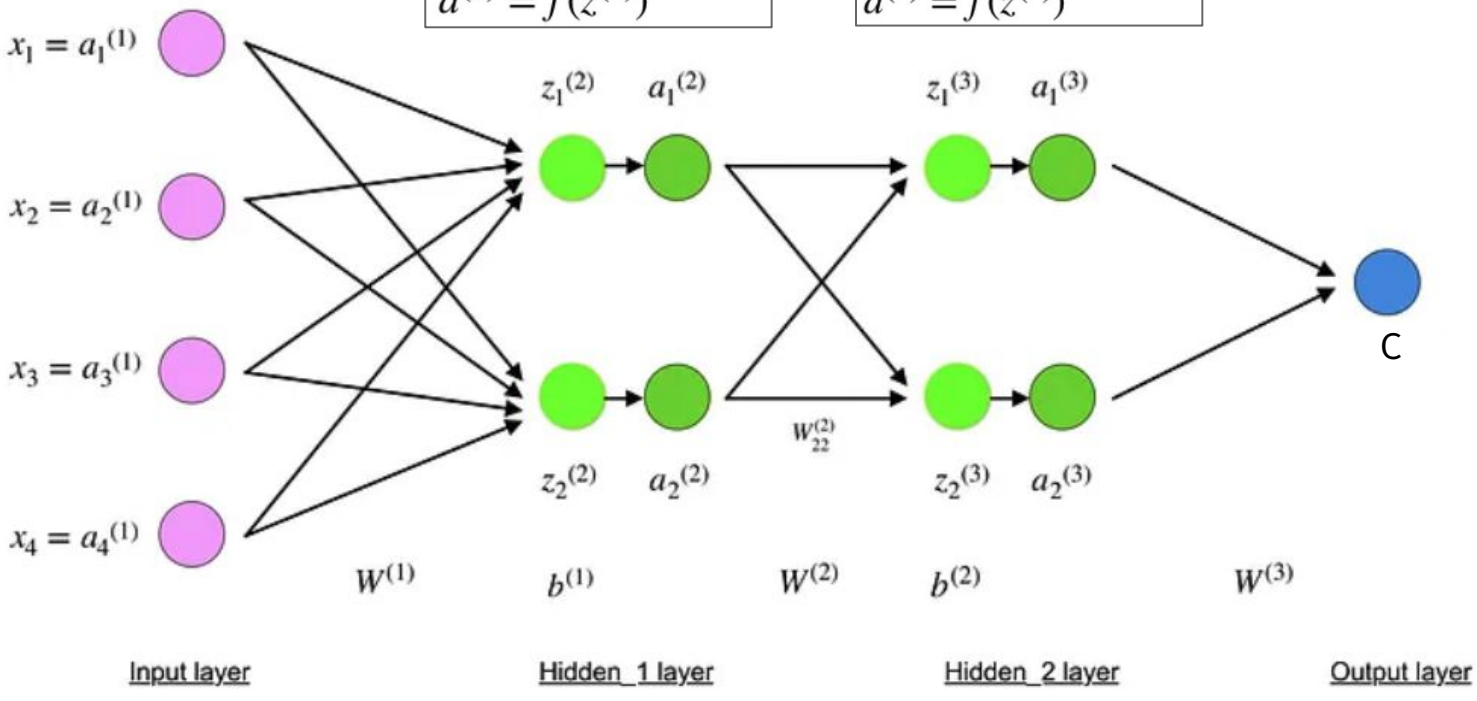
$\{y_1, y_2, \ldots y_n\}$ = successors of x

$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Example

$$z^{(2)} = W^{(1)}x + b^{(1)}$$
$$a^{(2)} = f(z^{(2)})$$

$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$
$$a^{(3)} = f(z^{(3)})$$

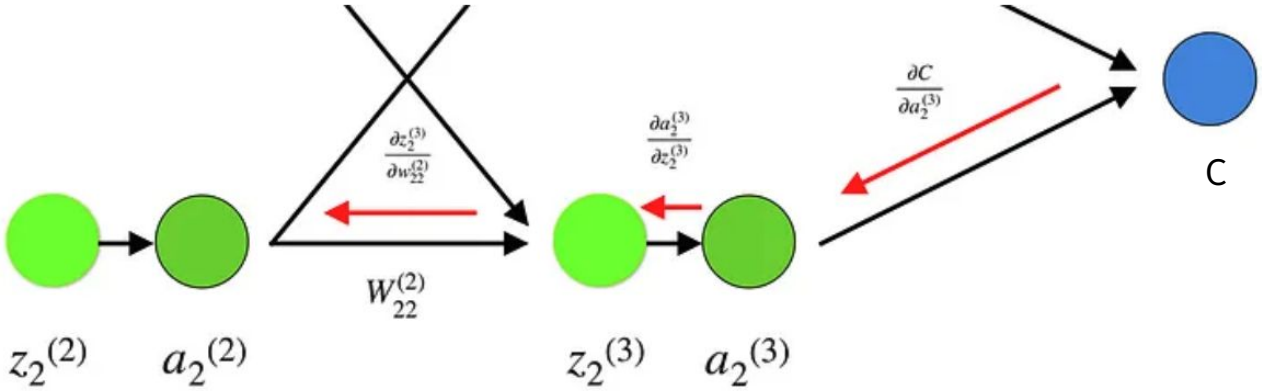


Simple 4-layer neural network illustration

Example

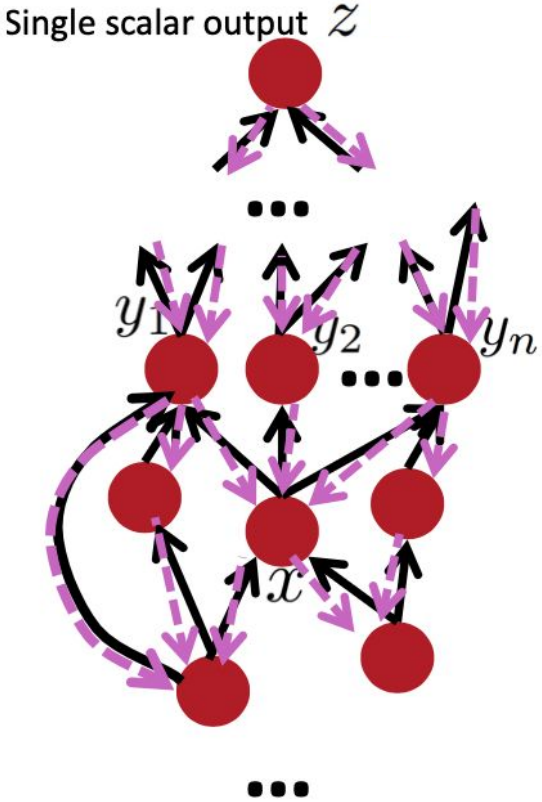
$$z^{(2)} = W^{(1)}x + b^{(1)}$$
$$a^{(2)} = f(z^{(2)})$$

$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$
$$a^{(3)} = f(z^{(3)})$$



$$\frac{\partial C}{\partial w_{22}^{(2)}} = \frac{\partial C}{\partial z_2^{(3)}} \cdot \frac{\partial z_2^{(3)}}{\partial w_{22}^{(2)}} = \frac{\partial C}{\partial a_2^{(3)}} \cdot \frac{\partial a_2^{(3)}}{\partial z_2^{(3)}} \cdot \frac{\partial z_2^{(3)}}{\partial w_{22}^{(2)}}$$

Backpropagation in General



1. Fprop: visit nodes in topo-sort order
   - Compute value of node given predecessors
2. Bprop:
   - initialize output gradient = 1
   - visit nodes in reverse order:
     Compute gradient wrt each node using gradient wrt successors

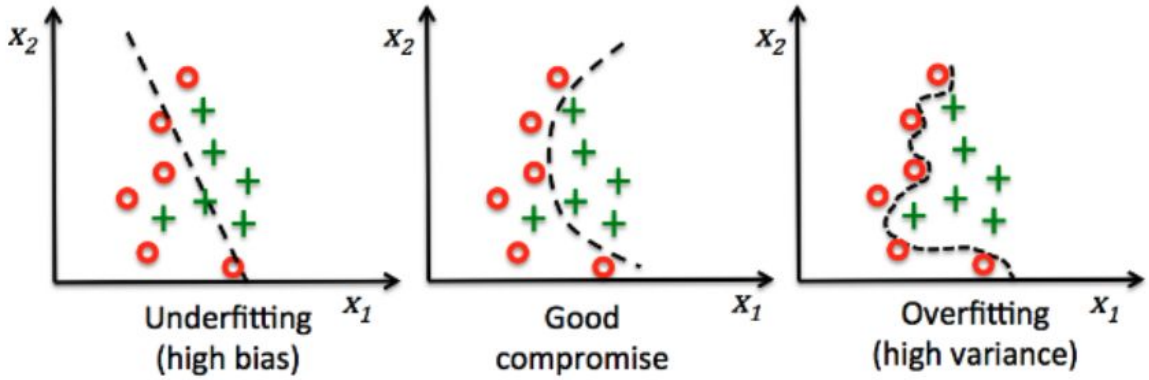
$\{y_1, y_2, \ldots y_n\}$ = successors of x

$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Source: Socher & Manning

Regularization

DNNs tend to overfit to the training data → poor generalisation performance.

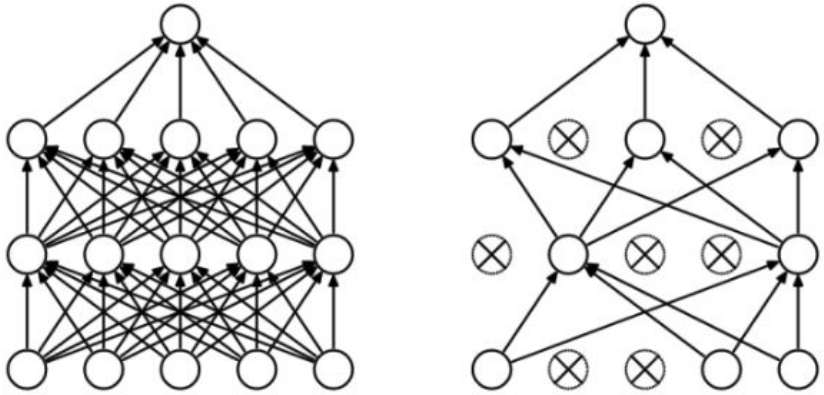


Generalization error increases due to overfitting.

We need to regularise the network

Dropout

- Simple, but powerful regulariser
- Randomly turnoff some nodes during training.
- Use all activations during inference

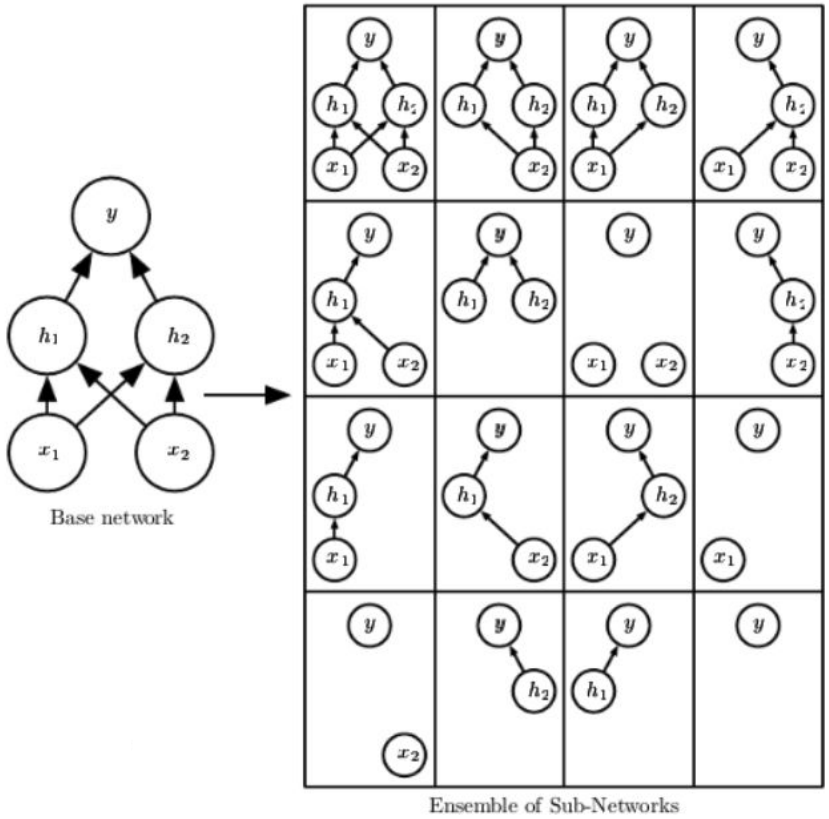


(a) Standard Neural Net (b) After applying dropout.

- Dropout has the effect of making the training noisy, forcing nodes within a layer to probabilistically take on more or less responsibility for the inputs.
- Dropout encourages the network to learn a sparse representation
- It breaks-up situations where network layers co-adapt to correct mistakes from prior layers, in turn making the model more robust

Dropout

- Has ensemble effect



L1/2 Regularization

If a particular feature f_j is usually positive, then it always improves the loss to increase θ_j.

Regularization: discourage every θ_j from getting too large in magnitude.

$$\arg\min_{\boldsymbol{\theta}} \text{loss}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_p^p$$

where $\lambda > 0$ is a "hyperparameter" and $p = 2$ or 1.

L1/2 Regularization

$$\min_{\mathbf{w}} \text{loss}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_1$$

Note that:

$$\|\boldsymbol{\theta}\|_1 = \sum_{j=1}^{d} |\theta_j|$$

- This results in **sparsity** (i.e., many $\theta_j = 0$).

Gradient Clipping

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \overbrace{\alpha}^{\text{learning rate}} \underbrace{\nabla_\theta J(\theta)}_{\text{gradient}}$$

- This can cause bad updates: we take too large a step and reach a bad parameter configuration (with large loss)
- In the worst case, this will result in Inf or NaN in your network (then you have to restart training from an earlier checkpoint)

Gradient Clipping

Gradient clipping: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

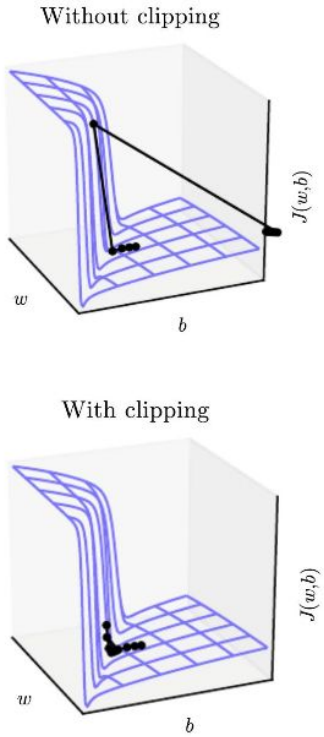
Algorithm 1 Pseudo-code for norm clipping

$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**
  $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|}\hat{\mathbf{g}}$
end if

- Intuition: take a step in the same direction, but a smaller step

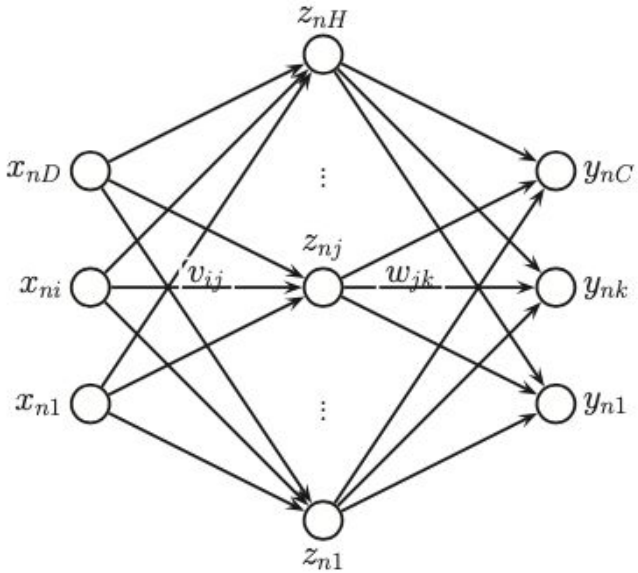
Gradient Clipping

- This shows the loss surface of a simple RNN (hidden state is a scalar not a vector)
- The "cliff" is dangerous because it has steep gradient
- In the Fig. at the top, gradient descent takes two very big steps due to steep gradient, resulting in climbing the cliff then shooting off to the right (both bad updates)
- At the bottom, gradient clipping reduces the size of those steps, so effect is less drastic



Summary

MLP



BackProp