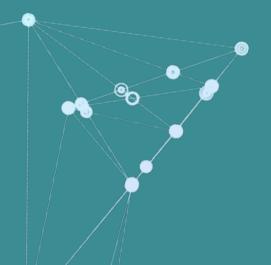
Deep Learning and Applications



DSA 5204 • Lecture 2 Dr Low Yi Rui (Aaron) Department of Mathematics



Homework 1

Homework 1 has been uploaded on Canvas

Submission through Canvas submission folder

Due: 4th Feb 2023

Take note of the late submission policies

Project Instructions

Please read Canvas for project instructions TLDR version

- Form groups of 5-7 by the end of Week 3
- Three main components
 - Proposal (Homework 2)
 - Presentation with Q&A (live, during last 2 classes)
 - Report
- Any questions, please post on Canvas forums

Last Time

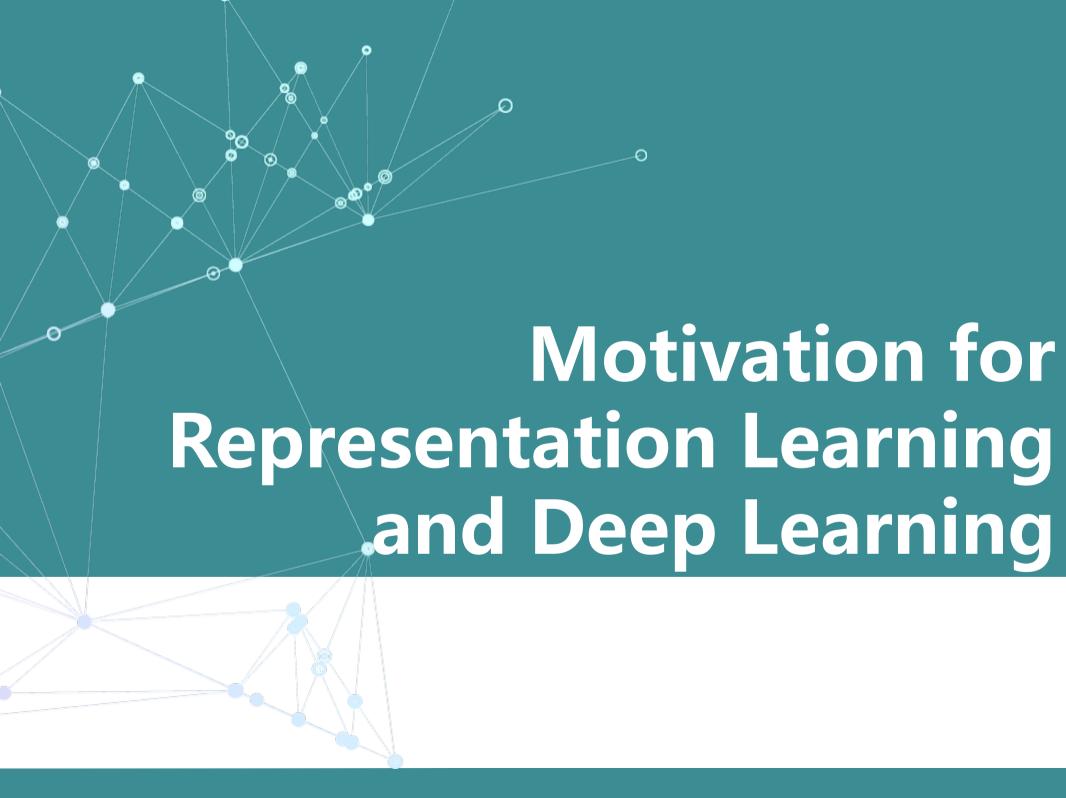
- Task, Experience, Performance
 Machine Learning = Improve P on T with E
- Linear regression models as a simplest example

$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$

Capture nonlinearity using linear basis model

$$f(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

 Today, we will look at a further extension of these ideas to neural networks



Let's play a game – Round 1

- 1. Choose 3 different numbers out of {0,1, ..., 9}
- 2. Write them down on a piece of paper. Don't change them!
- 3. Now, for the game:
 - 1. I will give you a "magic" number
 - 2. You add 0, 1, 2 or all 3 of your chosen numbers, to get as close to this number as possible. Record the absolute difference
 - 3. Example: You chose $\{3,5,9\}$. I give 15. The closest you can get is 5+9=14. Difference is 1. This is your score
 - 4. Example: You chose {3,5,9}. I give 1. The closest you can get is 0. Difference is 1. This is your score



Round 1.1: The magic number is 12. What is your score?

0

1

7

3

Z



Round 1.2: The magic number is 2. What is your score?

0

1

フ

3

4



Round 1.3: The magic number is 20. What is your score?

0

1

2

3

1

Round 2

For the next round, implement the following changes

- instead of picking 3 numbers out of {0,1, ..., 9}, pick 6 instead
- Now, you can pick either 0, 1, 2 or 3 of the 6 numbers you picked to get close to the answer
- Example: you picked {0,1,2,3,4,8}
 - The given number is 5, you can pick 2, 3, and your score is
 - The given number is 18, you can pick 3, 4, 8, and your score is 3 (note that you cannot pick more than 3)



Round 2.1: The magic number is 4. What is your score?

0

1

つ

3

7



Round 2.2: The magic number is 10. What is your score?

n

1

J

3

4



Round 2.3: The magic number is 19. What is your score?

0

1

J

3

Z

Recap



Score =
$$f - \sum_{i=1}^{3} w_i \phi_i$$
 $w_i \in \{0,1\}$

Given number Your numbers

Score =
$$\left| f - \sum_{i=1}^{3} w_i \phi_i(f) \right|$$
 $w_i \in \{0,1\}$
 $\phi(f) = \{3 \text{ choices based on } f\}$

Why did we do better in round 2?

Back to linear basis models

Recall that linear basis models can be chosen with universality

Examples (1D):

$$\phi(x) = (1, x, x^{2}, x^{3}, ...)$$

$$\phi(x) = (1, \cos(x), \sin(x), \cos(2x), \sin(2x), ...)$$

$$\phi(x) = \left(2^{\frac{n}{2}}\psi(2^{n}x - k)\right)_{n, k=1,2,...}$$

Haar Wavelet:
$$\psi(x) = \begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 1.0 \\ 1.5 \end{bmatrix}$$

Why don't we just use linear basis models with a large m?

Approximation Efficiency

Goal: approximate some function f^*

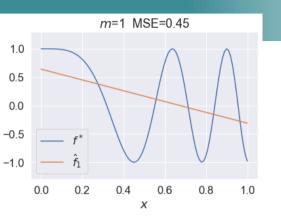
Consider two basis sets:

$$\phi_m(x) = (1, x, x^2, x^3, ..., x^m)$$

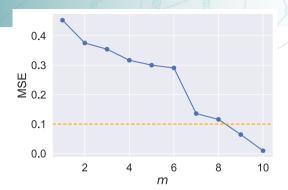
 $\phi_m(x) = (1, \cos(x), \cos(2x), ..., \cos(mx))$

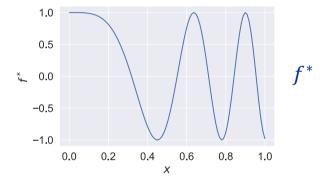
Let us consider fitting some function f^* with varying basis and varying m

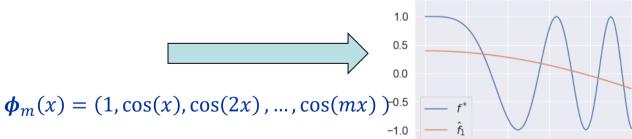
$$\boldsymbol{\phi}_m(x) = (1, x, x^2, x^3, \dots, x^m)$$



m=1 MSE=0.49







0.2

0.4

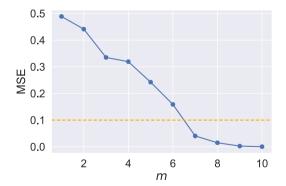
Х

0.6

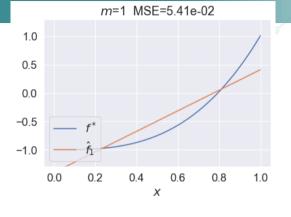
0.8

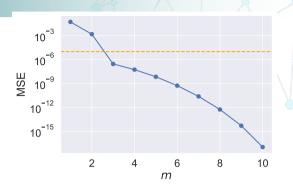
1.0

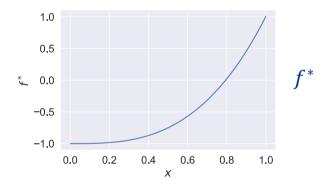
0.0

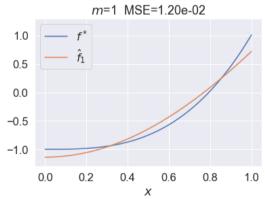


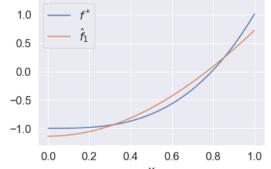
$$\boldsymbol{\phi}_m(x) = (1, x, x^2, x^3, \dots, x^m)$$

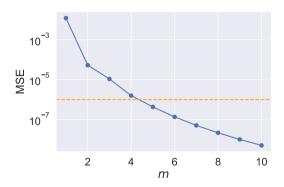












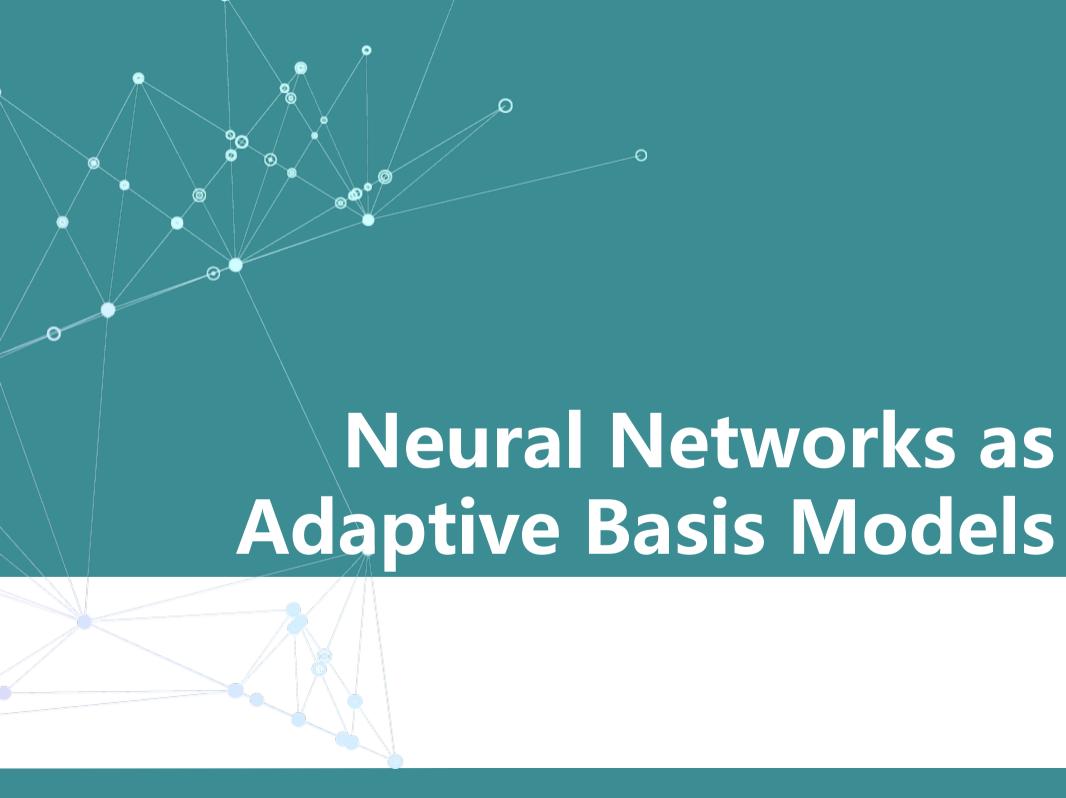


 $\boldsymbol{\phi}_m(x) = (1, \cos(x), \cos(2x), \dots, \cos(mx))$

Adaptive Approach

Previous experiments show

- How well we can learn with a given computational budget (m) depends **both** on the target (f^*) and the choice of basis (ϕ)
- No ϕ works universally well for **all** f^*
- Adapt the choice of ϕ to data!



Adaptive Basis Models

Usual linear basis models have the form

$$f(x) = w^T \phi(x)$$
 $x \in \mathbb{R}^d, w \in \mathbb{R}^m$

Adaptive models

$$f(x) = w^T \phi(x; \theta)$$
 $x \in \mathbb{R}^d, w \in \mathbb{R}^m, \theta \in \mathbb{R}^p$

The parameters θ are learned from data to find the best possible basis.

Example (Nonlinear Approximation)

Consider

$$f^* = 1 + x^{10}$$

Polynomial basis

$$\phi_m(x) = (1, x, x^2, ..., x^{m-1})$$

Adaptive polynomial basis

$$\boldsymbol{\phi}_{m}(x;\boldsymbol{\theta}) = \left(x^{\theta_{0}}, x^{\theta_{1}}, \dots, x^{\theta_{m-1}}\right)$$
$$\boldsymbol{\theta} \in \mathbb{N}^{m}$$

Learned Basis as Feature Maps

The basis $\{\phi(x; \theta): \theta \in \mathbb{R}^p\}$ is adapted to data by adjusting θ .

For this reason, we also call

$$\phi_i(\cdot; \boldsymbol{\theta}) : \mathbb{R}^d \to \mathbb{R}$$

feature maps, as they extract information from dataset.

Equivalently, they give good representation of the data

Example (Learning XOR)

The exclusive or (XOR) function on two binary variables

$$f^*(x_1, x_2) = \begin{cases} 1 & \text{exactly one of } x_i \text{ is 1} \\ 0 & \text{otherwise} \end{cases}$$

Let us build a simple linear model to represent this function

Data Matrix:

$$X = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix} \qquad y = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

Empirical Risk:

$$R(\boldsymbol{\theta}) = \frac{1}{4} \sum_{i=1}^{4} (f^*(\boldsymbol{x}_i) - f(\boldsymbol{x}_i; \boldsymbol{\theta}))^2$$

Linear Model:

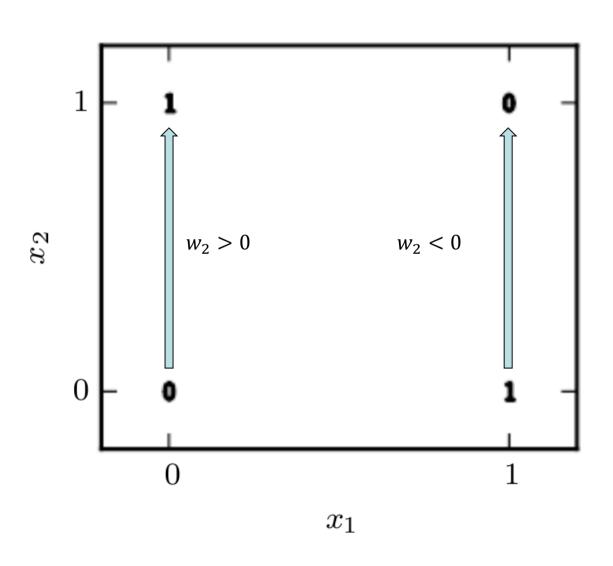
$$f(\mathbf{x}; \boldsymbol{\theta}) = f(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^T \mathbf{x} + b$$

Solving the regression problem gives

$$w = (0,0)$$
 $b = \frac{1}{2}$

Hence,
$$f(x; w, b) \equiv \frac{1}{2}$$

Why is linear model not enough?



Neural Network for the XOR Function

We are going to write $f = f^{(2)} \circ f^{(1)}$:

$$h = f^{(1)}(x; W, c)$$

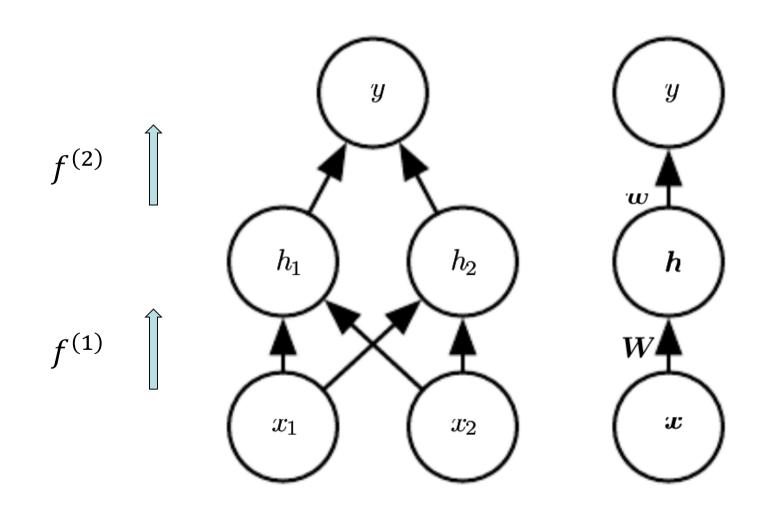
 $y = f^{(2)}(h; w, b)$

The vector h is called a vector of **hidden units** Its dimension is m, also known as the *width* of the hidden layer

The combined model is

$$f(\mathbf{x};\boldsymbol{\theta}) \equiv f(\mathbf{x}; W, \boldsymbol{c}, \boldsymbol{w}, b) = f^{(2)}(f^{(1)}(\mathbf{x}; W, \boldsymbol{c}); \boldsymbol{w}, b)$$

Graph Representation of Neural Networks



Activation Functions

We have not specified how to choose $f^{(1)}$ and $f^{(2)}$

Simplest choice: linear functions

$$f^{(1)}(x; W, c) = Wx + c$$

 $f^{(2)}(h; w, b) = w^{T}h + b$

$$f^{(2)}(f^{(1)}(x)) = \mathbf{w}^T(W\mathbf{x} + \mathbf{c}) + b$$
$$= (W^T\mathbf{w})^T\mathbf{x} + (\mathbf{w}^T\mathbf{c} + b)$$
$$\mathbf{w}'$$

We need some form of **nonlinearity**!
We pick the simplest type of nonlinearity

$$h = f^{(1)}(x; W, c) = g(Wx + c)$$

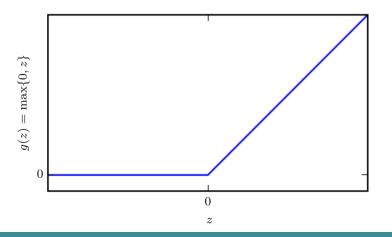
 $y = f^{(2)}(h; w, b) = w^{T}h + b$

The function $g: \mathbb{R} \to \mathbb{R}$ is called an **activation function**, and is applied **element-wise** to a vector

$$g(\mathbf{z})_i = g(z_i)$$

Simplest choice of activation:

$$g(z) = \max(0, z)$$



A Solution to the XOR Problem

Neural network model:

$$f(\mathbf{x}; W, \mathbf{c}, \mathbf{w}, b) = \mathbf{w}^T \max(0, W\mathbf{x} + \mathbf{c}) + b$$

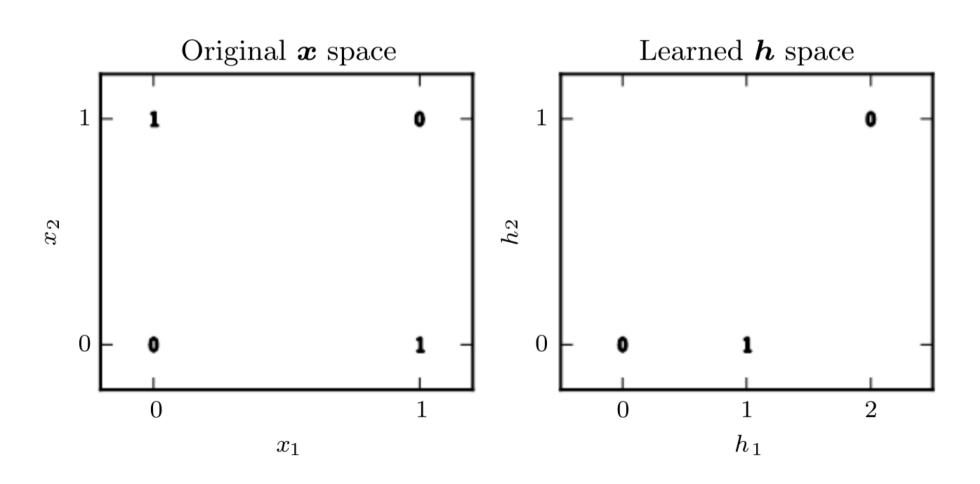
Let

$$W = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \mathbf{c} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \quad \mathbf{w} = \begin{pmatrix} 1 \\ -2 \end{pmatrix} \quad b = 0$$

Then

$$f(X; W, \boldsymbol{c}, \boldsymbol{w}, b) = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = f^*(X)$$

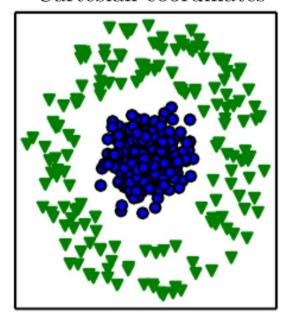
What is the role of the hidden units?



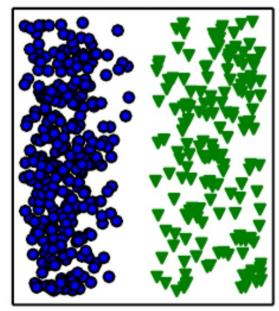
Feature Space



Cartesian coordinates



Polar coordinates



General Shallow (1-hidden-layer) Neural Networks



$$f(\mathbf{x}; W, \mathbf{c}, \mathbf{w}, b) = \mathbf{w}^{T} \underbrace{g(W\mathbf{x} + \mathbf{c})}_{\mathbf{\phi}(\mathbf{x}; \mathbf{\theta})} + b$$

Variables: $W \in \mathbb{R}^{m \times d}$, $\boldsymbol{c} \in \mathbb{R}^m$, $\boldsymbol{w} \in \mathbb{R}^m$, $b \in \mathbb{R}$

- W and w are called weights
- c and b are called biases
- g is the activation function

Activation Functions

 Rectified Linear Unit (ReLU)

$$g(z) = \max(0, z)$$

Sigmoid

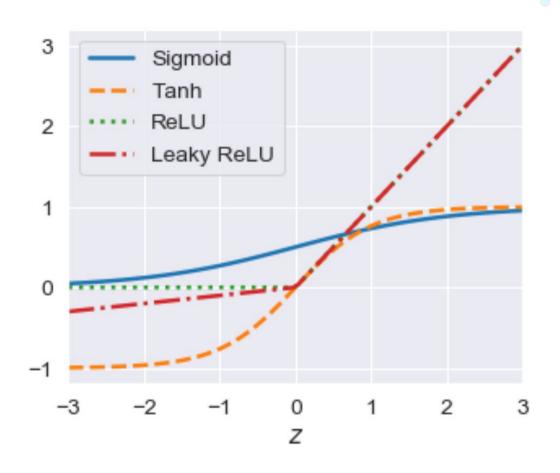
$$g(z) = \frac{1}{1 + e^{-z}}$$

Tanh

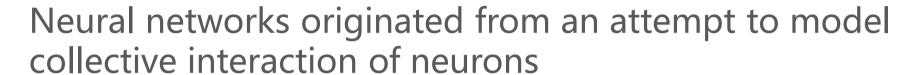
$$g(z) = \tanh(z)$$

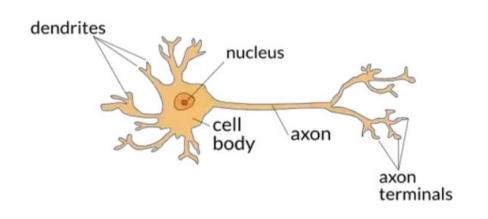
Leaky-ReLU

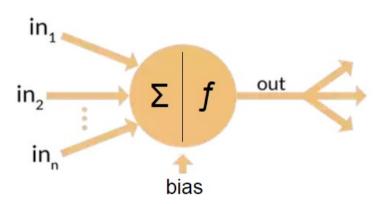
$$g(z) = \begin{cases} z & \text{if } z \ge 0\\ \delta z & \text{if } z < 0 \end{cases}$$



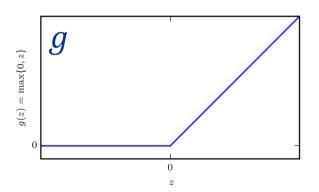
Historical Motivation: Modelling Neurons







Neuron: $g(W_i \cdot x + c_i)$



Picture: https://towardsdatascience.com/the-differences-between-artificial-and-biological-neural-networks-a8b46db828b7

Universal Approximation Theorem

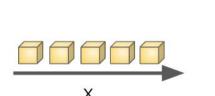
One of the foundational results for neural networks is the universal approximation theorem.

In words, it says the following:

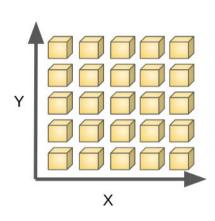
Any continuous function f^* on a compact domain can be approximated by neural networks to arbitrary precision, provided there are enough neurons (m large enough).

Why NNs over linear basis models?

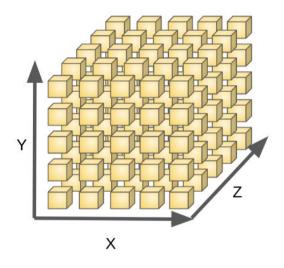
Curse of Dimensionality



$${x^j: j = 0,1, ...}$$



$$\left\{x_1^{j_1}x_2^{j_2}: j_1, j_2 = 0, 1, \dots\right\}$$



$$\left\{x_1^{j_1}x_2^{j_2}: j_1, j_2 = 0, 1, \dots\right\} \qquad \left\{x_1^{j_1}x_2^{j_2}x_3^{j_3}: j_1, j_2, j_3 = 0, 1, \dots\right\}$$

Under some technical assumptions, for any continuous (+ other conditions) function $f^*: [0,1]^d \to \mathbb{R}$, there exists a width-m neural network f_m such that

$$||f^* - f_m||^2 \le \mathcal{O}(m^{-1})$$

This result is first proved in [Baron, 1993]

This is a **tremendous** improvement over linear basis models, where we usually have [Jackson, 1912]

$$||f^* - f_m||^2 \le \mathcal{O}\left(m^{-\frac{2\alpha}{d}}\right)$$

The constant α measures the smoothness of f^*

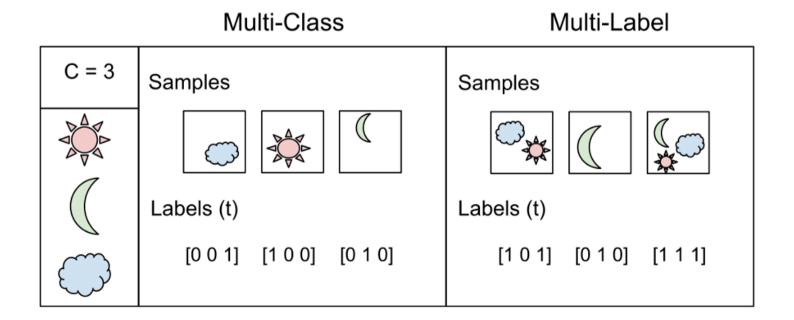
Neural Networks for Classification

Neural networks can be modified to handle classification problems, exactly in the same way as linear models

Choice of Output Units

The soft-max output unit is appropriate for multi-class classification problems

There are also multi-label classification problems...



In multilabel classification, a sigmoid output unit is more appropriate

Softmax(
$$\mathbf{z}$$
)_i = $\frac{\exp(z_i)}{\sum_j \exp(z_j)}$

Sigmoid(
$$\mathbf{z}$$
)_i = $\frac{1}{1 + \exp(-z_i)}$

Loss Functions

Empirical risk minimization requires the definition of loss functions

$$R_{\text{emp}}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} L(f^*(\boldsymbol{x}_i), f(\boldsymbol{x}_i, \boldsymbol{\theta}))$$

For regression problems, we usually pick the square loss (why?)

$$L(y, y') = \frac{1}{2}(y - y')^2$$

Loss Functions for Classification

Multiclass classification problem

- Here, $y = f(x; \theta)$ and $y' = f^*(x)$ are probability vectors
- Usually pick the cross-entropy loss

$$L(\mathbf{y}, \mathbf{y}') = -\sum_{j} y_{j}' \log y_{j}$$

Multilabel classification problem

- Here, each y, y' is a vector whose coordinates are in [0,1]
- Usually pick the binary cross-entropy loss

$$L(y, y') = -\sum_{j} (y'_{j} \log y_{j} + (1 - y'_{j}) \log(1 - y_{j}))$$

Why cross-entropy over square?

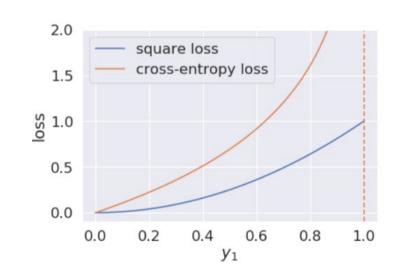
There are some good reasons to choose cross-entropy over the square loss for classification problems

- Better statistical interpretation
- Better numerical stability

2-Class case:

MSE: $L(y, y') = (y_1 - y_1')^2$

CE: $L(y, y') = -y'_1 \log y_1 - (1 - y'_1) \log(1 - y_1)$



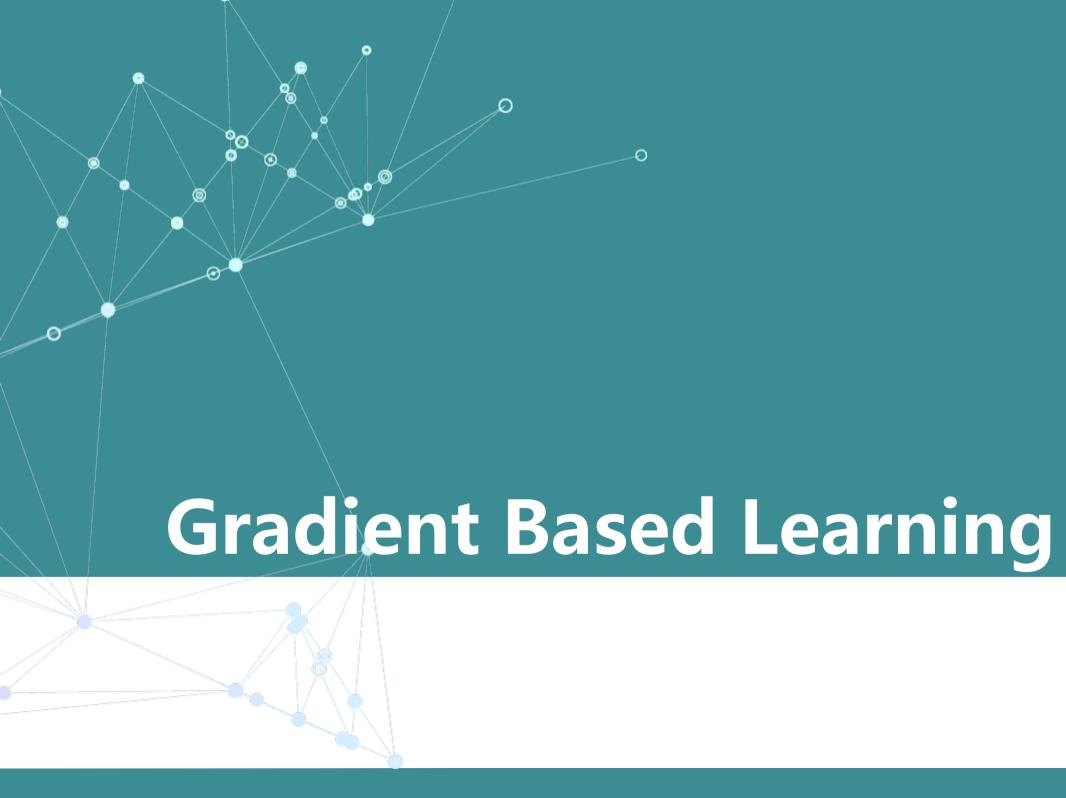
Surrogate Losses

Importantly, for classification problems, whatever loss you choose, they are often **surrogates** for the true loss, which is the **accuracy**:

$$L(y, y') = \mathbb{I}_{y \neq y'}$$

This is known as the **zero-one loss**.

Why is this usually not used for optimization?



Empirical Risk Minimization

Essentially, empirical risk minimization is an optimization problem

$$\min_{\boldsymbol{\theta}} R(\boldsymbol{\theta})$$

Recall that in linear regression, we solved the problem by setting

$$\nabla R(\boldsymbol{\theta}) = 0$$

However, very often there are no easy way to solve this equation

Iterative Methods

In this case, we will resort to iterative methods, where we make the loss smaller successively

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k + F(\boldsymbol{\theta}_k)$$

And hopefully we achieve

$$R(\boldsymbol{\theta}_{k+1}) \le R(\boldsymbol{\theta}_k)$$

Gradient Descent as an Iterative Method

Let us consider the optimization problem

$$\min_{\boldsymbol{\theta}} R(\boldsymbol{\theta}) \qquad R: \mathbb{R}^p \to \mathbb{R}$$

Given θ , we want to make a small change to θ in some appropriate direction ϕ , so that

$$R(\boldsymbol{\theta} + \epsilon \cdot \boldsymbol{\phi}) \le R(\boldsymbol{\theta})$$

Here, ϵ is a small positive number

Taylor Expansion:

$$R(\boldsymbol{\theta} + \epsilon \boldsymbol{\phi}) = R(\boldsymbol{\theta}) + \epsilon \boldsymbol{\phi}^T \nabla R(\boldsymbol{\theta}) + \mathcal{O}(\epsilon^2)$$

We want the term $\epsilon \phi^T \nabla R(\theta)$ to be as negative as possible, so we should take

$$\phi \propto -\nabla R(\theta)$$

In other words, we want to push θ in the negative gradient direction

$$\boldsymbol{\theta} \to \boldsymbol{\theta} - \epsilon \nabla R(\boldsymbol{\theta})$$

The Gradient Descent Algorithm

The direction $-\nabla R$ is called the **steepest descent direction**

This gives rise to a simple iterative algorithm for minimization

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \epsilon \nabla R(\boldsymbol{\theta}_k)$$

This is called **Gradient Descent** (GD) The number ϵ is called the **step size** or the **learning rate**

Can we take ϵ as large as we like?

Example

Consider minimizing a quadratic function

$$R(\boldsymbol{\theta}) = \frac{1}{2} \|\boldsymbol{\theta}\|^2$$

Gradient descent iterates

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \epsilon \boldsymbol{\theta}_k$$

$$\boldsymbol{\theta}_k = (1 - \epsilon)^k \boldsymbol{\theta}_0$$

Example (Iterative Solution of Linear Regression)

Recall linear regression problem

$$\min_{\mathbf{w}} R(\mathbf{w}) = \frac{1}{2} ||X\mathbf{w} - \mathbf{y}||^2$$

Gradient descent iterates

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \epsilon X^T (X \mathbf{w}_k - \mathbf{y})$$

= $(I - \epsilon X^T X) \mathbf{w}_k + \epsilon X^T \mathbf{y}$

Suppose $w_k \to w_\infty$ for some w_∞ , what is w_∞ ?

$$\mathbf{w}_{\infty} = (I - \epsilon X^T X) \mathbf{w}_{\infty} + \epsilon X^T \mathbf{y} \Rightarrow \mathbf{w}_{\infty} = (X^T X)^{-1} X^T \mathbf{y}$$

Convergence Analysis (Optional)

When does $w_k \rightarrow w_\infty$?

To see this, we can rewrite the GD iterations as

$$\mathbf{w}_{k+1} - \mathbf{w}_{\infty} = A(\mathbf{w}_k - \mathbf{w}_{\infty})$$
 where $A = (I - \epsilon X^T X)$

Denote by $e_k = w_k - w_\infty$ the error vector, then

$$\boldsymbol{e}_k = A^k \boldsymbol{e}_0$$

Let $\{\lambda_1(A), ..., \lambda_d(A)\}$ be the real eigenvalues of A (why real?)

Then, if $\lambda_i(A) < 0$ for all i,

$$\boldsymbol{e}_k = A^k \boldsymbol{e}_0 \to 0$$

This is ensured by $\epsilon \leq \frac{1}{\max_{i} \lambda_{i}(X^{T}X)}$ (Is this necessary?)

Suppose we take

$$\epsilon = \frac{1}{\max_{i} \lambda_{i}(X^{T}X)}$$

Then,

$$\|\boldsymbol{e}_k\| \le \left(1 - \frac{1}{\kappa(X^T X)}\right)^k \|\boldsymbol{e}_0\|$$

The quantity

$$\kappa(X^T X) \coloneqq \frac{\max_{i} \lambda_i(X^T X)}{\min_{i} \lambda_i(X^T X)} \ge 1$$

is called the **condition number** of X^TX . The bigger the condition number, the slower the convergence.

Convergence for General Losses

In general, one can prove that if ∇R is Lipschitz and $\nabla^2 R$ is uniformly bounded, then for small enough ϵ we have

$$\|\nabla R(\boldsymbol{\theta}_k)\| \to 0$$
 as $k \to \infty$

Does this mean that $\theta_k \to \theta_\infty$ for some θ_∞ ?

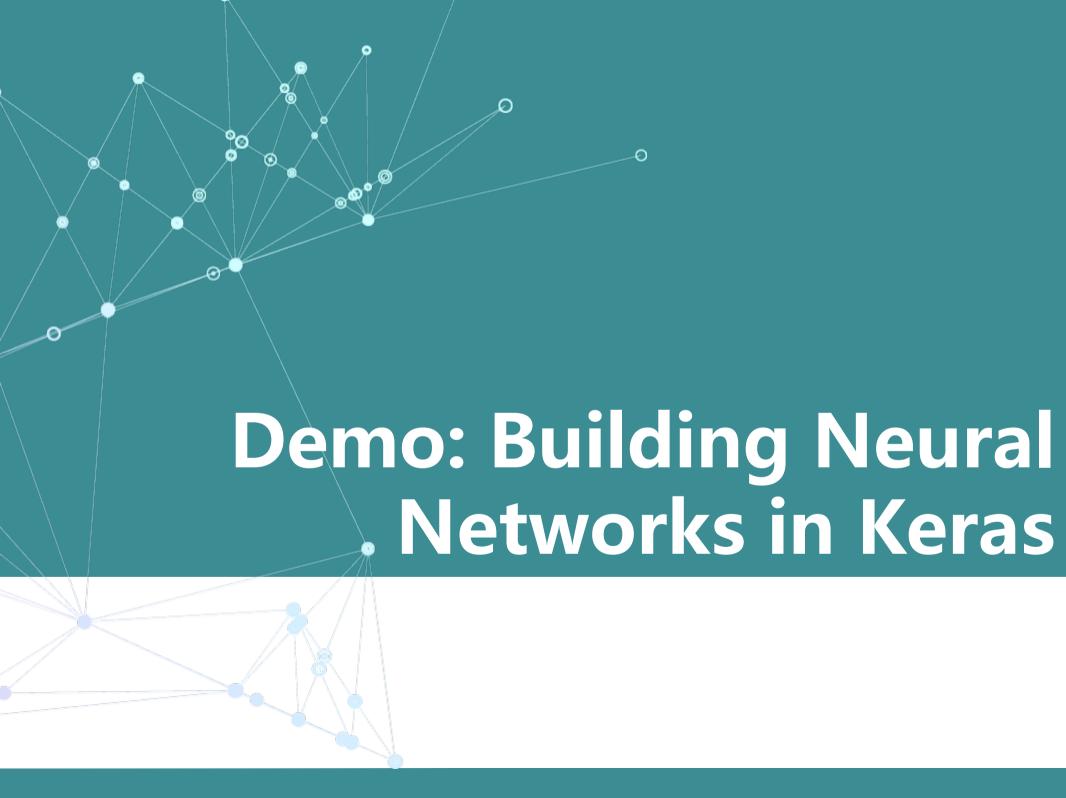
Steepest Descent to Optimize Neural Networks

Recall that the empirical risk minimization problem for NNs can be cast as an optimization problem

$$\min_{W,c,w,b} R(W,c,w,b) = \sum_{i=1}^{N} L(f^*(x_i), f(x_i; W, c, w, b))$$

And hence can be solved* iteratively by gradient descent

$$W_{k+1} = W_k - \nabla_W R(W_k, \boldsymbol{c}_k, \boldsymbol{w}_k, b_k)$$
:



Tensorflow

Tensorflow is a open source deep learning framework developed by Google.

Main features

- Automatic differentiation
- Same code can be run on GPU (CUDA)
- Deployable to all sorts of devices (e.g. mobile phones)
- Eager execution starting from Tensorflow v2.0

Further Information and Tutorials https://www.tensorflow.org/



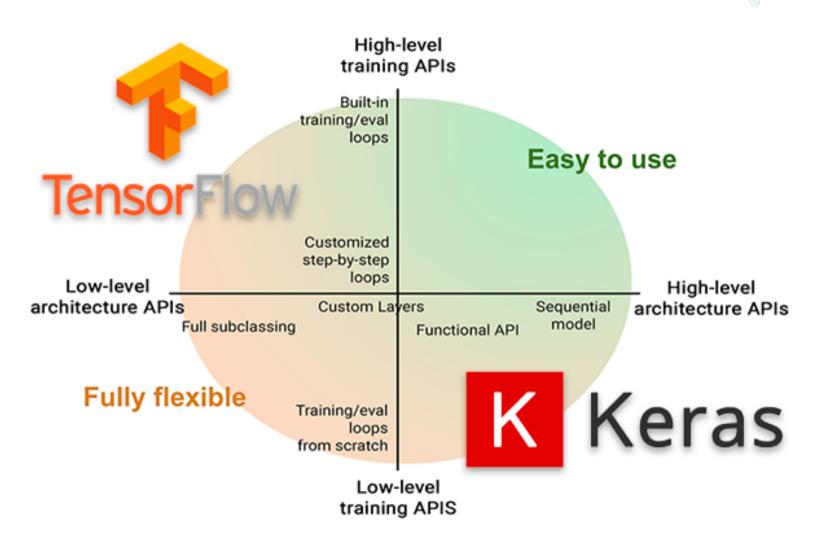
Keras

Keras is a high-level neural network API that makes model building and prototyping easier

- Uses Tensorflow (or CNTK, Theano) backend
- High-level abstraction (layers, models)
- "Disadvantage": may need some lower level (tensorflow) knowledge to do some meaningful tinkering



Keras vs Tensorflow



Alternatives

The main alternative to the tensorflow/keras framework is **pytorch**

- Similar API and behavior to numpy
- Flexible for model and algorithm development
- See: https://pytorch.org/



Computational Resources

For your project, you may require GPU computing resources for application-heavy type of problems

There are two sources for computational resources available to you:

- University HPC cluster (https://nusit.nus.edu.sg/hpc/)
- National Supercomputing Center (NSCC) (<u>https://www.nscc.sg</u>)