SUMMER SCHOOL 2020

MACHINE LEARNING DAY 2

DEEP LEARNING

Session III: Multi-Layer Perceptron

Isaac Ye, HPTC @ York University

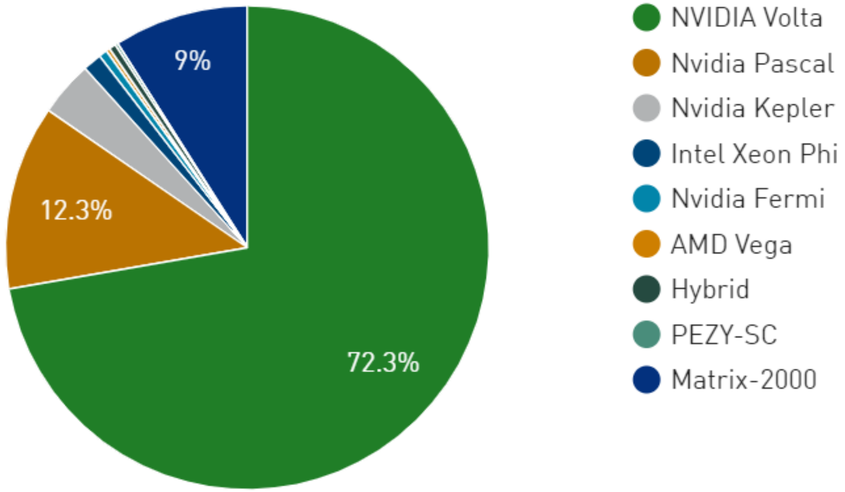
Isaac@sharcnet.ca

Running DL in Graham

DL and HPC architectures

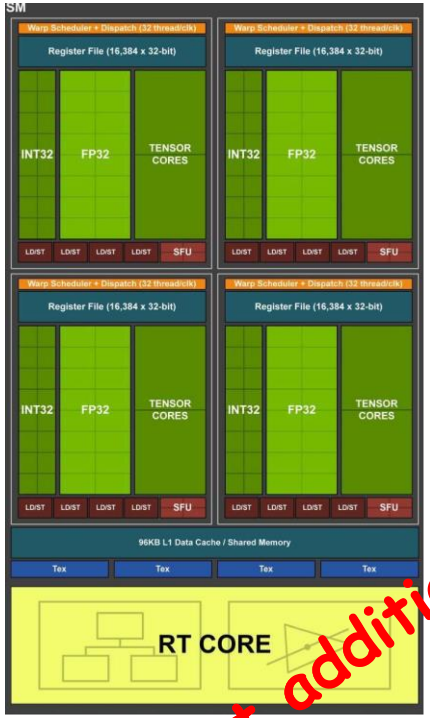
NVIDIA GPUs are the main driving force for faster training DL models

Accelerator/CP Family Performance Share



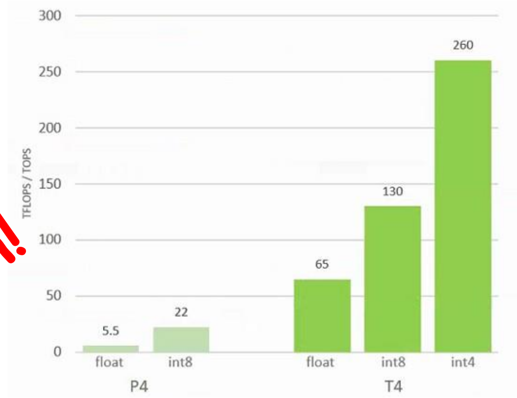
https://top500.org

NVIDIA T4 Turing GPU on Graham



Streaming Multiprocessor
8 Tensor cores

40 SM in T4
8.1 Tflops FP32
65 Tflops FP16



Latest addition!

GPU resources in Compute Canada

As of Feb, 2020

	# of nodes	GPU type	Note
Graham	160	P100 Pascal	--gres=gpu:1
	7	V100 Volta	CPU/GPU ≤ 3.5 --gres=gpu:v100:1
	36	T4 Turing (DL target)	CPU/GPU ≤ 3.5 --gres=gpu:t4:2
Cedar	146	P100 Pascal	--gres=gpu:1
Beluga	172	V100 Volta	CPU/GPU ≤ 3.5 --gres=gpu:v100:1
Niagara	None		

Virtual environment

Allows users to create virtual environments so that one can install Python modules easily

Many versions of same module are possible

```
[isaac@gra-login3 ~]$ module load python
[isaac@gra-login3 ~]$ module list

Currently Loaded Modules:
  1) nixpkgs/16.09   (S)      3) gcccore/.5.4.0  (H)    5) ifort/.2016.4.258 (H)    7) openmpi/2.1.1 (m)    9) python/3.7.4 (t)
  2) imkl/11.3.4.258 (math)   4) icc/.2016.4.258 (H)    6) intel/2016.4      (t)    8) StdEnv/2016.4 (S)

  Where:
   S:     Module is Sticky, requires --force to unload or purge
   m:     MPI implementations / Implémentations MPI
   math:  Mathematical libraries / Bibliothèques mathématiques
   t:     Tools for development / Outils de développement
   H:                Hidden Module



[isaac@gra-login3 ~]$ virtualenv --no-download ~/tf5
Using base prefix '/cvmfs/soft.computecanada.ca/easybuild/software/2017/Core/python/3.7.4'
New python executable in /home/isaac/tf5/bin/python
Installing setuptools, pip, wheel...
done.
[isaac@gra-login3 ~]$ source tf5/bin/activate
(tf5) [isaac@gra-login3 ~]$ deactivate
[isaac@gra-login3 ~]$ █
```

Lab 3A – Working in Graham

1. Log into graham.computecanada.ca with guest account and p/w

   (Use MobaXterm or Putty for Windows / Open terminal in Linux or Mac)

2. Load modules and make a virtual environment
   https://docs.computecanada.ca/wiki/Python#Creating_and_using_a_virtual_environment

```
module load python
module load scipy-stack
virtualenv --no-download ~/ENV
```

3. Activate, Upgrade 'PIP' and install 'PyTorch'
   https://docs.computecanada.ca/wiki/PyTorch#Installation

```
source ~/ENV/bin/activate
pip install --no-index --upgrade pip
pip install --no-index torch
pip install --no-index torch torchvision torchtext torchaudio
```

4. Getting out of virtual enviornment

```
deactivate
```

Lab 3A – Running simple code

Break room

1. Download *Lab2A_Linear_Reg_Vanilla.ipynb* as .py file from Google Colab
2. File transfer *Lab2A_Linear_Reg_Vanilla.py* to Graham using WinScp or MobaXterm (Windows) / sftp (Linux, Mac)
3. Activate virtual environment (make sure you load python and scipy-stack module)
4. Run it by 'python *Lab2A_Linear_Reg_Vanilla.py*'
5. Note you need to collect all import commands into the beginning of code using text editor (Nano/emacs/VI)

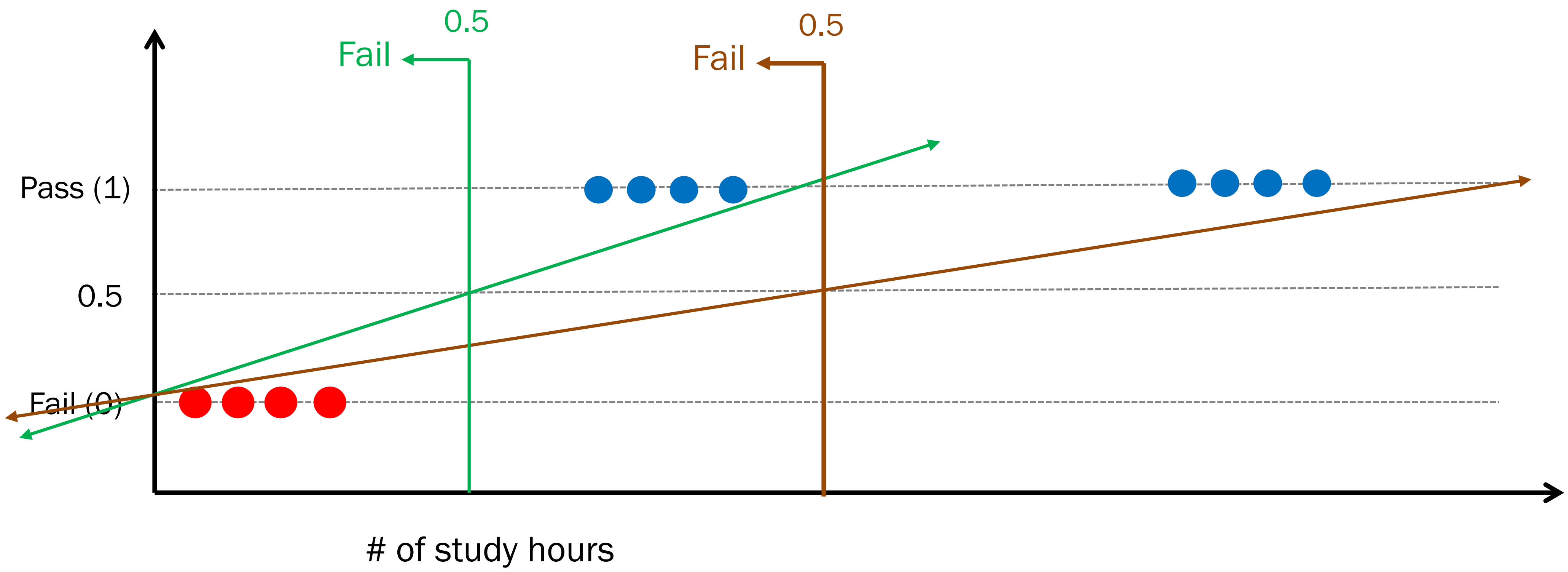
```
import matplotlib.pyplot as plt
import numpy as np
```

6. Note that you need to save/close your plots with proper filename for each plotting command like below

```
plt.scatter(X,Y)
plt.savefig('datascatter.png')
plt.close()
```

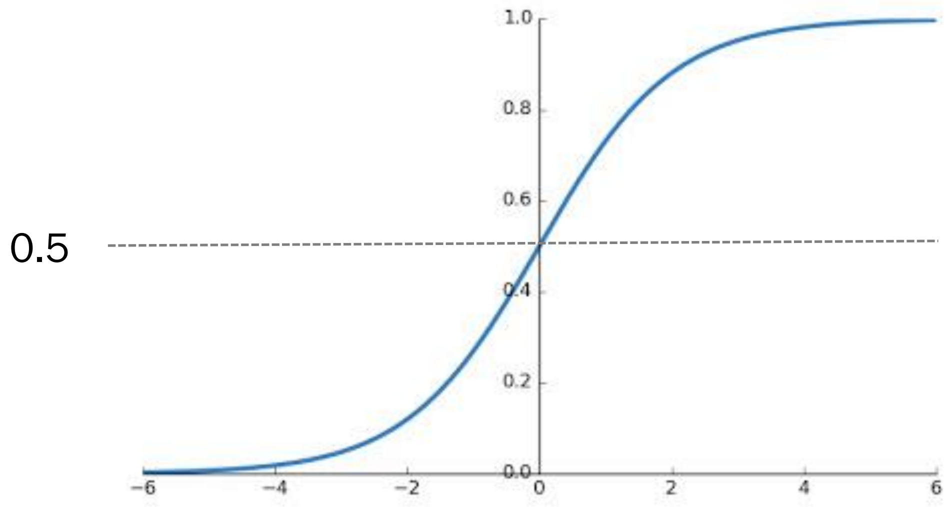
7. File transfer plotting files to your local computer using WinScp or MobaXterm (Windows) / sftp (Linux, Mac) and check it out

Binary classification



Linear regression is not good to solve binary problem!

Model: Logistic (Sigmoid) hypothesis



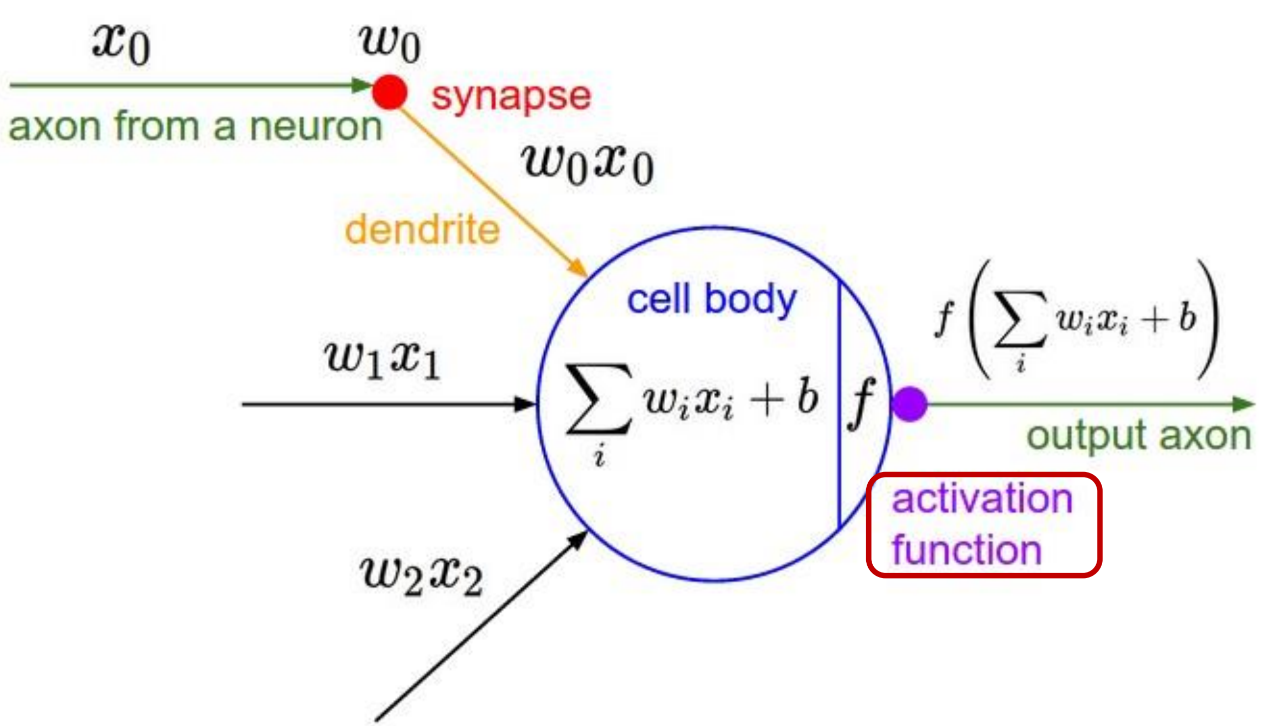
$$H(x) = f(Wx + b)$$

$$z = Wx + b$$

$$H(z) = f(z)$$

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

Neural Network



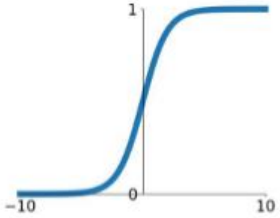
http://cs231n.github.io/neural-networks-1/

Mathematical model

Activation functions

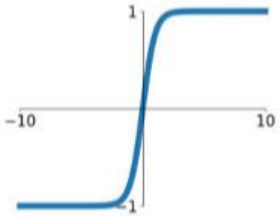
Sigmoid

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



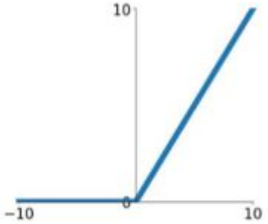
tanh

$\tanh(x)$



ReLU

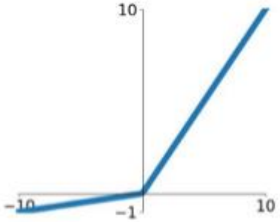
$\max(0, x)$



Most commonly used

Leaky ReLU

$\max(0.1x, x)$

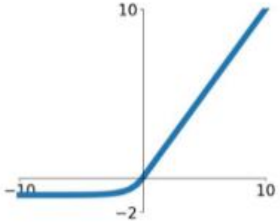


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Cost function: Cross Entropy

Cross entropy: difference between two probability distribution

$$H(P,Q) = -\sum P(x)\log Q(x)$$

$P(x)$: actual probability

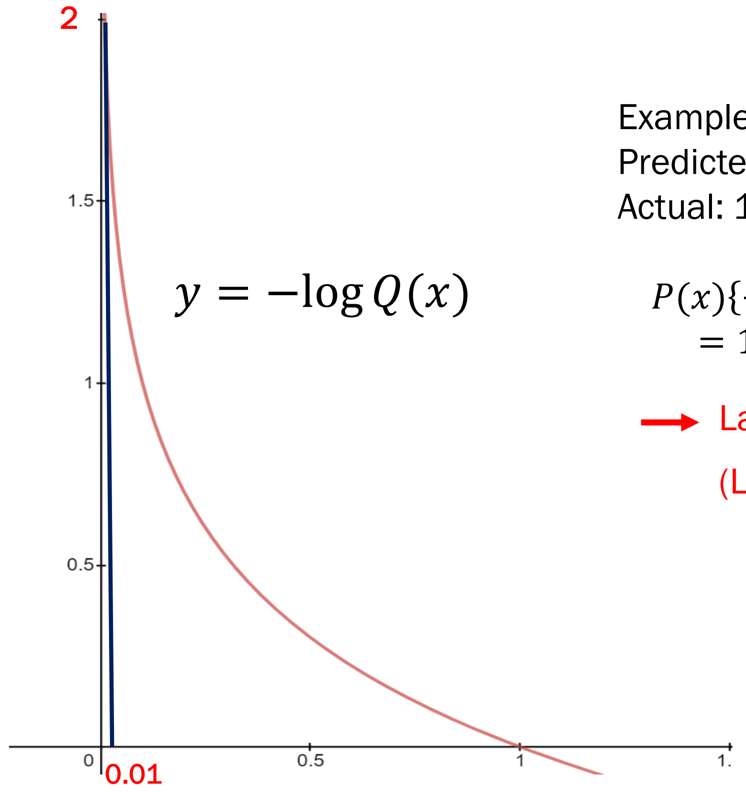
$Q(x)$: predicted probability

CROSSENTROPYLOSS

CLASS `torch.nn.CrossEntropyLoss(weight=None, size_average=None, ignore_index=-100, reduce=None, reduction='mean')` [SOURCE]

This criterion combines `nn.LogSoftmax()` and `nn.NLLLoss()` in one single class.

It is useful when training a classification problem with C classes. If provided, the optional argument `weight` should be a 1D *Tensor* assigning weight to each of the classes. This is particularly useful when you have an unbalanced training set.



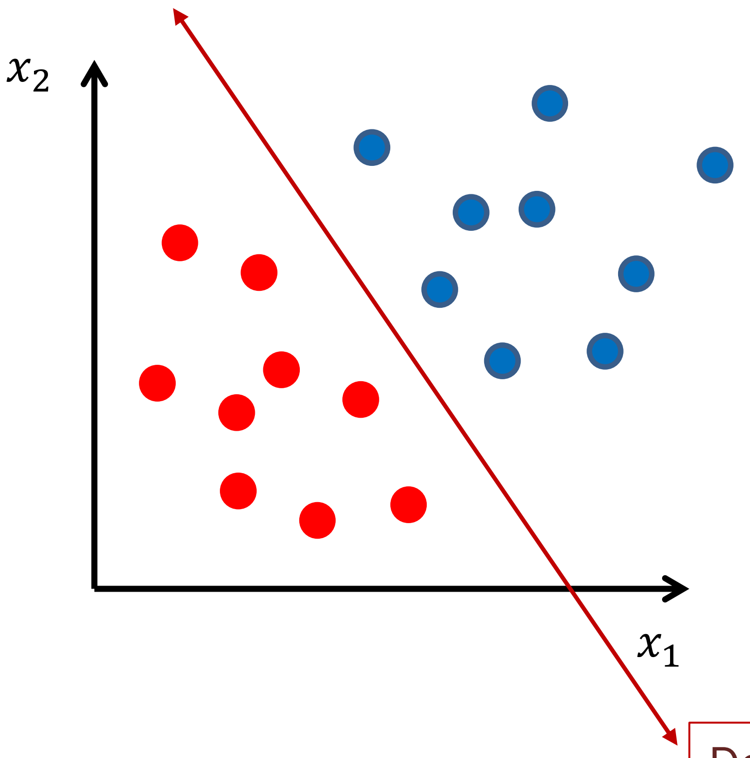
Example
Predicted: 0.01
Actual: 1

$$P(x)\{-\log Q(x)\}$$
$$= 1\{2\} = 2$$

→ Large entropy

(Large error)

Decision boundary



Decision boundary line

$$H(x) = G(Wx + b)$$

Sigmoid$(wx + b)$ = 0.5

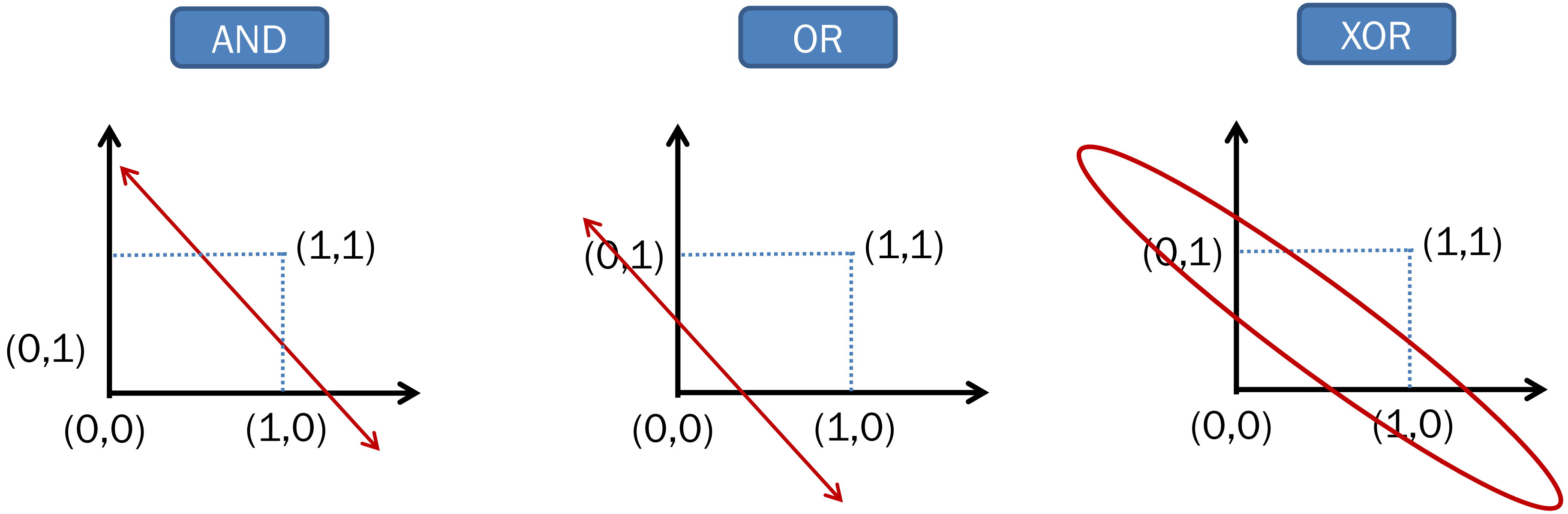
$\rightarrow$ $wx + b = 0$

For two input feature problem, one can have

$$w_1x_1 + w_2x_2 + b = 0$$

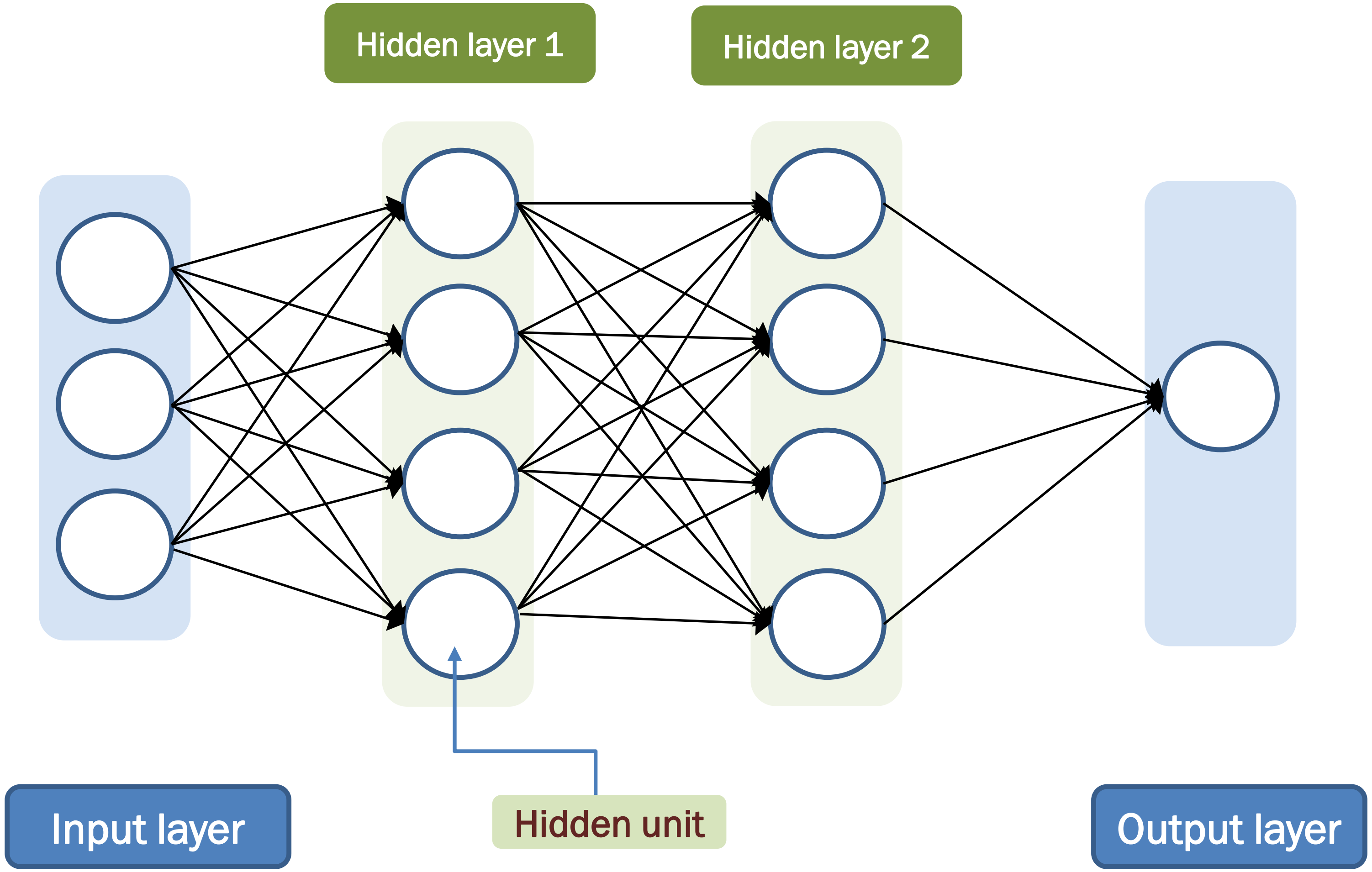
$\rightarrow$ Linear line!

XOR problem



Fail to find a decision line !

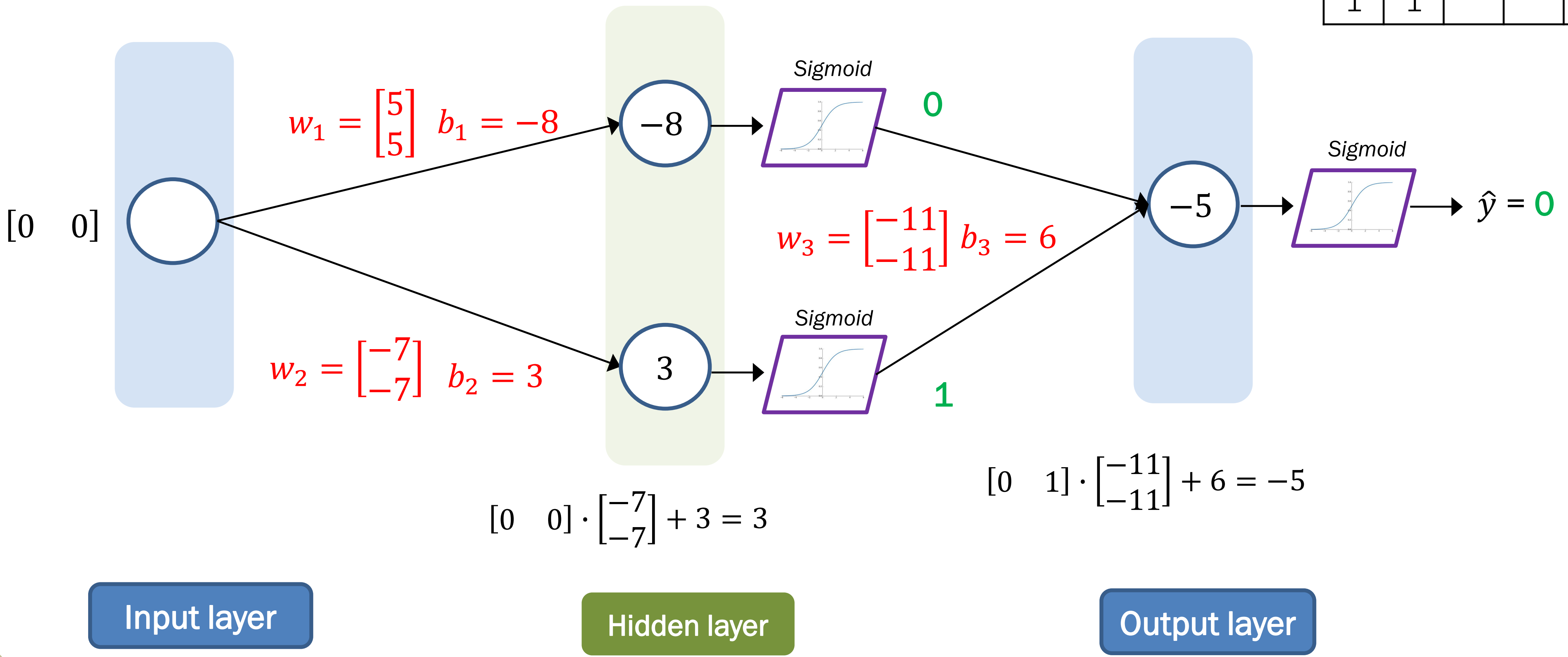
Multi-Layer Perceptron



XOR problem

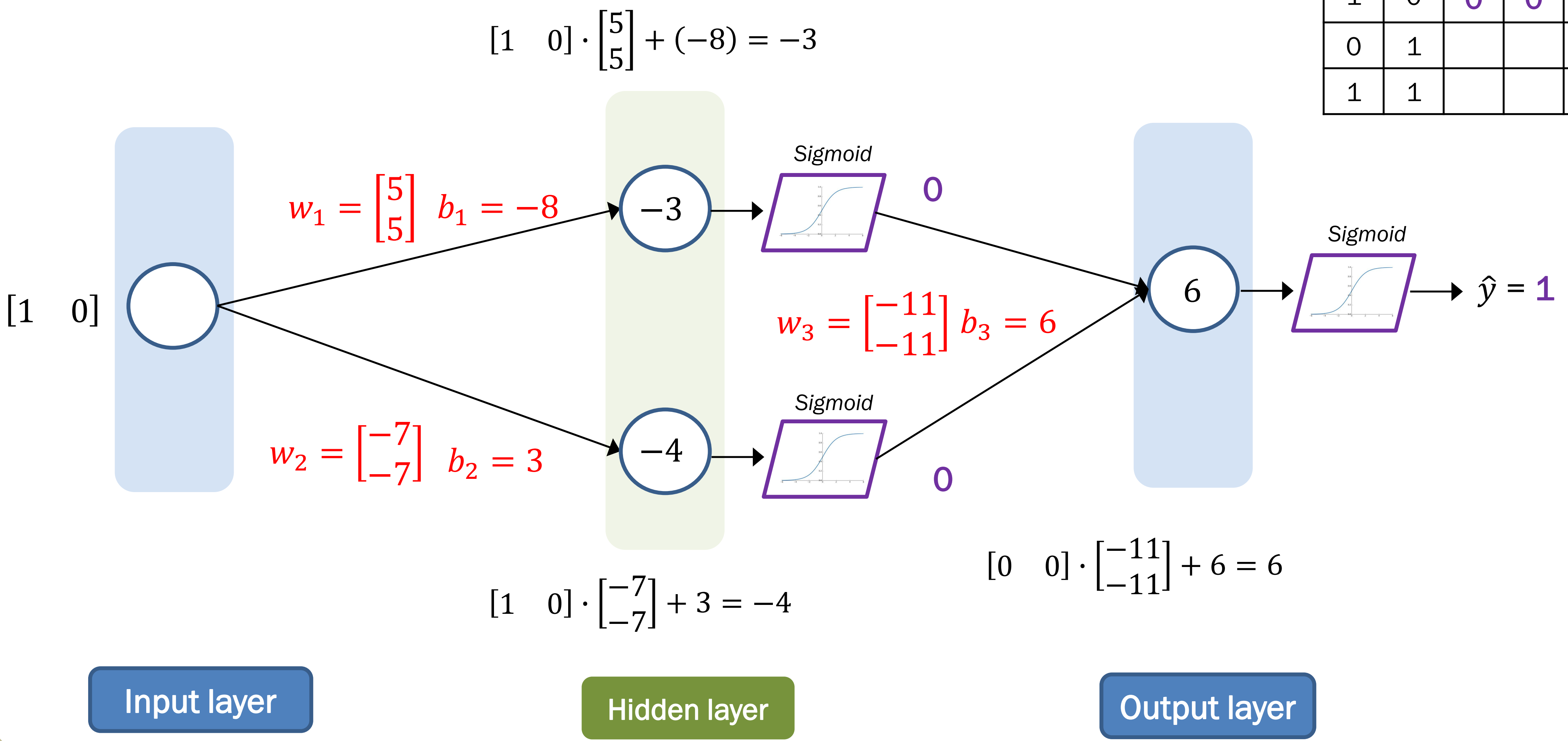
x_1	x_2	y_1	y_2	$\hat{y}$	y
0	0	0	1	0	0
1	0				1
0	1				1
1	1				0

$$[0 \quad 0] \cdot \begin{bmatrix} 5 \\ 5 \end{bmatrix} + (-8) = -8$$



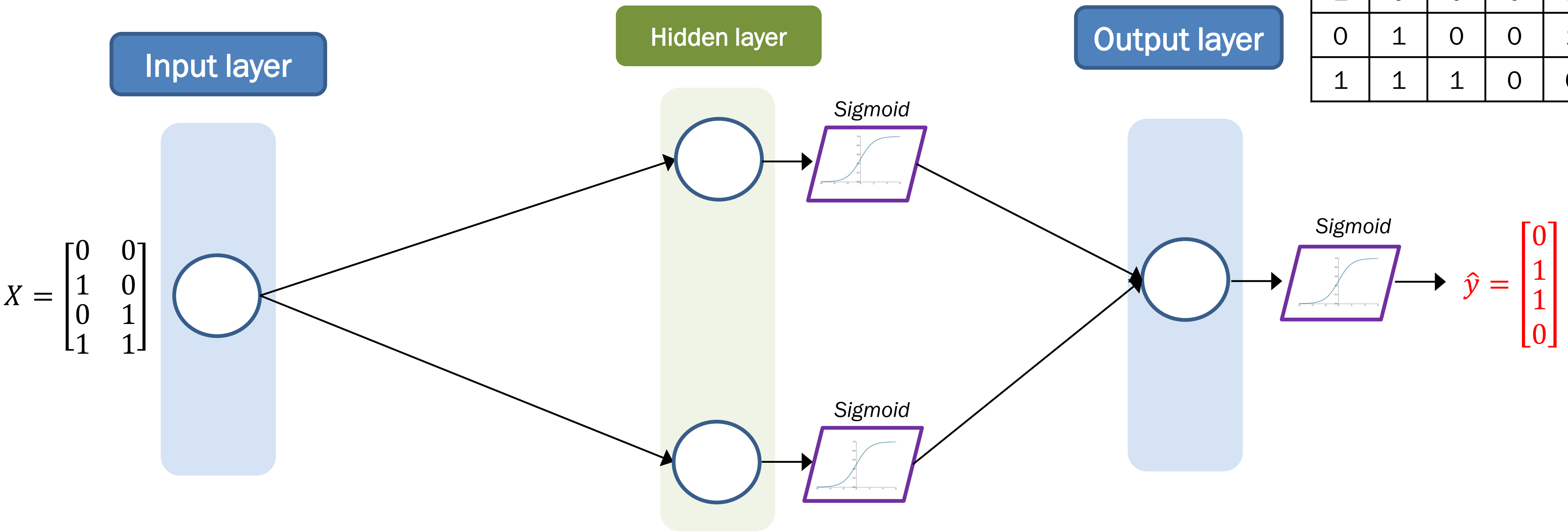
XOR problem

x_1	x_2	y_1	y_2	$\hat{y}$	y
0	0	0	1	0	0
1	0	0	0	1	1
0	1				1
1	1				0



XOR problem

x_1	x_2	y_1	y_2	$\hat{y}$	y
0	0	0	1	0	0
1	0	0	0	1	1
0	1	0	0	1	1
1	1	1	0	0	0

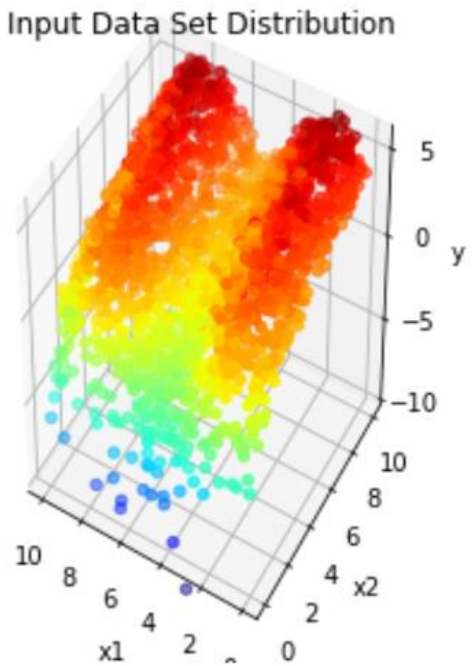


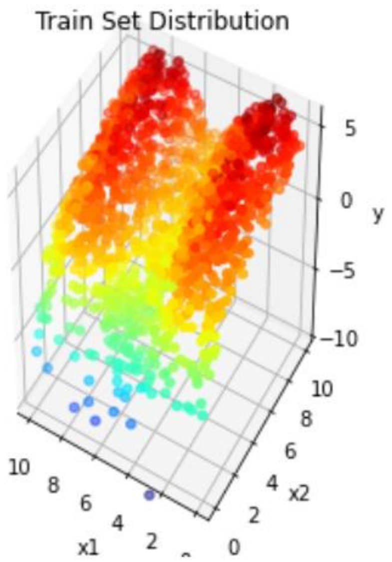
$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 5 & -7 \\ 5 & -7 \end{bmatrix} + \begin{bmatrix} -8 & 3 \\ -8 & 3 \\ -8 & 3 \\ -8 & 3 \end{bmatrix} = \begin{bmatrix} -8 & 3 \\ -3 & -4 \\ -3 & -4 \\ 2 & -11 \end{bmatrix} \xrightarrow{\text{Sigmoid}} \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} -11 \\ -11 \end{bmatrix} + \begin{bmatrix} 6 \\ 6 \\ 6 \\ 6 \end{bmatrix} = \begin{bmatrix} -5 \\ 6 \\ 6 \\ -5 \end{bmatrix} \xrightarrow{\text{Sigmoid}} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

Data preparation

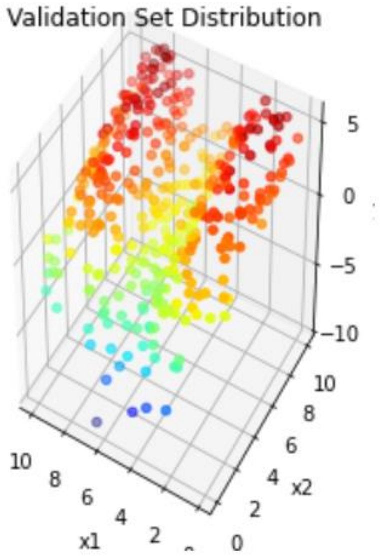
Data Preparation

x_1	x_2	y
3.91870851	2.32626914	0.73817558
2.59194437	6.00656071	4.3940048
6.46991632	3.57514815	0.61488728
:	:	:
4.56486433	2.14296641	3.95964088
1.29483514	1.67730041	3.48018992

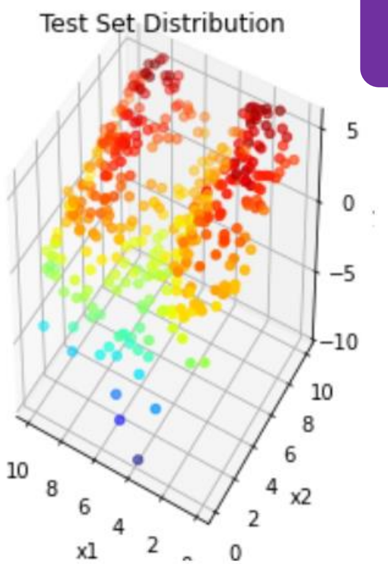




Train set



Validation set



Testing set

In the code

```
train_X, train_y = X[:1600, :], y[:1600]
val_X, val_y = X[1600:2000, :], y[1600:2000]
test_X, test_y = X[2000:, :], y[2000:]
```

Model define

Model define

In the code

```
import torch
import torch.nn as nn

class MLPModel(nn.Module):
    def __init__(self):
        super(MLPModel, self).__init__()
        self.linear1 = nn.Linear(in_features=2, out_features=200)
        self.linear2 = nn.Linear(in_features=200, out_features=1)
        self.relu = nn.ReLU()

    def forward(self, x):
        x = self.linear1(x)
        x = self.relu(x)
        x = self.linear2(x)
        return x
```

Cost (loss) function + Optimizer

Cost function + optimizer

Loss function

In the code

```
cls_loss = nn.CrossEntropyLoss()
```

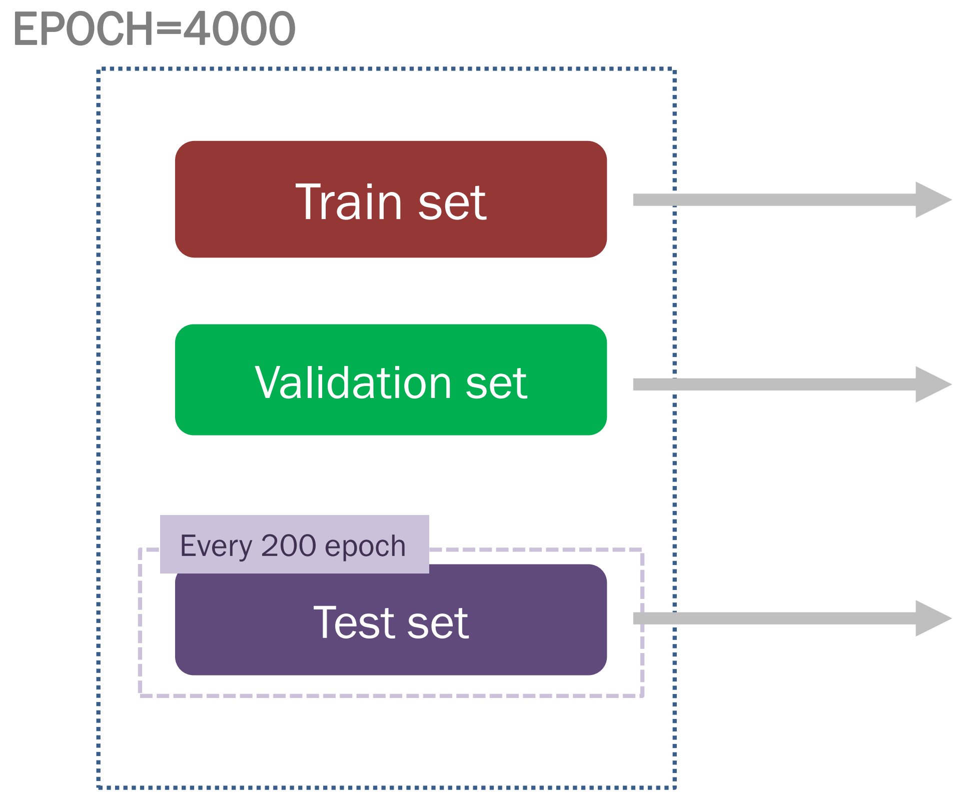
Optimizer

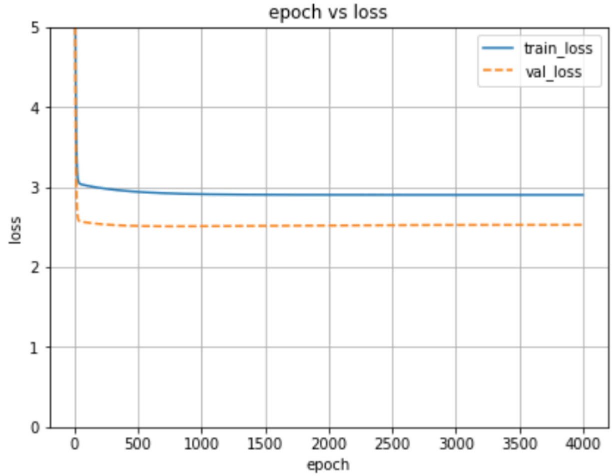
In the code

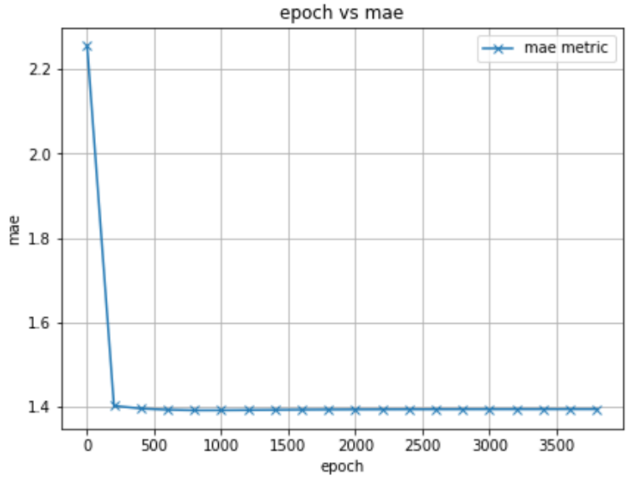
```
lr = 0.005
optimizer = optim.SGD(model.parameters(), lr =lr)
```

Model test

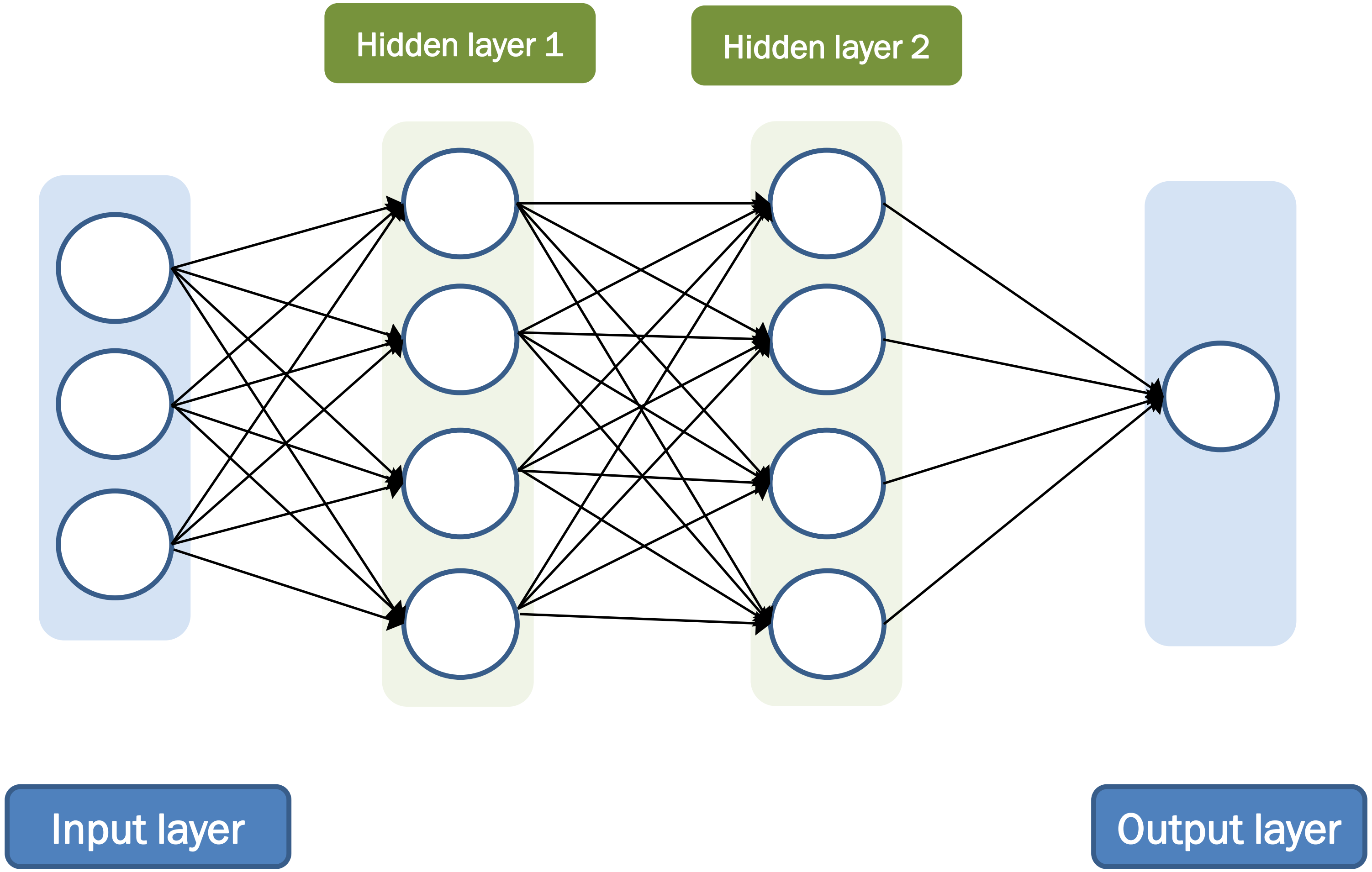
Model Test







Multi-Layer Perceptron



Lab 3B: Linear regression – MLP

1. Check the model define (MLP)
2. Check the result by varying learning rate
3. Check the result with different number of Epoch
4. Check the result with more fully connected layers

   /different number of hidden units
5. Check the result with different activation functions(Sigmoid, ReLU, Leaky ReLU)
6. Check the result with different loss function

Break room

Lab 3B – Running it on Graham (Interactive mode)

1. Download *Lab3B_Linear_Reg_MLP.ipynb* as .py file from Colab
2. File transfer *Lab3B_Linear_Reg_MLP.py* to Graham using WinScp or MobaXterm (Windows) / sftp (Linux, Mac)
3. Start interactive running mode

   `salloc --time=0:30:0 --ntasks=1 --cpus-per-task=3 --gres=gpu:t4:1 --node=1 --mem=1000M --account=def-training-wa`
4. Activate virtual environment (make sure you load python and scipy-stack module)
5. Run it by 'python *Lab3B_Linear_Reg_MLP.py*'
6. Note you need to collect all import commands into the beginning of code using text editor (Nano/emacs/VI)
6. Note that you need to save/close your plots with proper filename for each plotting command like below
7. File transfer plotting files to your local computer using WinScp or MobaXterm (Windows) / sftp (Linux, Mac) and check it out

Lab 3B – Running it on Graham (batch mode)

1. Download *Lab3B_Linear_Reg_MLP.ipynb* as .py file from Google Colab
2. File transfer *Lab3B_Linear_Reg_MLP.py* to Graham using WinScp or MobaXterm (Windows) / sftp (Linux, Mac)
3. Write a submission script *'job_s.sh'* like below text editor

```
[isaac@gra-login3 ~]$ cat job_s.sh
#!/bin/bash
#
#SBATCH --nodes=1
#SBATCH --gres=gpu:t4:1
#SBATCH --cpus-per-task=3
#SBATCH --nodes=1
#SBATCH --mem=20000M
#SBATCH --time=0-30:00
#SBATCH --account=def-training-wa
#SBATCH --output=slurm.%x.%j.out

module load python scipy-stack
source ~/ENV/bin/activate
python Lab3A_Linear_Reg_MLP.py
```

4. Submit it by typing *'sbatch job_s.sh'*
5. Check it by typing *'squeue -u $USER'*

Session break:

Please come back by 3:45 PM