Lecture 1: Introduction

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SIST, ShanghaiTech
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Outline

- Course logistics
  - Overall objective
  - Grading policy
  - Pre-requisite / Syllabus
- Introduction to deep learning
- Machine learning review
- Artificial neurons

Course objectives

- Learning to use deep networks
  - How to write from scratch, debug and train neural networks
  - Toolboxes commonly used in practice
- Understanding deep models
  - Key concepts and principles
- State of the art
  - Some new topics from research field
  - Focusing on vision-related problems

Syllabus & Schedule

- Piazza:
  - piazza.com/shanghaitech.edu.cn/fall2020/cs280
  - The schedule for the latter half of the semester may vary a bit
- Part I: Basic neural networks (1~1.5 weeks by Prof He)
  - Linear models
  - Multiple layer networks
  - Gradient descent and BP
- Part II: Convolutional neural networks
- Part III: Recurrent neural networks
- Part IV: Generative neural networks
- Part V: Advanced Topics

Syllabus & Schedule

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  - The schedule for the latter half of the semester may vary a bit
- Part I: Basic neural networks (1~1.5 weeks)
- Part II: Convolutional neural networks (4 weeks by Prof He)
  - CNN basics
  - Understanding CNN
  - CNN in Vision
- Part III: Recurrent neural networks
- Part IV: Generative neural networks
- Part V: Advanced Topics

Syllabus & Schedule

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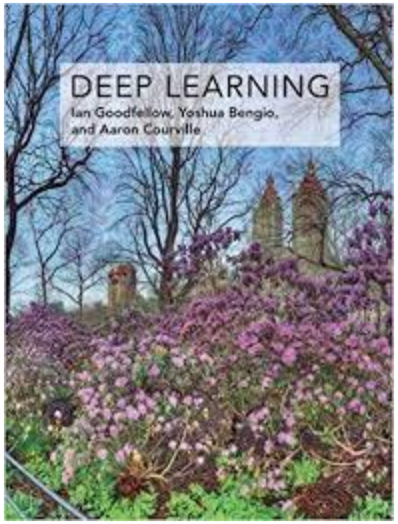
  - The schedule for the latter half of the semester may vary a bit
- Part I: Basic neural networks (1~1.5 weeks)
- Part II: Convolutional neural networks (4 weeks)
- Part III: Recurrent neural networks (3 weeks by Prof Xu)
  - LSTM, GRU
  - Attention modeling
  - RNN in Vision/NLP
  - Transformer and Graph Neural Networks
- Part IV: Generative neural networks
- Part V: Advanced Topics

Syllabus & Schedule

- Piazza:
  - piazza.com/shanghaitech.edu.cn/fall2020/cs280
  - The schedule for the latter half of the semester may vary a bit
- Part I: Basic neural networks (1~1.5 weeks)
- Part II: Convolutional neural networks (4 weeks)
- Part III: Recurrent neural networks (3 weeks)
- Part IV: Generative neural networks (2 weeks by Prof Xu)
  - Variational Auto Encoder (VAE)
  - Generative deep nets (GAN)
- Part V: Advanced Topics (2 weeks)
- Note: no lectures in the following weeks
  - Nov 9 ~ Nov 16 (CVPR)

Reference books and materials

- Deep learning:
  - http://www.deeplearningbook.org/
  - https://d2l.ai/



- Online deep learning courses:
  - Stanford: CS230, CS231n
  - CMU: 11-785
  - MIT: 6.S191

- Additional reading materials on Piazza
  - Survey papers, tutorials, etc.

Instructor and TAs

- Instructor: Prof Xuming He and Prof Lan Xu
  - hexm@shanghaitech.edu.cn ; xulan1@shanghaitech.edu.cn
  - SIST 1A-304D ; 1C-203D
- TAs:
  - Haozhe Wang, Qiuyue Wang, Guoxing Sun, Yannan He, Quan Meng, Yinwenqi Jiang
- Office hours: To be announced on Piazza
- We will use Piazza as the main communication platform

Grading policy

- 4 Problem sets: 10% x 4 = 40%
  - Write-up problem sets + Programming tasks
- Final course project: 40% (+10%)
  - Proposal
  - Final report (Conference format)
  - Presentation
  - Bonus points for novel results: 10%
- 10 Quizzes (in class): 2% x 10 = 20%
- Late policy
  - A total of 7 free late (calendar) days to use, but no more than 4 late days can be used on any single assignment.
  - After that, 25% off per day late
  - Does not apply to Final course project/Quizzes
- Collaboration policy
  - Project team: 3~5 students
  - Grading according to each member's contribution

Administrative Stuff

- Plagiarism
  - All assignments must be done individually
    - You may not look at solutions from any other source
    - You may not share solutions with any other students
    - Plagiarism detection software will be used on all the programming assignments
    - You may discuss together or help another student but you cannot give the exact solution

- Plagiarism punishment
  - When one student copies from another student, both students are responsible
  - Zero point on the assignment or exam in question
  - Repeated violation will result in an F grade for this course as well as further discipline at the school/university level

Pre-requisite

- Proficiency in Python
  - All class assignments will be in Python (and use numpy)
  - A Python tutorial available on Piazza
- Calculus, Linear Algebra, Probability and Statistics
  - Undergrad course level
- Equivalent knowledge of Andrew Ng's CS229 (Machine Learning)
  - Formulating cost functions
  - Taking derivatives
  - Performing optimization with gradient descent
- Will be evaluated in next quiz (Wednesday)

Outline

- Course logistics
- Introduction to deep learning
  - What & Why deep learning?
- Machine Learning review
- Artificial neurons

Acknowledgement: Bhiksha Raj@CMU's course notes

Introduction

- Our goal: Build intelligent algorithms to make sense of data
  - Example: Recognizing objects in images

red panda (*Ailurus fulgens*)

  - Example: Predicting what would happen next

Vondrick et al. CVPR2016

Introduction

- Our goal: Build intelligent algorithms to make sense of data
  - Example: Recognizing objects in images

  - Example: Predicting what would happen next

Given an initial still frame,

Introduction

- A broad range of real-world applications
  - Speech recognition
    - Input: sound wave → Output: transcript
  - Language translation
    - Input: text in language A (Eng) → Output: text in language B (Chs)
  - Image classification
    - Input: images → Output: image category (cat, dog, car, house, etc.)
  - Autonomous driving
    - Input: sensory inputs → Output: actions (straight, left, right, stop, etc.)
- Main challenges: difficult to manually design the algorithms

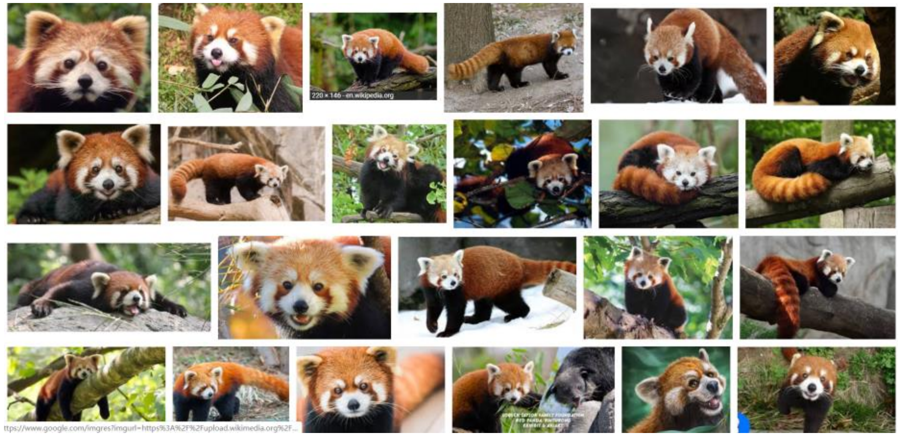
A data-driven approach

- Each task as a mapping function (or a model)

Input data $\xrightarrow{\text{Mapping function}}$ Expected output

  - input data: images
  - expected output: object or action names

- Building such mapping functions from data



→ Mapping function

red panda (*Ailurus fulgens*)

A data-driven approach

- Building a mapping function (model)

$$y = f(x; \theta)$$

  - x: input data
  - y: expected output
  - θ: parameters to be estimated

- Learning the model from data
  - Given a dataset $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^{N}$
  - Find the 'best' parameter $\hat{\theta}$, such that

$$y_n \simeq f(x_n; \hat{\theta}) \quad \forall n$$

  - And it can be generalized to unseen input data

What is deep learning?

- Using deep neural networks as the mapping function

- Model: Deep neural networks
  - A family of parametric models
  - Consisting of many 'simple' computational units
  - Constructing a multi-layer representation of input

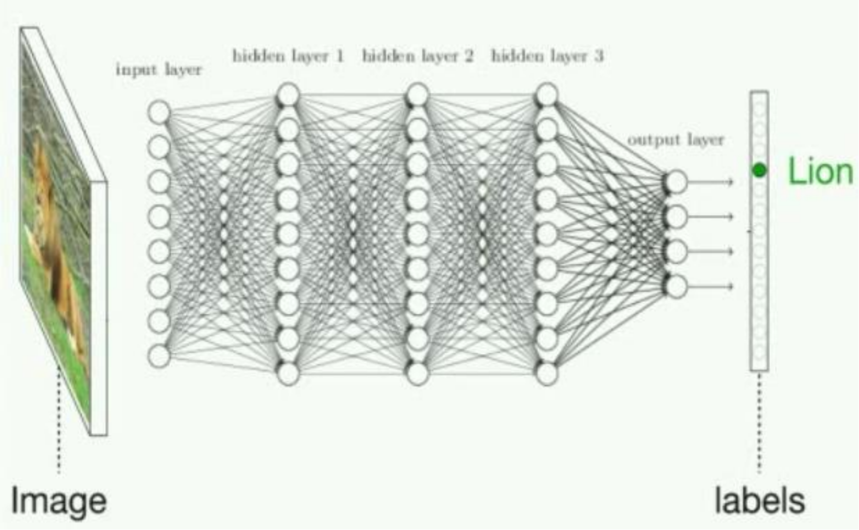
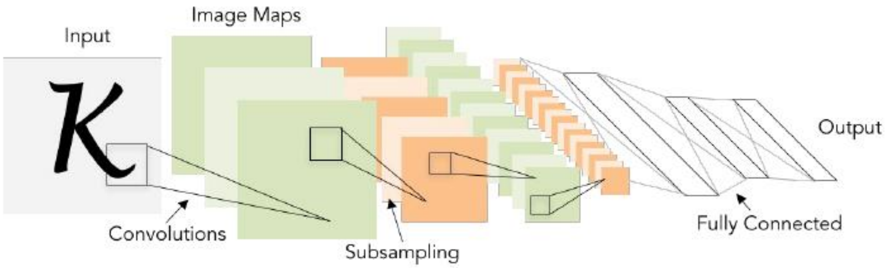


Image from Jeff Clune's Deep Learning Overview

What is deep learning?

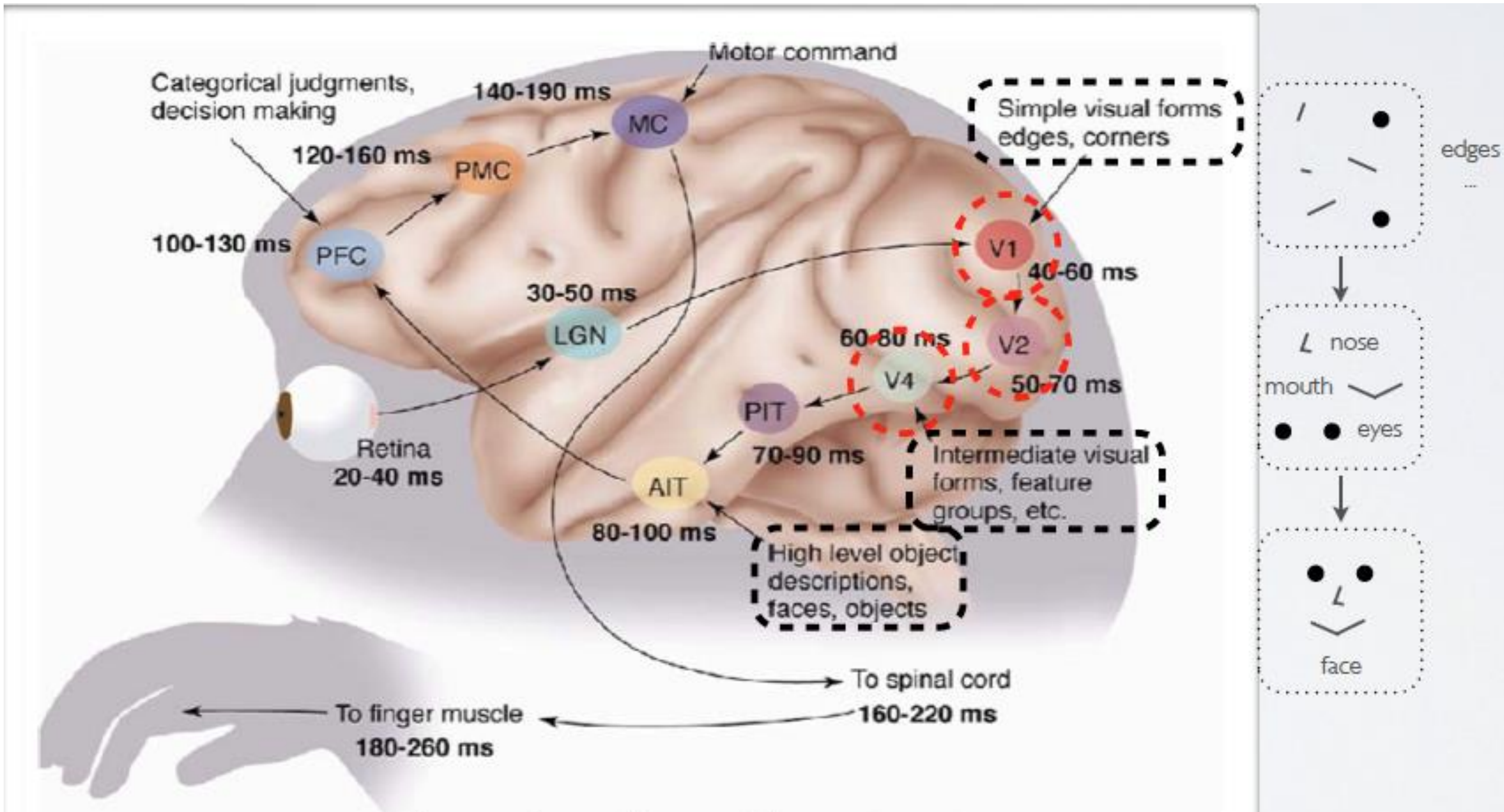
- Using deep neural networks as the mapping function
- Learning: Parameter estimation from data
  - Parameters: connection weights between units
  - Formulated as an optimization problem
  - Efficient algorithms for handling large-scale models & datasets



LeNet-5

Why deep networks?

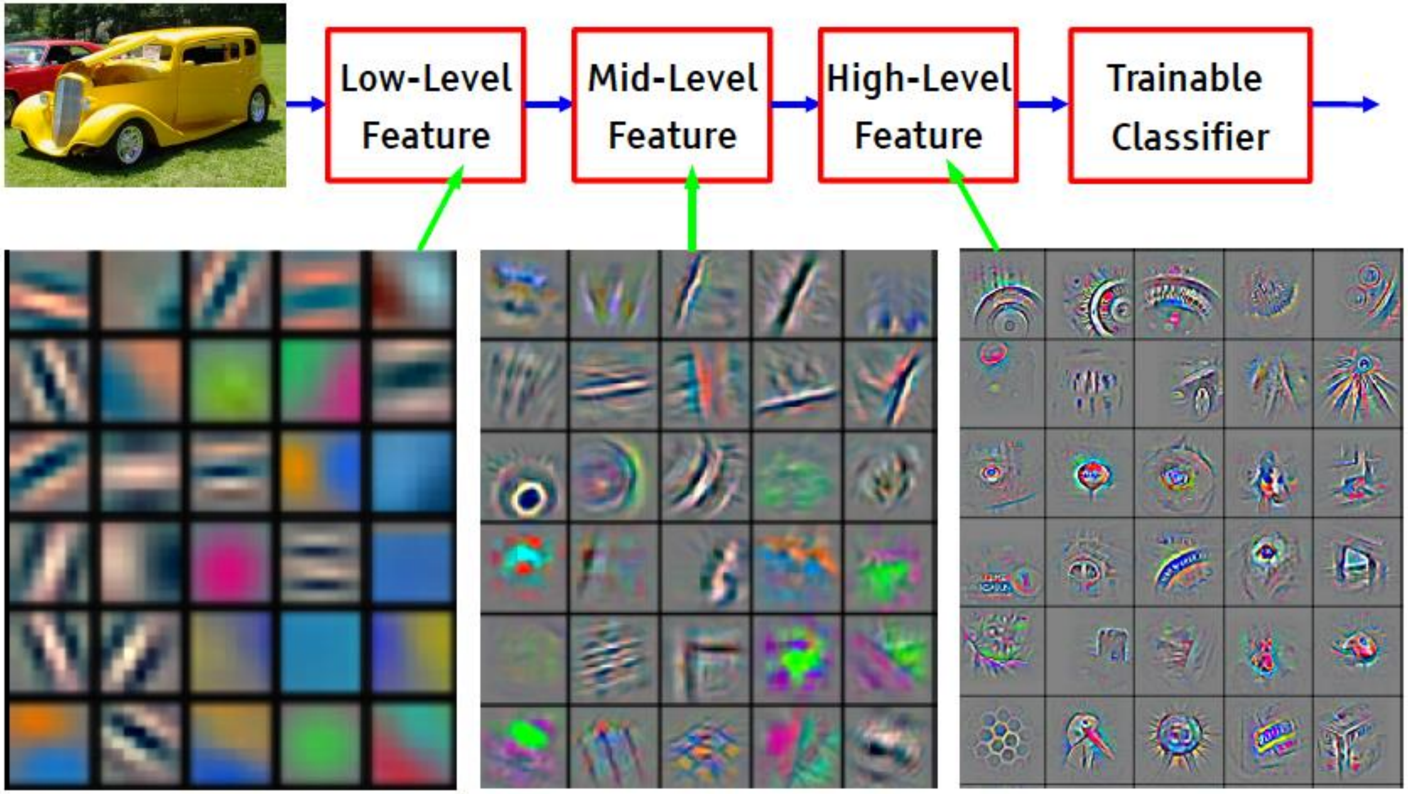
- Inspiration from visual cortex



[picture from Simon Thorpe]

Why deep networks?

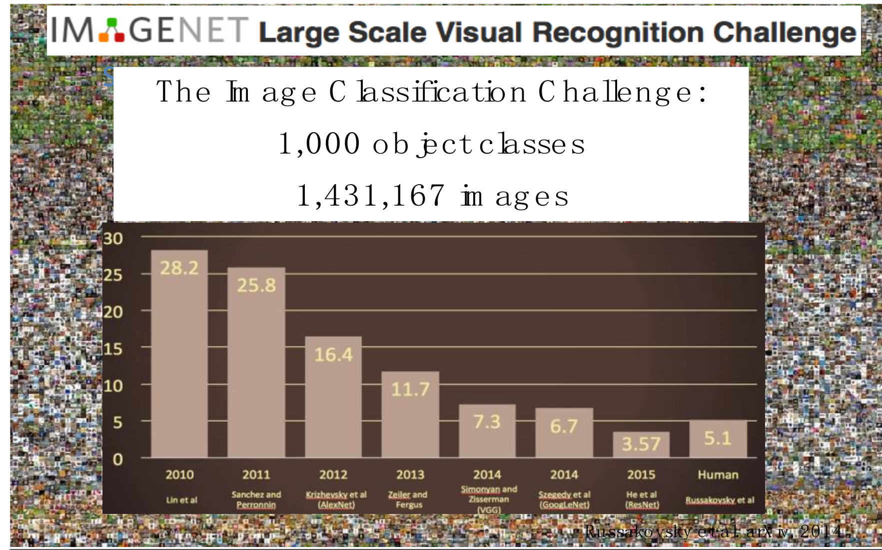
- A deep architecture can represent certain functions (exponentially) more compactly
- Learning a rich representation of input data

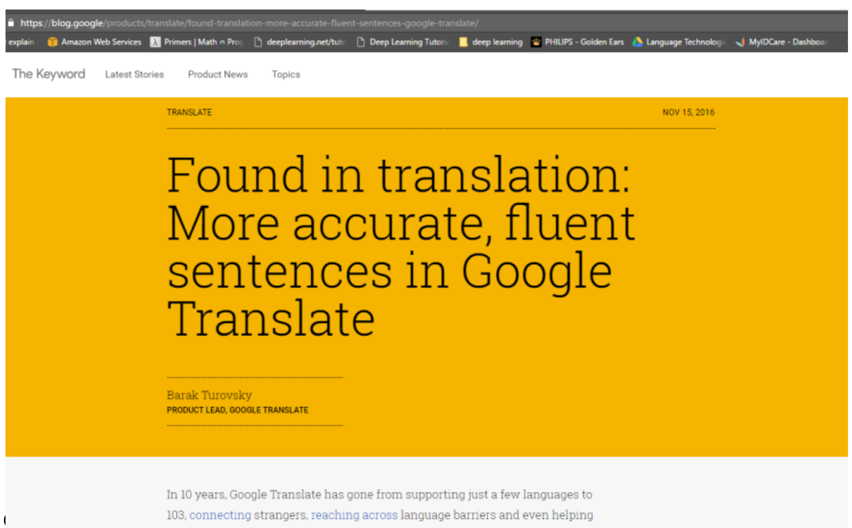


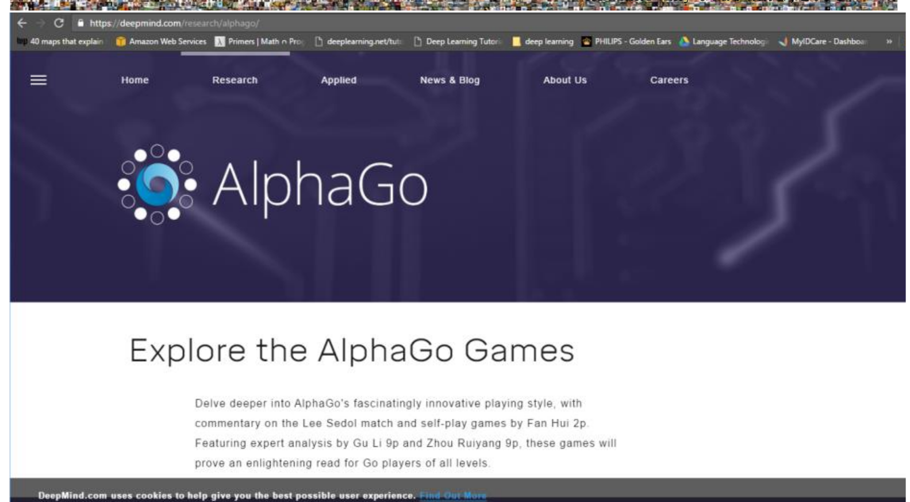
Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

Recent success with DL

- Some recent success with neural networks







Summary: Why deep learning?

- One of the major thrust areas recently in various pattern recognition, prediction and data analysis
  - Efficient representation of data and computation
  - Other key factors: large datasets and hardware

- The state of the art in many problems
  - Often exceeding previous benchmarks by large margins
  - Achieve better performances than human for certain “complex” tasks.

- But also somewhat controversial …
  - Lack of theoretical understanding
  - Sometimes difficult to make it work in practice

Is it alchemy?

Questions to ask

- Understanding neural networks
  - What is different from traditional ML methods?
  - How it works for specific problems?
  - Why get great performance?
- Future development
  - Its limitation and weakness?
  - After more than 10 years, what is on-going or next?
  - The road to general-purpose AI?

Outline

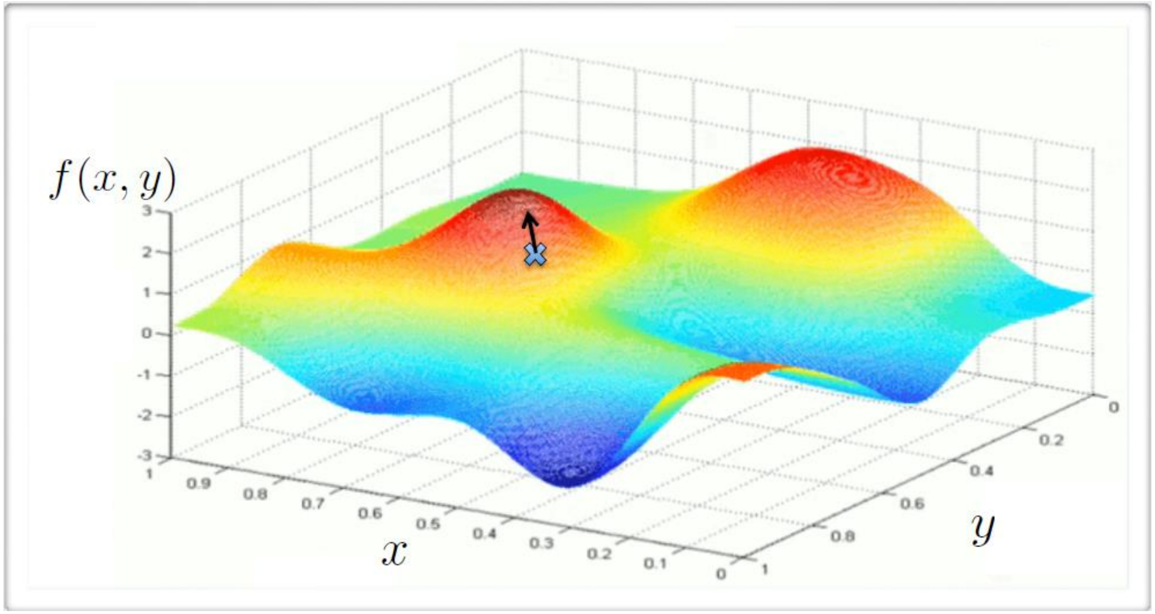
- Course logistics
- Introduction to deep learning
- Machine learning review
  - Math review
  - Supervised learning
- Artificial neurons

Acknowledgement: Hugo Larochelle's, Mehryar Mohri@NYU's & Yingyu Liang@Princeton's course notes

Math review – Calculus

- Gradient

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = [\frac{\partial}{\partial x_1} f(\mathbf{x}), \cdots, \frac{\partial}{\partial x_d} f(\mathbf{x})]^\mathsf{T} = \begin{bmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_d} f(\mathbf{x}) \end{bmatrix}$$



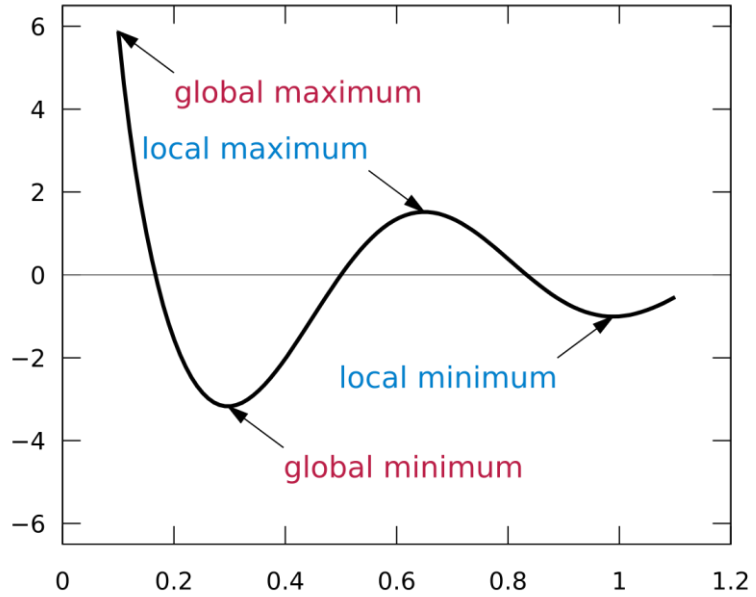
Math review – Calculus

- Local and global minima
  - Necessary condition

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = 0$$

  - Sufficient condition
    - Hessian is positive definite

$$f(\mathbf{x}) \approx f(\mathbf{x}^*) + (\mathbf{x} - \mathbf{x}^*)^\intercal \nabla_{\mathbf{x}} f(\mathbf{x}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^*)^\intercal \nabla_{\mathbf{x}}^2 f(\mathbf{x})(\mathbf{x} - \mathbf{x}^*)$$



Math review – Probability

- Factorization

- Probability chain rule: $p(s,o) = p(s|o)p(o) = p(o|s)p(s)$
  - in general:

$$p(\mathbf{x}) = \prod_i p(x_i | x_1, \ldots, x_{i-1})$$

- Bayes rule:

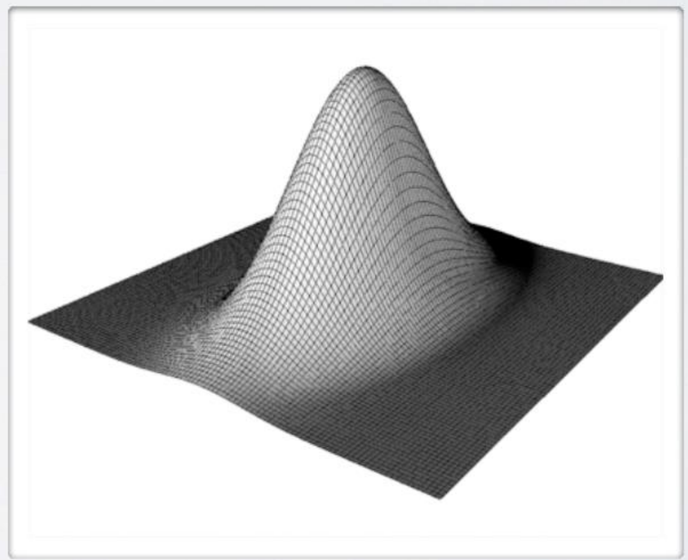
$$p(O=o|S=s) = \frac{p(S=s|O=o)p(O=o)}{\sum_{o'} p(S=s|O=o')p(O=o')}$$

Math review – Probability

- Common distributions

• Gaussian variable: $\mathbf{X} \in \mathbb{R}^d$

  - $p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$
  - $\mathrm{E}[\mathbf{X}] = \boldsymbol{\mu}$
  - $\mathrm{Cov}[\mathbf{X}] = \Sigma$



Math review – Statistics

- Monte Carlo estimation
  - a method to approximate an expensive expectation

$$\mathrm{E}[f(\mathbf{X})] = \sum_{\mathbf{x}} f(\mathbf{x})\, p(\mathbf{x}) \approx \frac{1}{K} \sum_k f(\mathbf{x}^{(k)})$$

  - the $\mathbf{x}^{(k)}$ must be sampled from $p(\mathbf{x})$

- Maximum likelihood

$$\widehat{\theta} = \arg\max_{\theta} p(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(T)})$$

  - Independent and identically distributed

$$p(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(T)}) = \prod_t p(\mathbf{x}^{(t)})$$

ML tasks

- Classification: assign a category to each item (e.g., document classification)
- Regression: predict a real value for each item (e.g., prediction of stock values, economic variables)
- Ranking: order items according to some criterion (e.g., relevant web pages returned by a search engine)
- Clustering: partition data into ‘homogenous’ regions (e.g., analysis of very large data sets)
- Dimensionality reduction: find lower-dimensional manifold preserving some properties of the data

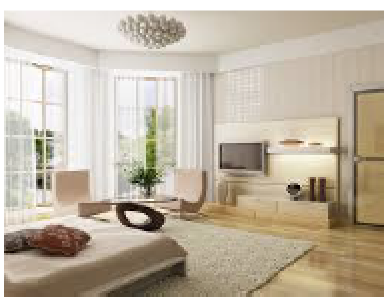
Standard learning scenarios

- Unsupervised learning: no labeled data
- Supervised learning: uses labeled data for prediction on unseen points
- Semi-supervised learning: uses labeled and unlabeled data for prediction on unseen points
- Reinforcement learning: uses reward to learn prediction on action policies.
- …

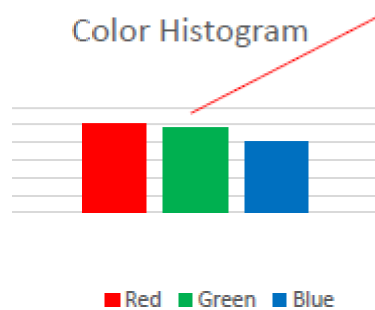
Supervised learning

- Task formulation

  - Learning example: $(\mathbf{x}, y)$
  - Task to solve: predict target y from input $\mathbf{x}$
    - classification: target is a class ID (from 0 to nb. of class - 1)
    - regression: target is a real number



Extract features



Feature vector: x_i

Indoor

0

Label: y_i

Supervised learning

- Task formulation

  - Learning example: $(\mathbf{x}, y)$
  - Task to solve: predict target y from input $\mathbf{x}$
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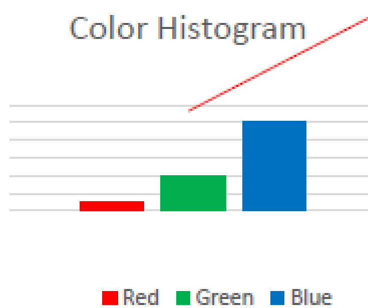
Extract features



Feature vector: x_j

Label: y_j

outdoor → 1

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$
  - Find $y = f(x)$ using training data
  - s.t. f correct on test data

What kind of functions?

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. f correct on test data

Hypothesis class

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. f correct on test data

Connection between training data and test data?

Learning problem

- Problem setup

  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. f correct on test data i.i.d. from distribution D

They have the same distribution

i.i.d.: independently identically distributed

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. f correct on test data i.i.d. from distribution D

What kind of performance measure?

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. the expected loss is small

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

Various loss functions

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. the expected loss is small

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

  - Examples of loss functions:
    - 0-1 loss: $l(f, x, y) = \mathbb{I}[f(x) \neq y]$ and $L(f) = \Pr[f(x) \neq y]$
    - l_2 loss: $l(f, x, y) = [f(x) - y]^2$ and $L(f) = \mathbb{E}[f(x) - y]^2$

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
  - Find $y = f(x) \in \mathcal{H}$ using training data
  - s.t. the expected loss is small

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

How to use?

Learning problem

- Problem setup
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Find $y = f(x) \in \mathcal{H}$ that minimizes $\hat{L}(f) = \frac{1}{n}\sum_{i=1}^{n} l(f, x_i, y_i)$
  - s.t. the expected loss is small

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

Empirical loss

Learning as iterative optimization

- Gradient descent
  - choose initial $w^{(0)}$, repeat

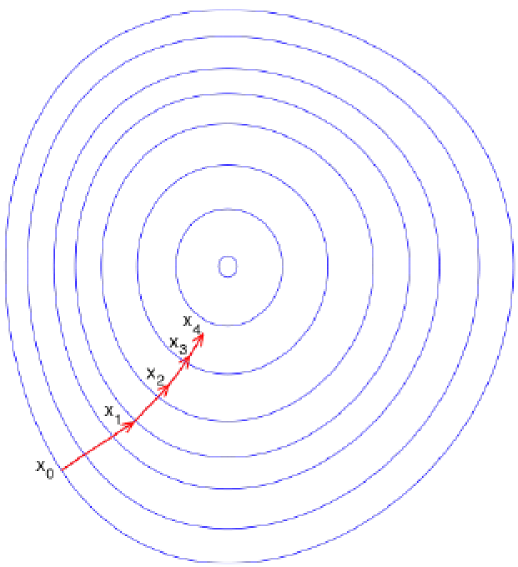
    $$w^{(t+1)} = w^{(t)} - \eta_t \cdot \nabla \mathrm{L}\left(w^{(t)}\right)$$

    until stop
  - η_t is the learning rate, and

    $$\nabla \mathrm{L}\left(w^{(t)}\right) = \frac{1}{n} \sum_i \nabla_w \mathrm{L_i}(w^{(t)}; y_i, x_i)$$

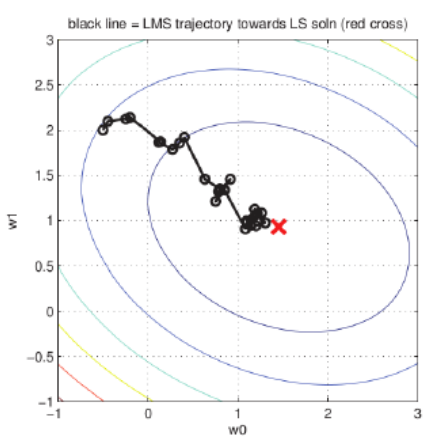
  - How to stop? $\|w^{(t+1)} - w^{(t)}\| \leq \epsilon$ or $\|\nabla \mathrm{L}(w^{(t)})\| \leq \epsilon$

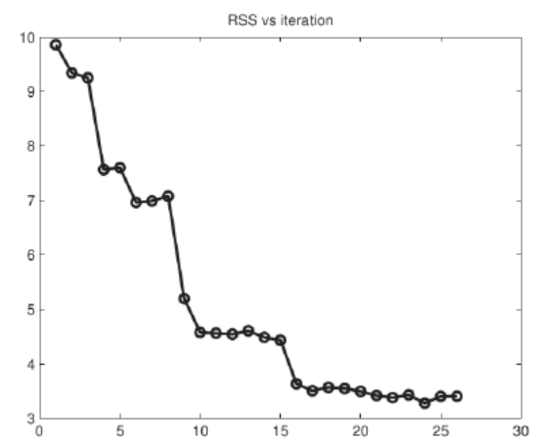
Two dimensional example:



Learning as iterative optimization

- Stochastic gradient descent (SGD)
  - Suppose data points arrive one by one
  - $\hat{L}(\mathrm{w}) = \frac{1}{n}\sum_{t=1}^{n} l(\mathrm{w}, x_t, y_t)$, but we only know $l(\mathrm{w}, x_t, y_t)$ at time t
  - Idea: simply do what you can based on local information
    - Initialize w_0
    - $\mathrm{w}_{t+1} = \mathrm{w}_t - \eta_t \nabla l(\mathrm{w}_t, x_t, y_t)$



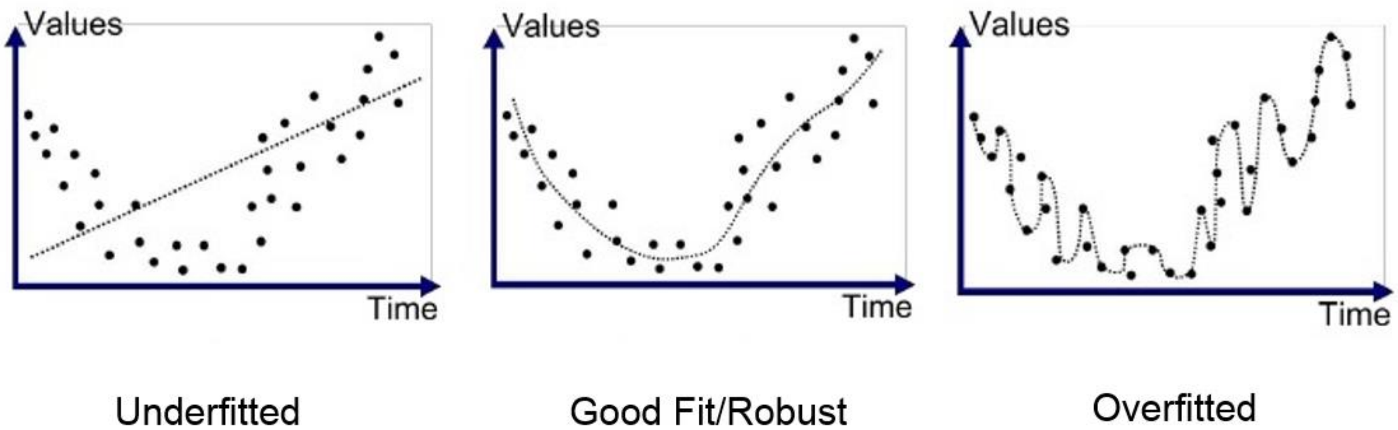


Supervised learning pipeline

- Three steps
  - Collect data and extract features
  - Build model: choose hypothesis class $\mathcal{H}$ and loss function l
  - Optimization: minimize the empirical loss
- Datasets & hyper-parameters
  - Hyper-parameter: a parameter of a model that is not trained (specified before training)
    - Training set $\mathcal{D}^{\text{train}}$ serves to train a model
    - Validation set $\mathcal{D}^{\text{valid}}$ serves to select hyper-parameters
    - Test set $\mathcal{D}^{\text{test}}$ serves to estimate the generalization performance (error)

Generalization

- Model selection for better generalization
  - Capacity: flexibility of a model
  - Underfitting: state of model which could improve generalization with more training or capacity
  - Overfitting: state of model which could improve generalization with less training or capacity
  - Model Selection: process of choosing the best hyper-parameters on validation set



Generalization

- Training/Validation curves

Questions

- Generalization
  - Interaction between training set size/capacity/training time and training error/generalization error
- If capacity increases:
  - Training error will ?
  - Generalization error will ?
- If training time increases:
  - Training error will ?
  - Generalization error will ?
- If training set size increases:
  - Generalization error will ?
  - Gap between the training and generalization error will ?

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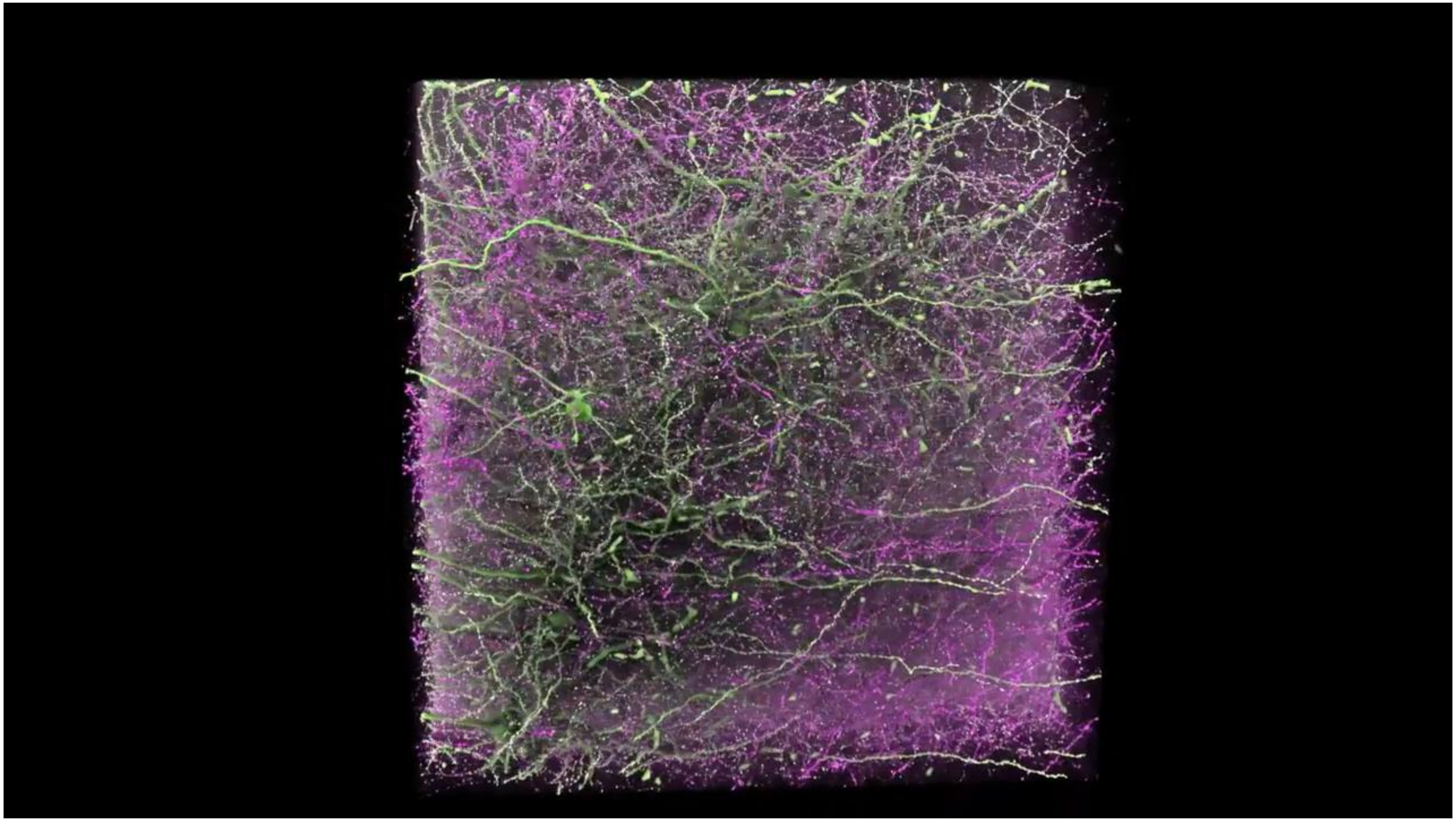
- Machine learning review
- Artificial neurons
  - Math model
  - Perceptron algorithm

Acknowledgement: Hugo Larochelle's, Mehryar Mohri@NYU's & Yingyu Liang@Princeton's course notes

Artificial Neuron

- Biological inspiration



https://www.youtube.com/watch?v=m0rHZ_RDdyQ

Artificial Neuron

- Biological inspiration
  - Our brain has $\sim 10^{11}$ neurons, each of which communicates (is connected) to $\sim 10^{4}$ other neurons

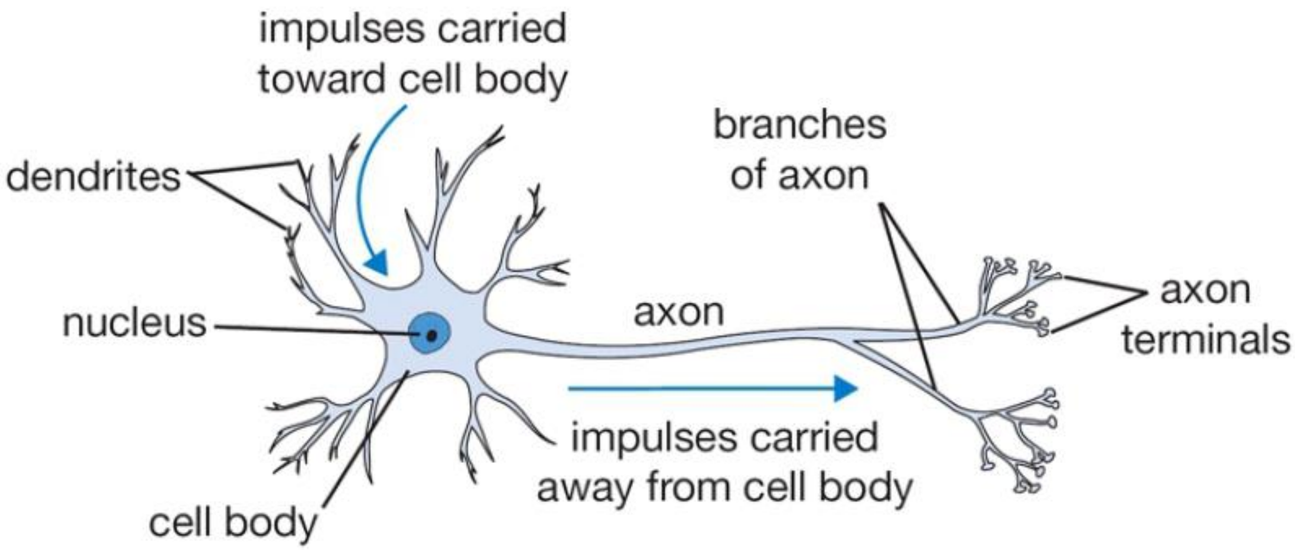
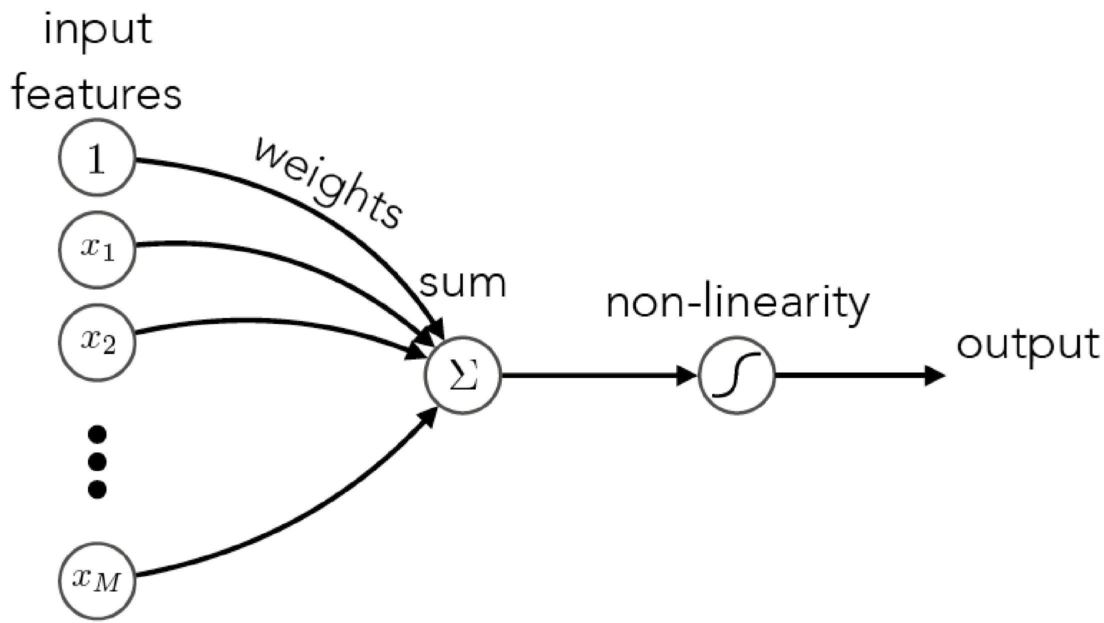


Figure : The basic computational unit of the brain: Neuron

Mathematical model of a neuron



artificial neuron: *weighted sum and non-linearity*

bias

input features

$$s = b + w_1 x_1 + w_2 x_2 + \cdots + w_M x_M = \mathbf{w}^\mathsf{T}\mathbf{x}$$

sum

weights

$$h = g(s)$$

output

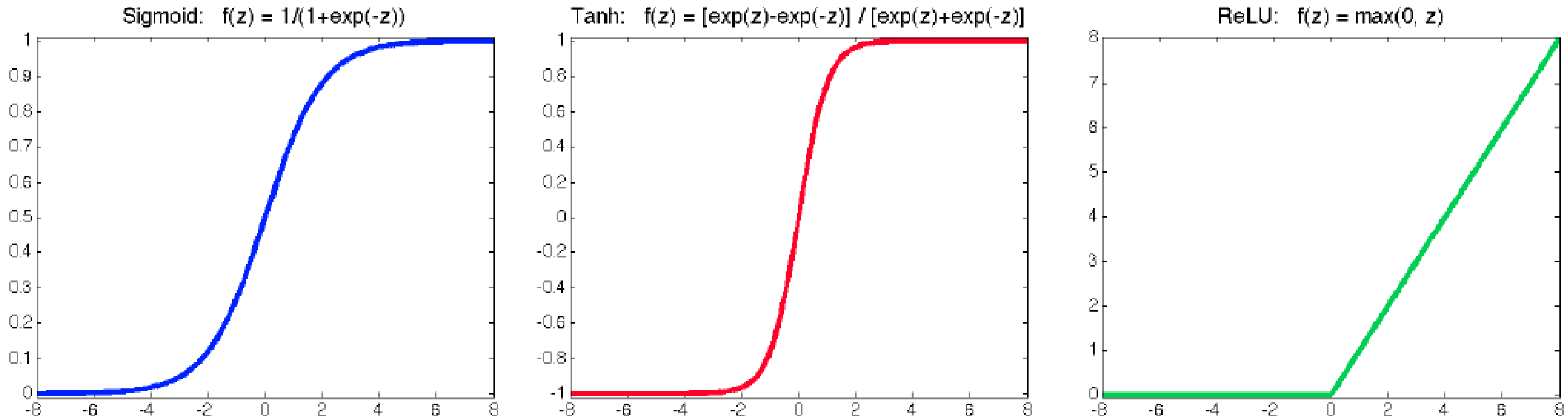
non-linearity

sum

Activation functions

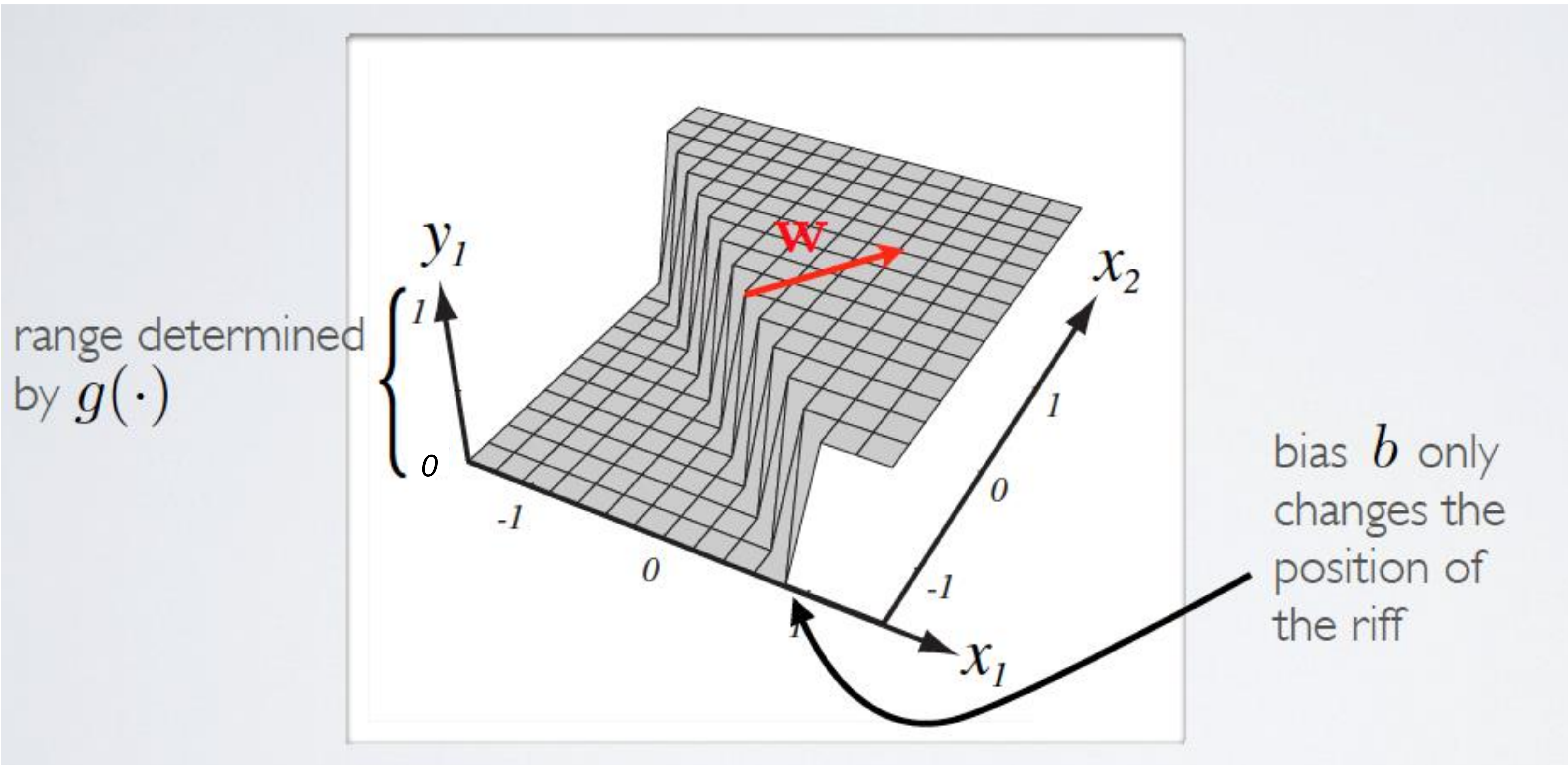
Most commonly used activation functions:

- Sigmoid: $\sigma(z) = \frac{1}{1+\exp(-z)}$
- Tanh: $\tanh(z) = \frac{\exp(z)-\exp(-z)}{\exp(z)+\exp(-z)}$
- ReLU (Rectified Linear Unit): $\mathrm{ReLU}(z) = \max(0, z)$



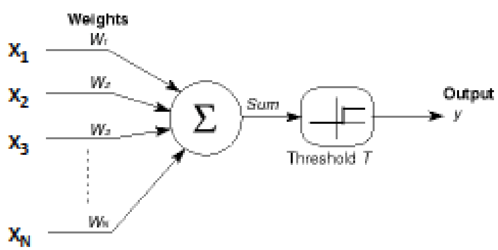
Capacity of single neuron

- Sigmoid activation function



What a single neuron does?

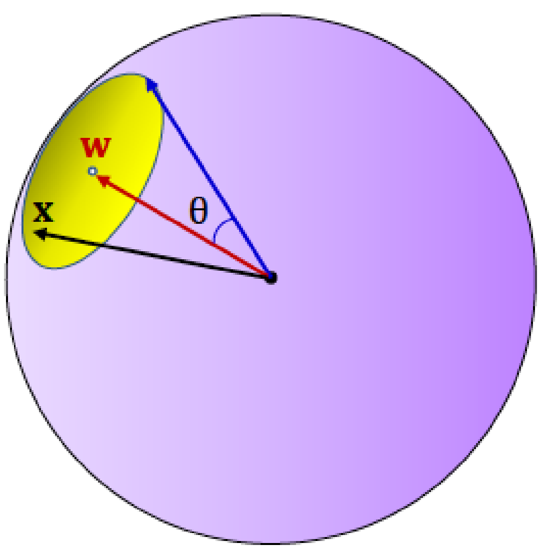
- A neuron (perceptron) fires if its input is within a specific angle of its weight
  - If the input pattern matches the weight pattern closely enough



$$\mathbf{x}^T\mathbf{w} > T$$

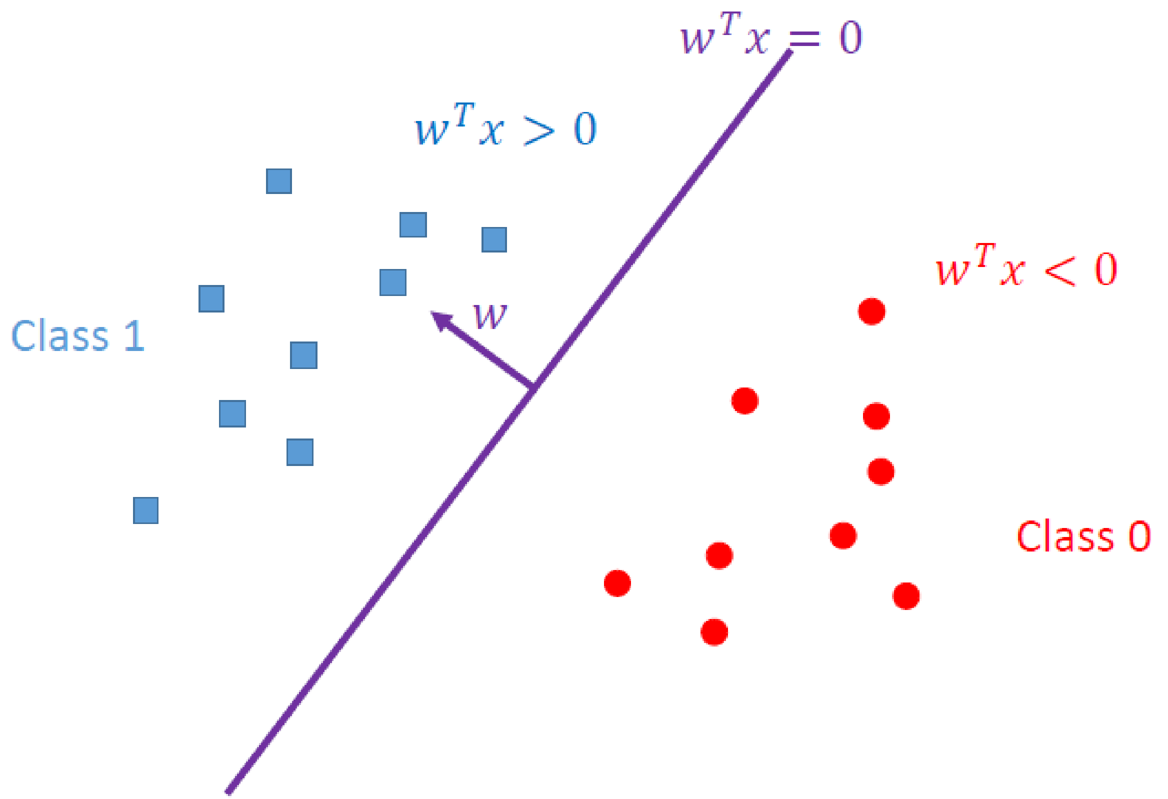
$$\Rightarrow \cos\theta > \frac{T}{|\mathbf{x}||\mathbf{w}|}$$

$$\Rightarrow \theta < \cos^{-1}\left(\frac{T}{|\mathbf{x}||\mathbf{w}|}\right)$$



Single neuron as a linear classifier

- Binary classification



Summary

- Introduction to deep learning
- Course logistics
- Review of basic math & ML
- Artificial neurons

- Next time
  - Basic neural networks
  - First Quiz on prerequisite