PRACTICAL MACHINE LEARNING: AN INTRODUCTION

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Universidad Católica del Norte, Chile
October 7th, 2024

Queen Mary
University of London

This Course: 4 Workshops (Lectures & Exercises)

First and foremost an interactive course! Please bring a laptop or share one with a friend!

- **Lecture 1 (Monday):** Introduction to machine learning with neural networks and linear regression.
- **Lecture 2 (Tuesday):** Optimisation and non-linear regression with neutral networks.
- **Lecture 3 (Thursday):** Classification and using convolutional neural networks for image classification.
- **Lecture 4 (Friday):** Robustness and adversarial examples in image classification problems.

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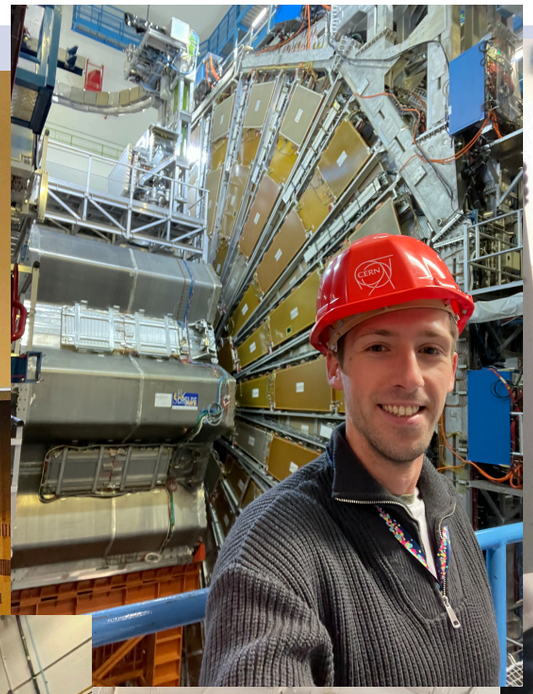
Software:

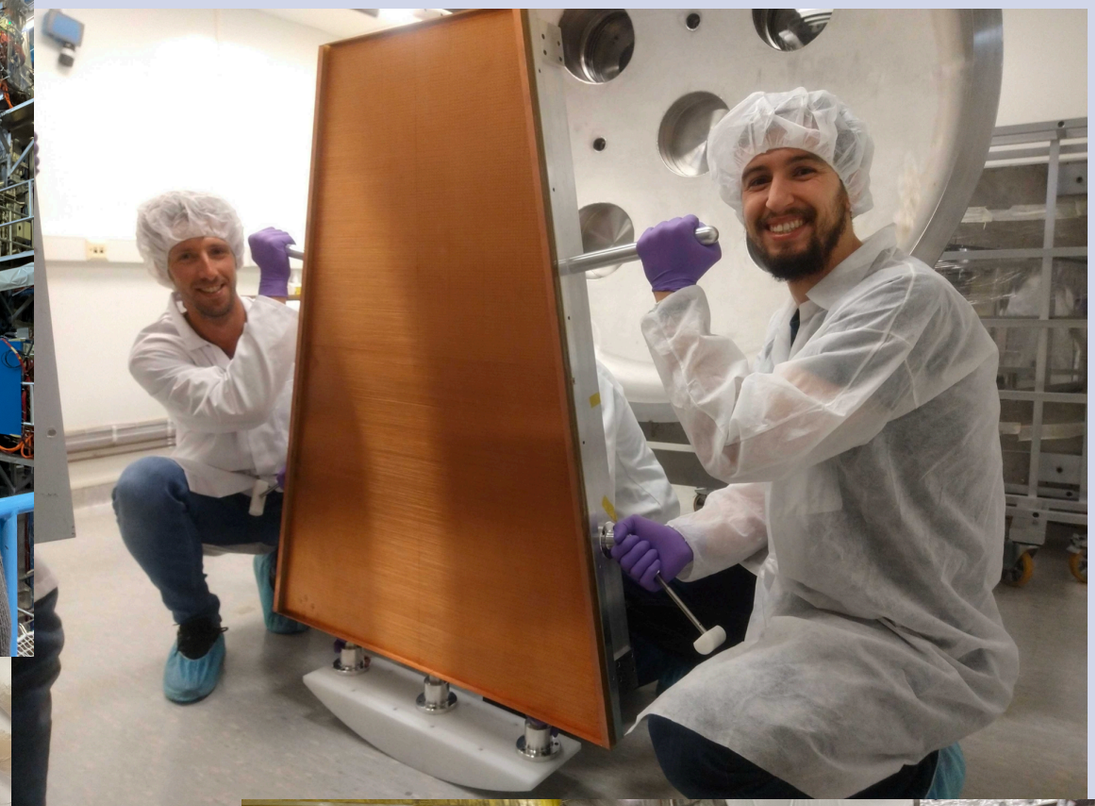
- **Python** and **TensorFlow 2.11** will be used throughout the course.
- Can access this software via **Binder** from the course Github.

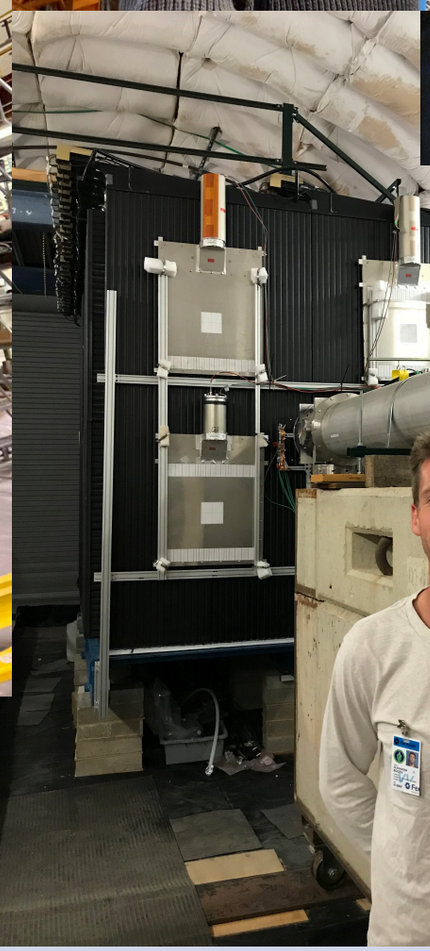
https://github.com/alexbooth92/workshop-UCDN_PracticalML.git

- Will interact with the software using **Jupyter Notebooks,** also in the Github.

I am a neutrino physicist!

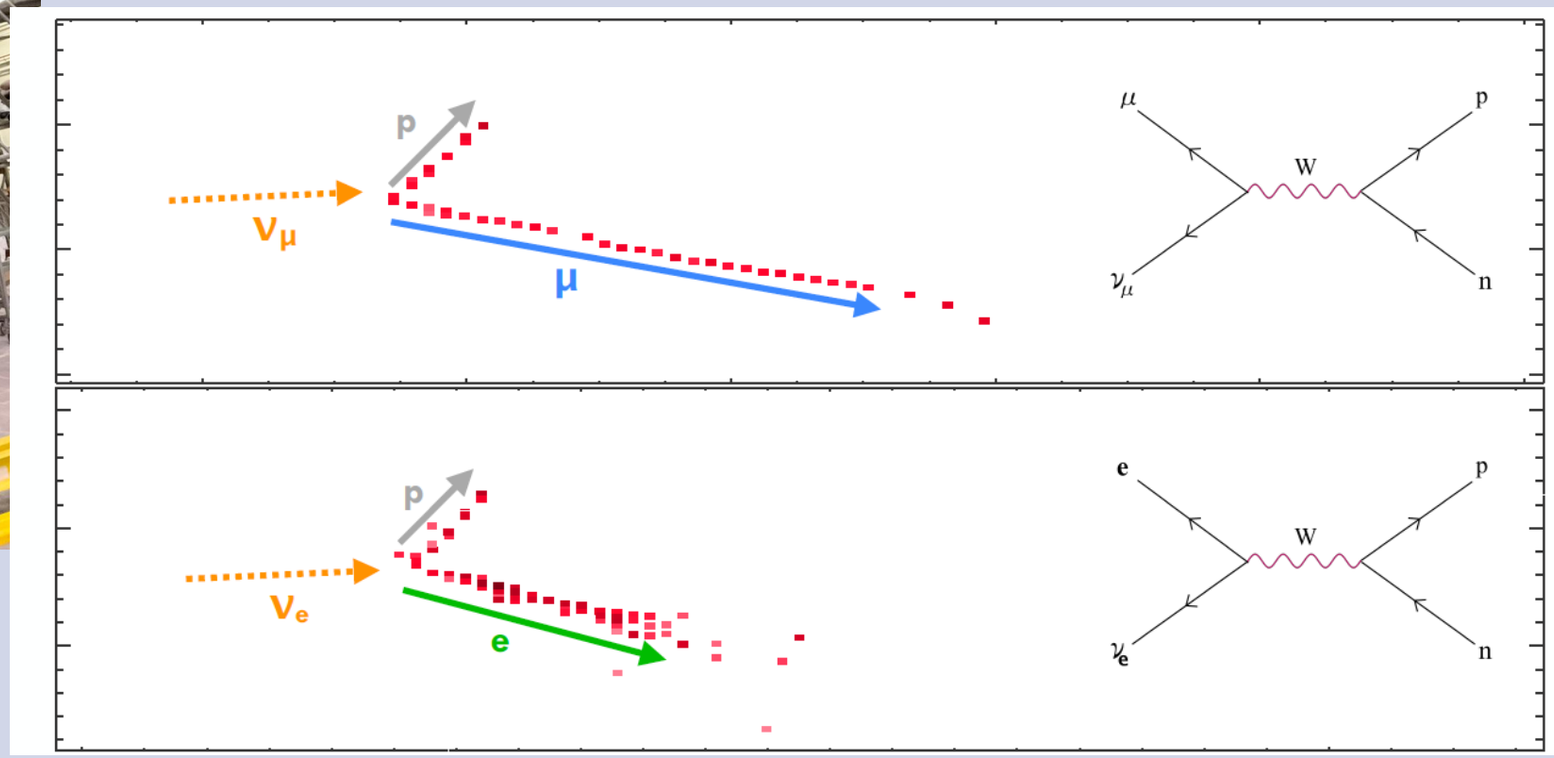






I am a neutrino physicist!

- Co-lead the Reconstruction & Machine Learning group in the NOvA experiment.
- Apply machine learning to the classification and energy estimation of neutrino interactions.



A Bit More About Me…

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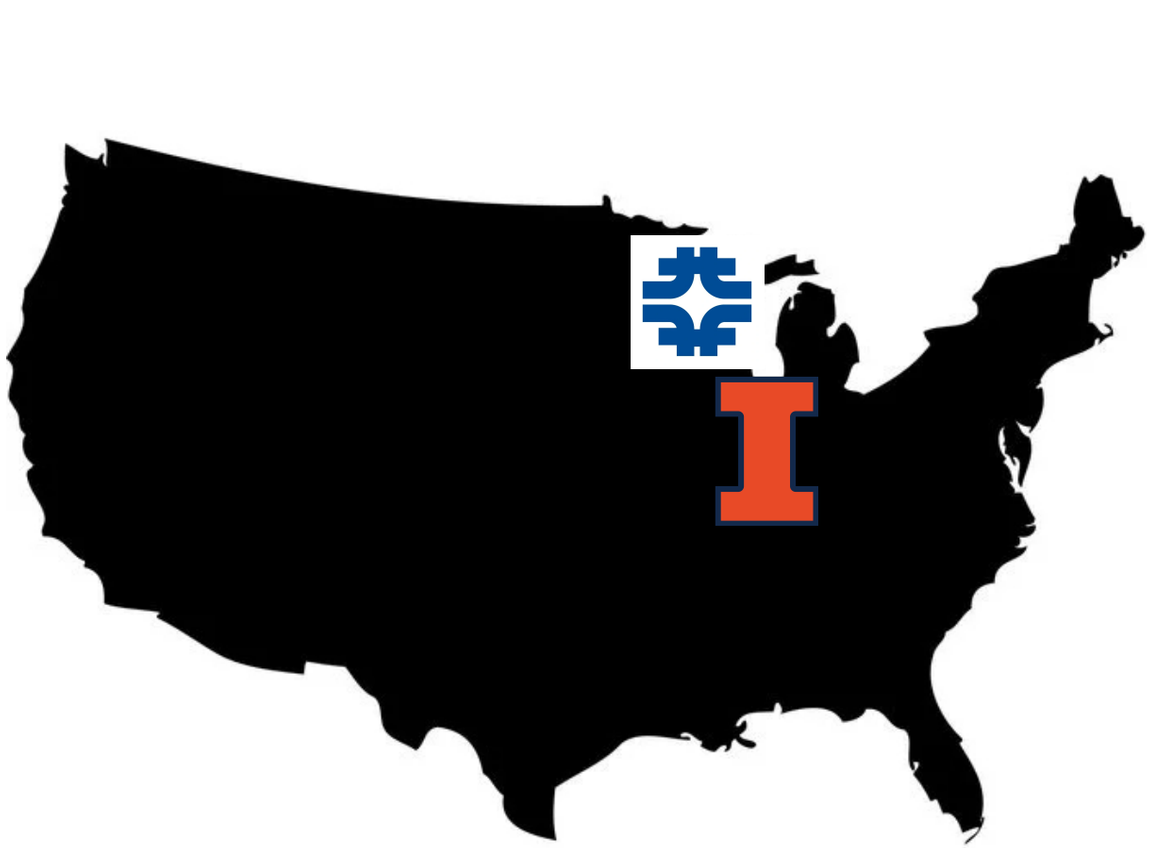

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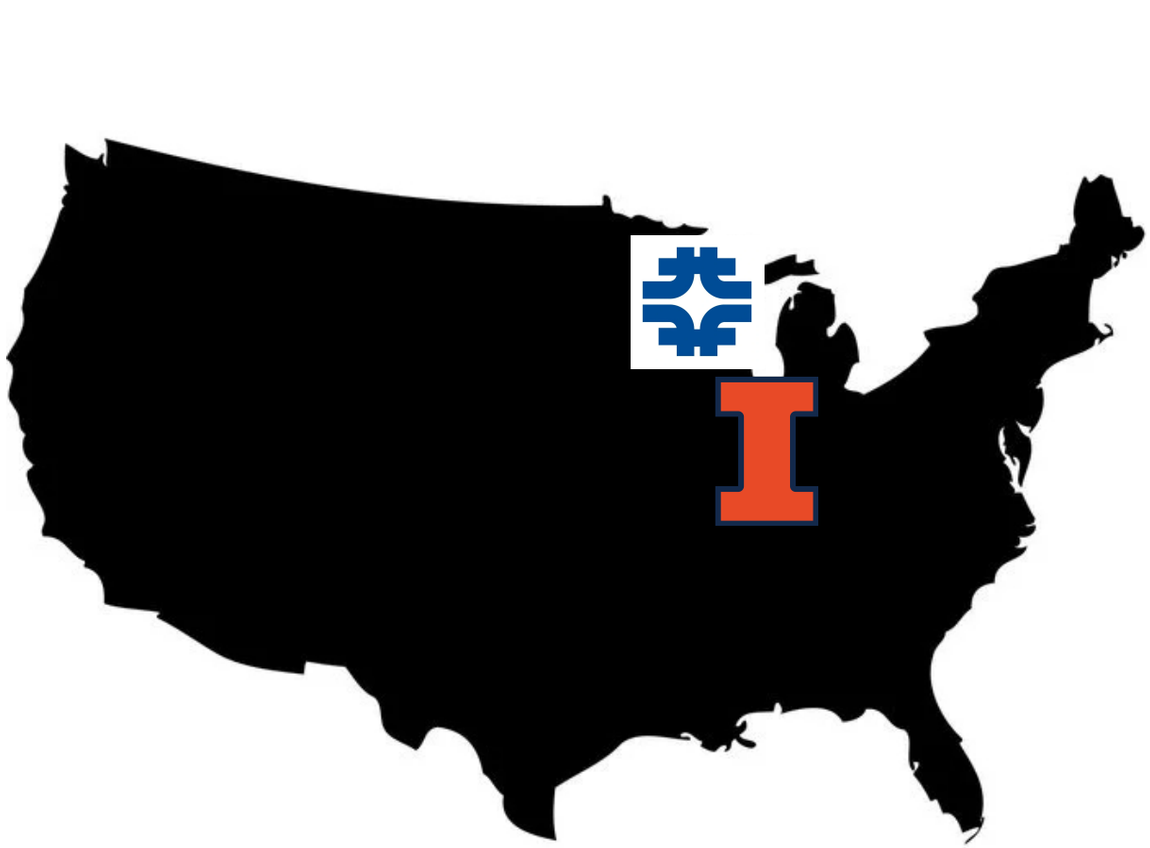

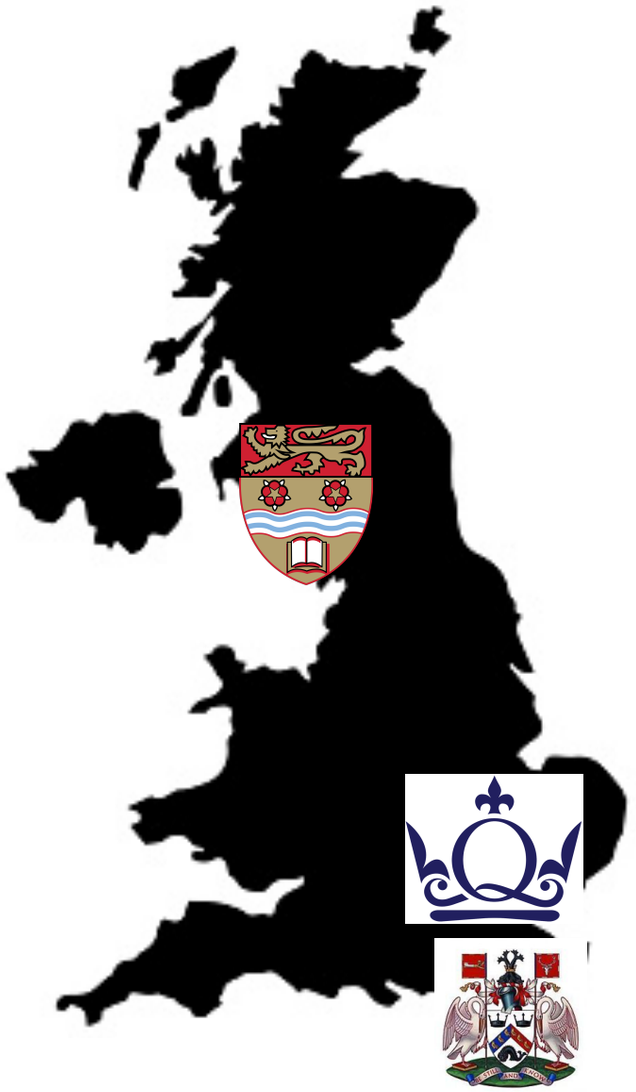

Let's find out about you!

PollEv.com/alexanderbooth769

What is Machine Learning?

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"The science (and art) of programming computers so that they can learn from data".

A. Géron

Queen Mary
University of London

Can you think of examples?

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Image recognition

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Speech recognition

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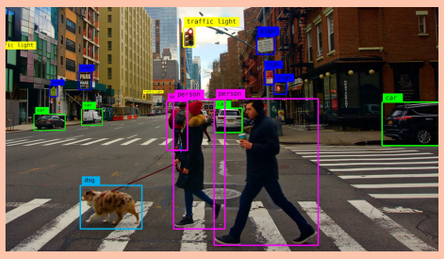
Object detection



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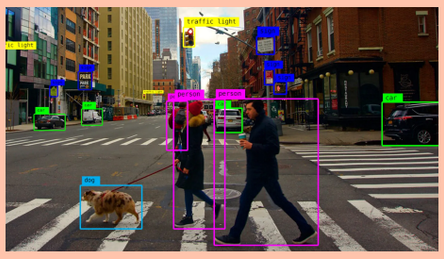

Art generation

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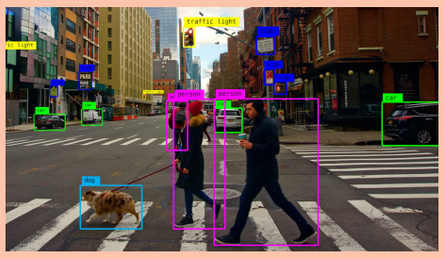

Art generation

Particle ID in fundamental particle physics

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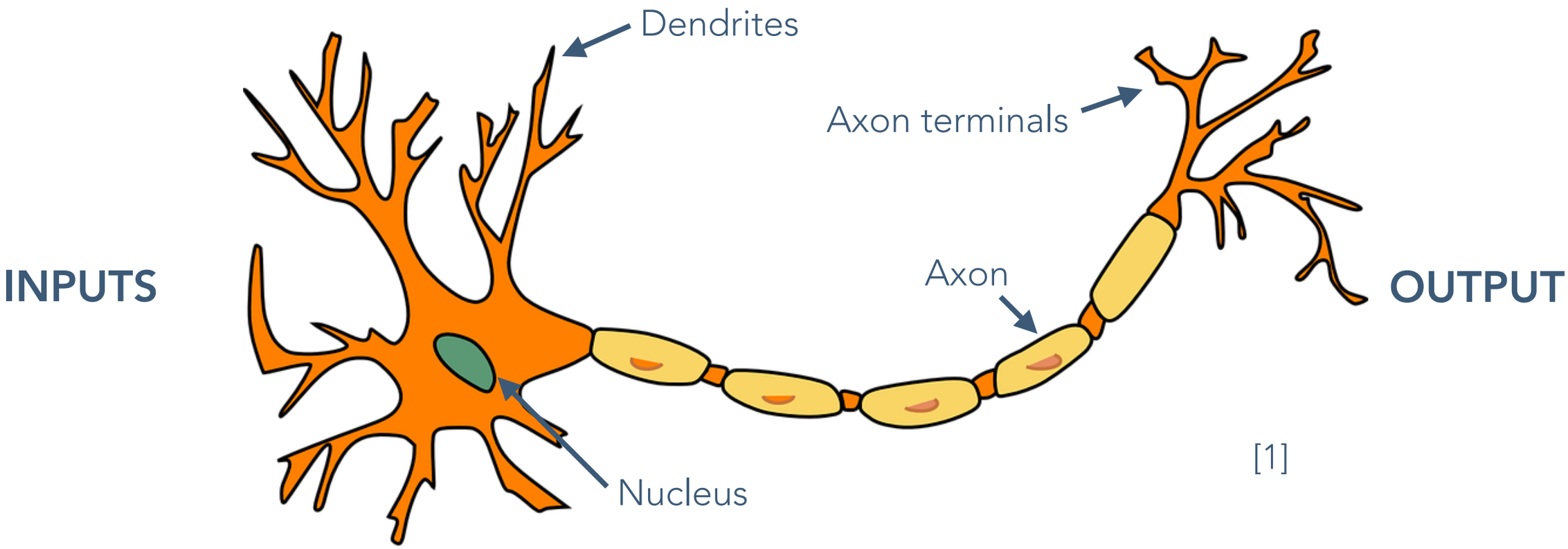
Neurons

Neurons

Biological Neuron



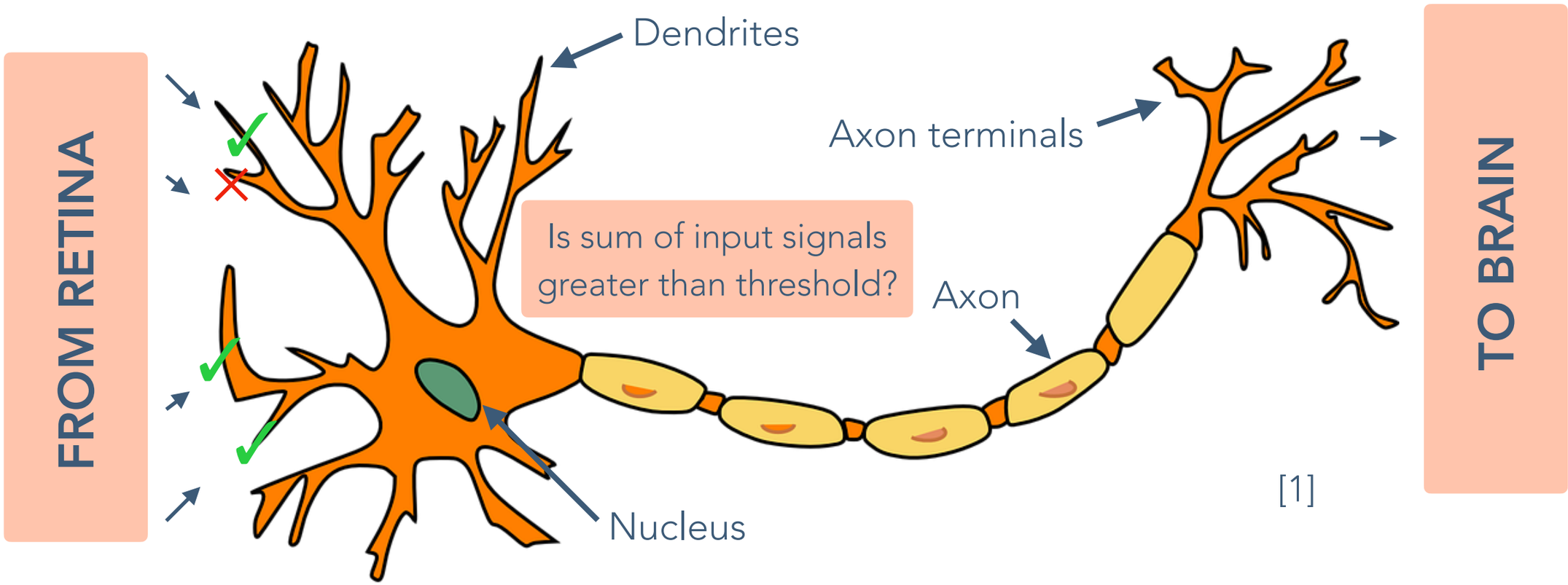
[1]

- Artificial neurons used in machine learning originate in trying to understand the operation of biological neurons.

- Responsible for processing and transmission of cellular signals.
  - Input signals arrive through dendrites - can scale signal importance.
  - Nucleus makes “decision” on if / how signals will be passed on.
  - Output signals transmitted via axon to axon terminals to be passed on.

Neurons

Biological Neuron



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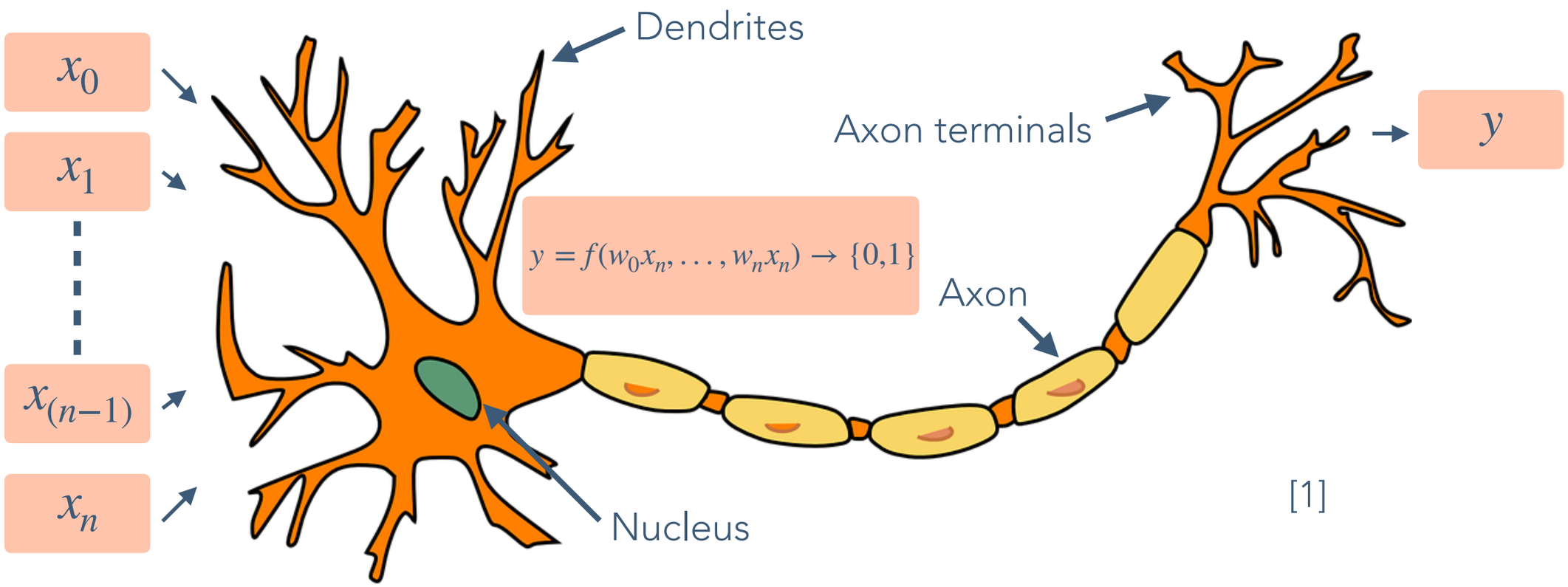
- Artificial neurons used in machine learning originate in trying to understand the operation of biological neurons.

- First artificial neuron, **"perceptron"** focussed on trying to understand how information from the retina is processed.
  - Gather input signals from several cells.
  - If total signal intensity is high enough "fire" response (all or nothing).

Neurons

Biological Neuron



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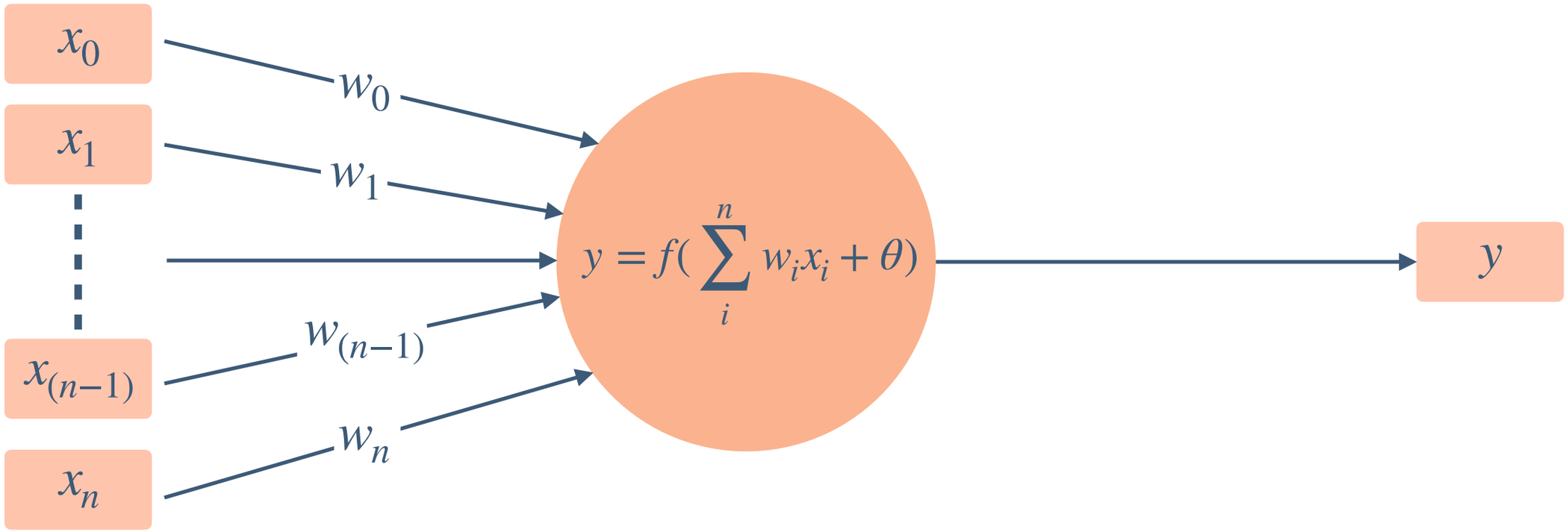
Neurons

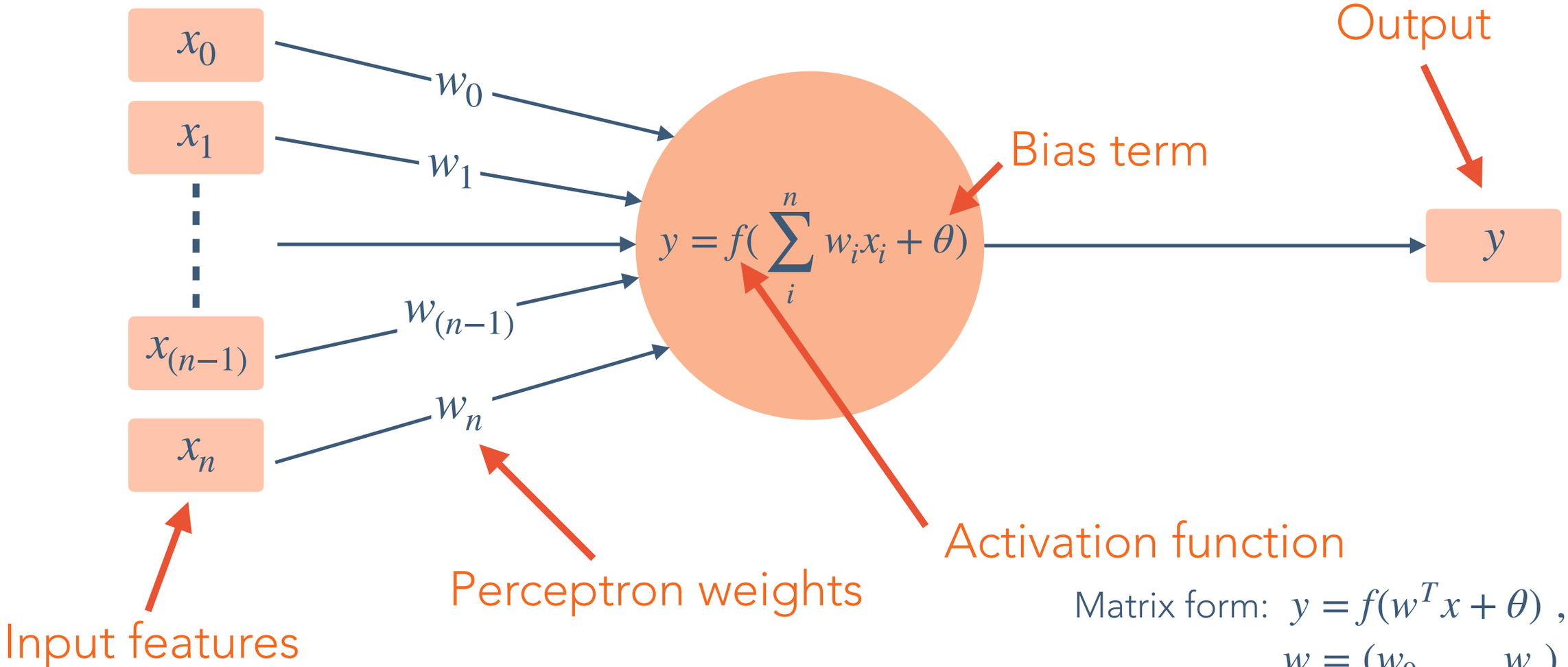
Artificial Neuron -> Perceptron (Node)



- Idea of perceptron can be extended to describe a more generalised picture.
  - Take some number, n, of **input features**.
  - Compute the sum of each of the features multiplied by some factor assigned to it (indicating the importance of that information).
  - Compare the sum against some reference threshold.
  - Perceptron is “active” (y=1) if above threshold, not active if below (y=0).

Neurons

Artificial Neuron -> Perceptron (node)

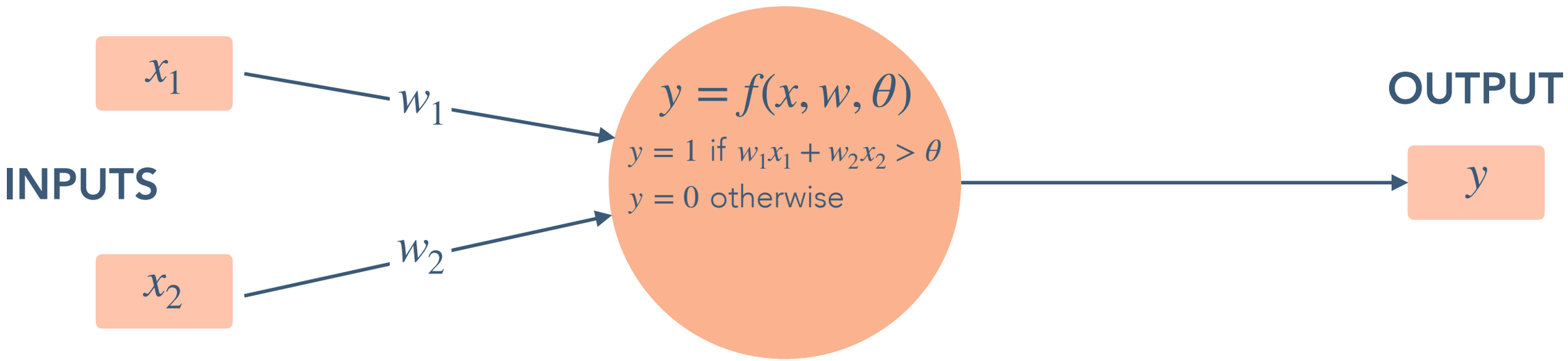


Matrix form: $y = f(w^T x + \theta)$,

$w = (w_0, \ldots, w_n)$,

$x = (x_0, \ldots, x_n)$

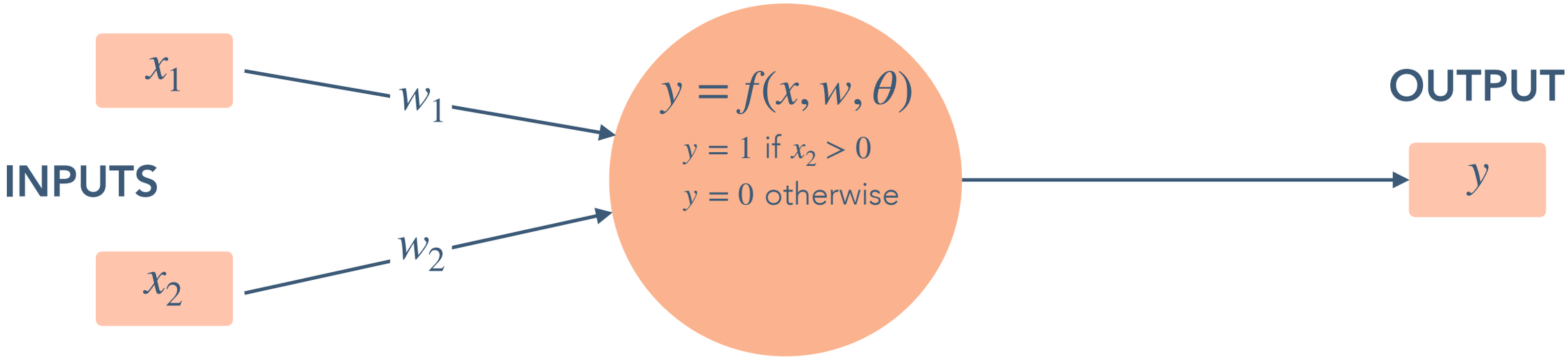
Perceptrons: Illustrative Example



- Consider a measurement of two quantities x_1 and x_2 and a perceptron with **binary activation function**.

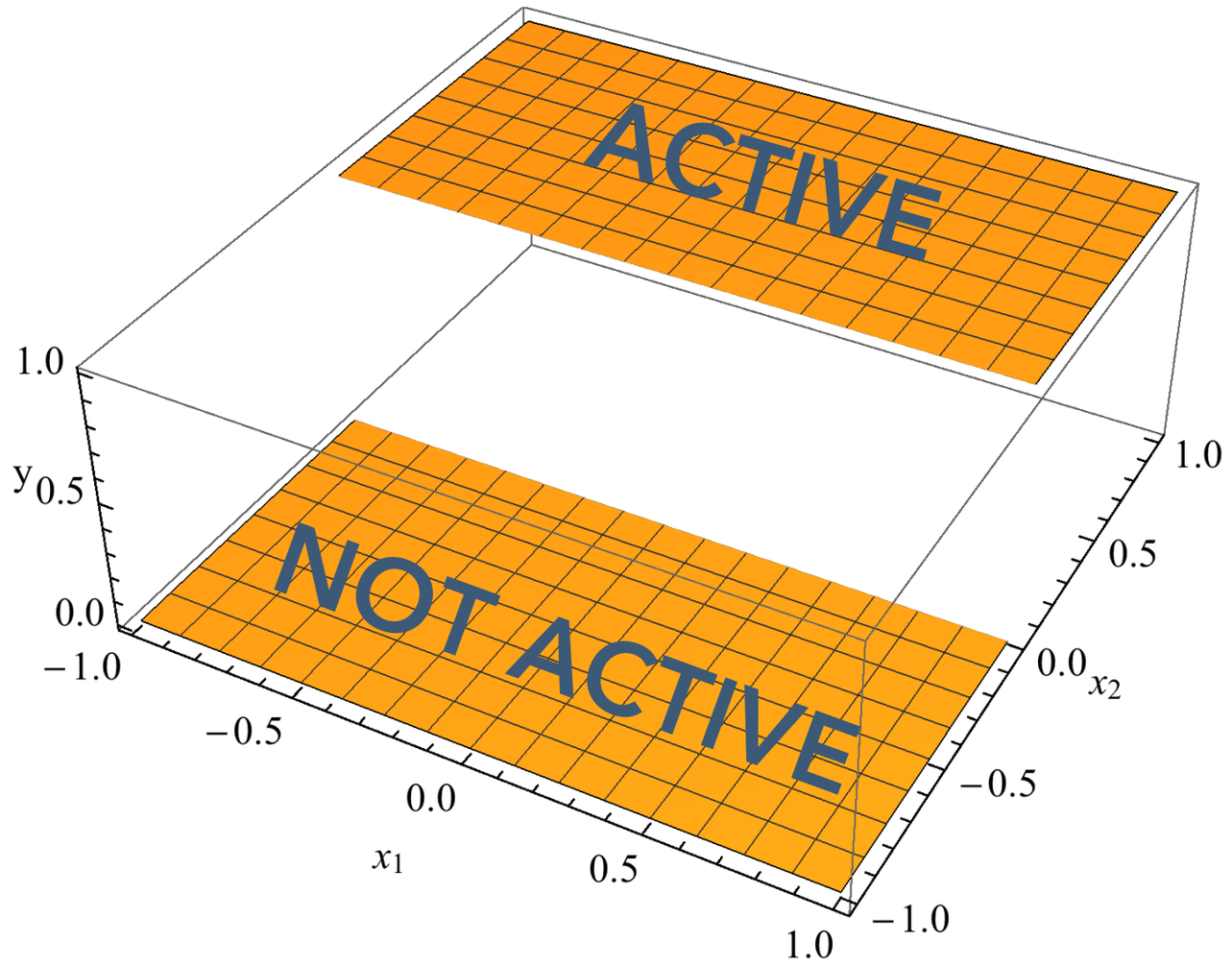
- Based on these measurements lets determine if the perceptron is active / to give an output (y = 1) or not (y = 0) **for a given choice of weights**.

Perceptrons: Illustrative Example



Weight choice 1: $w_1 = 0, w_2 = 1, \theta = 0$

Decision based on x_2 only.



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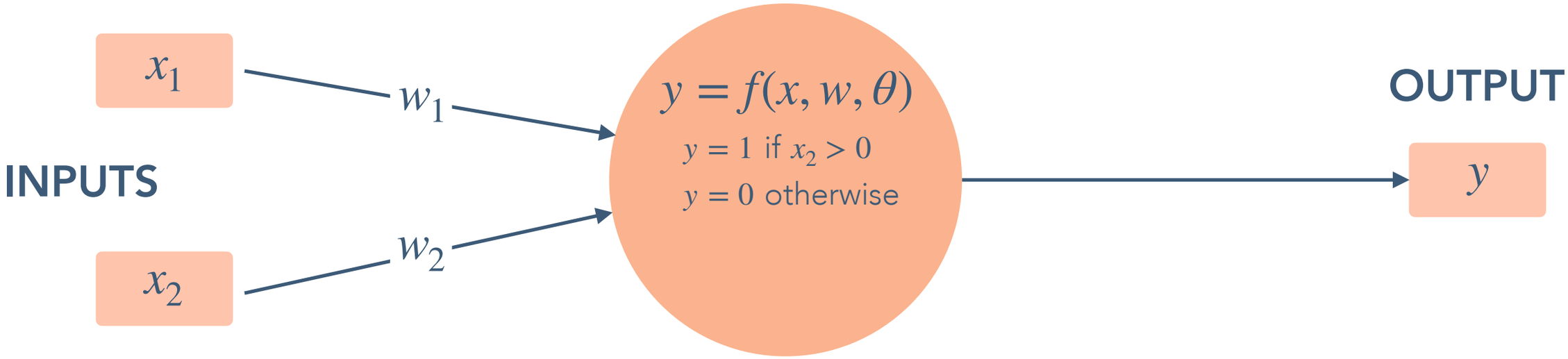
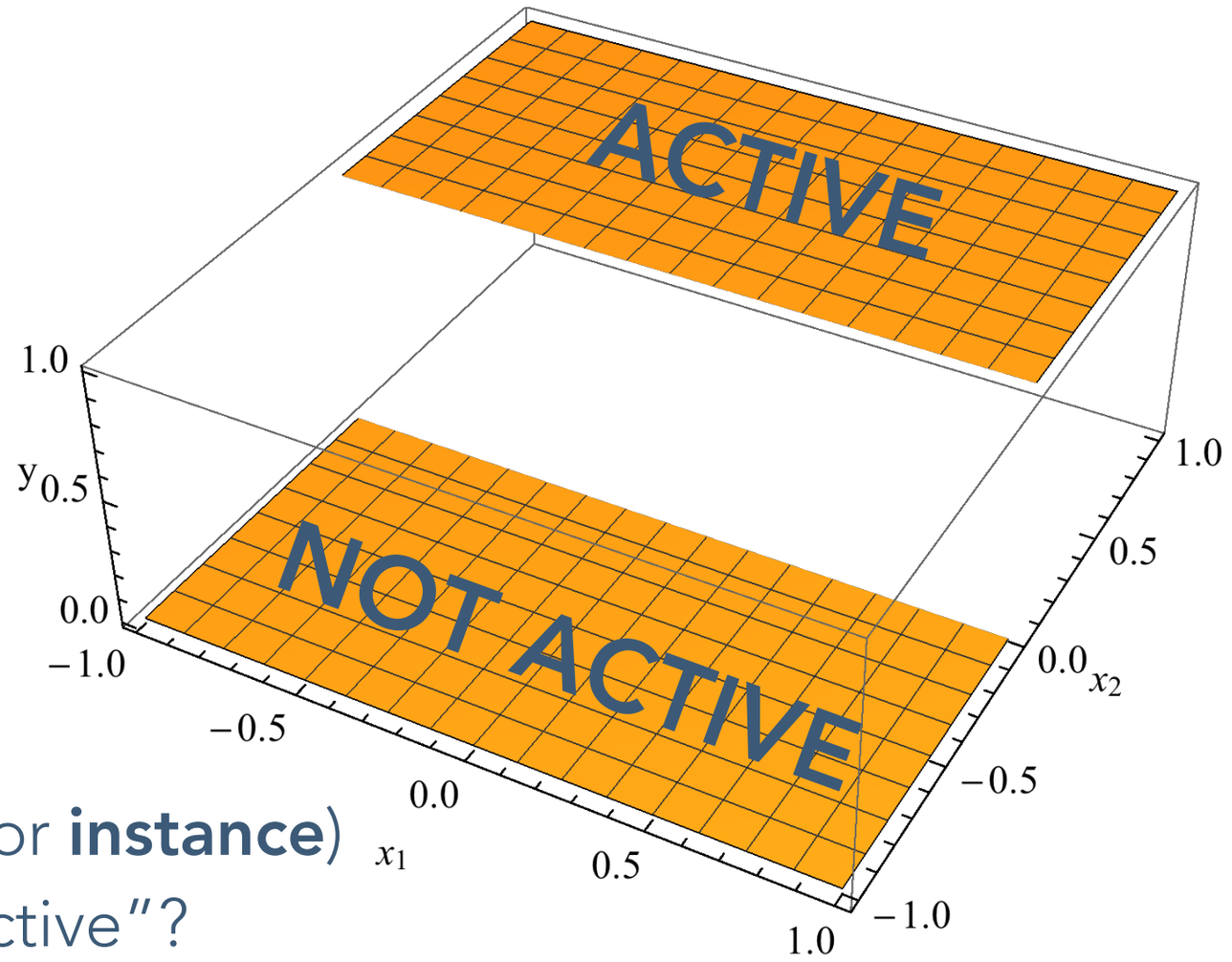


Weight choice 1: $w_1 = 0,\ w_2 = 1,\ \theta = 0$

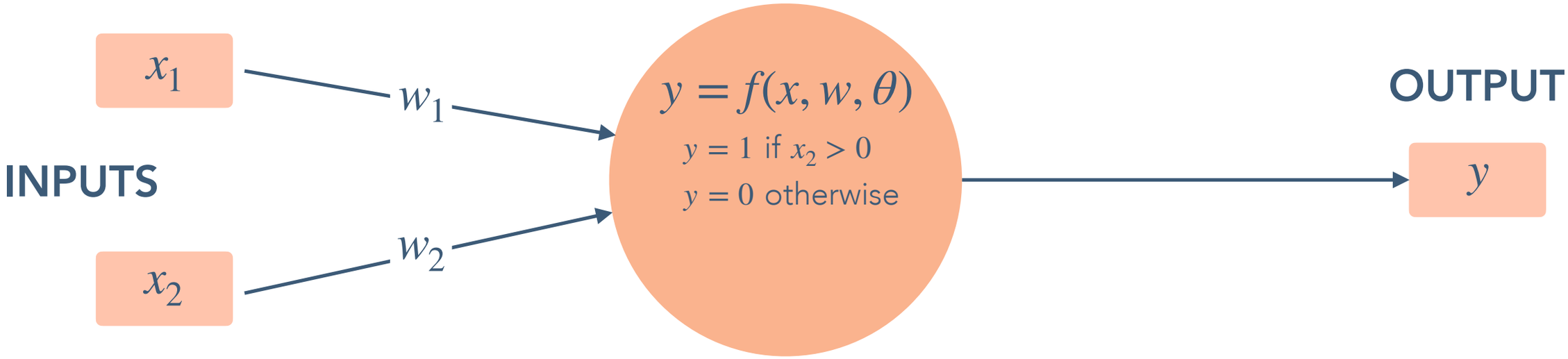
Input set 1: $x_1 = 0.2,\ x_2 = -0.5$

Input set 2: $x_1 = -0.6,\ x_2 = 0.8$



For which input set (or **instance**) is the perceptron "active"?

Perceptrons: Illustrative Example



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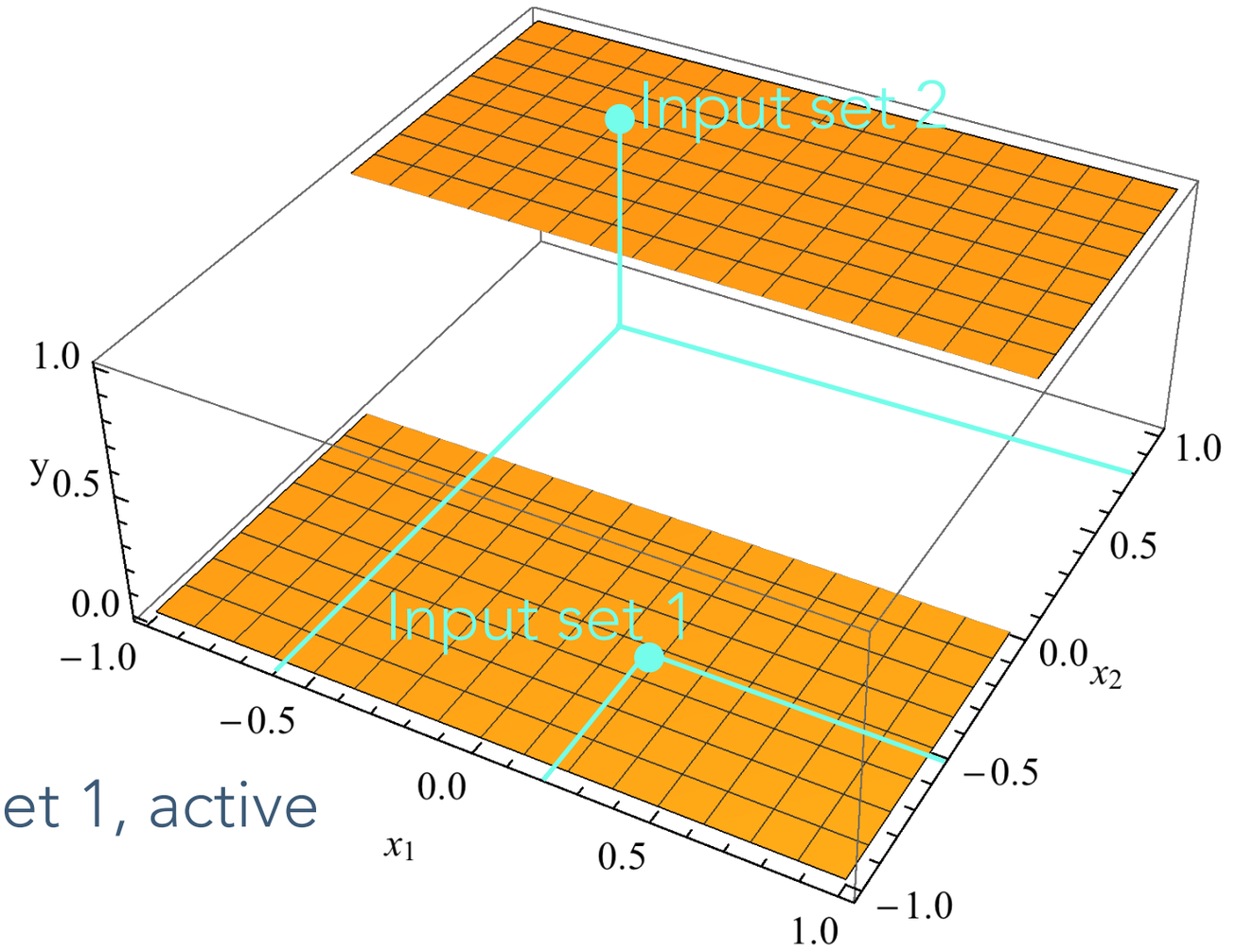
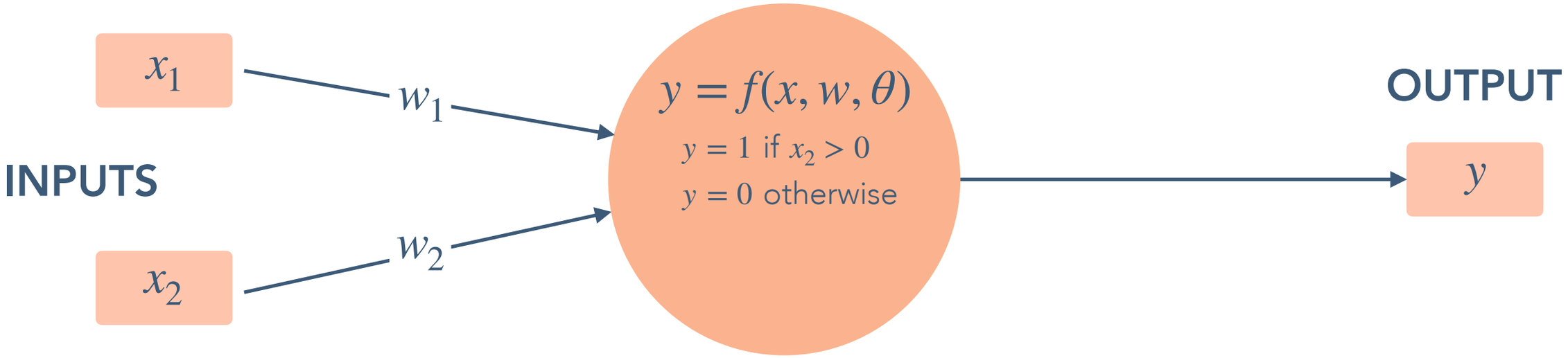


Not active for set 1, active for set 2

Perceptrons: Illustrative Example

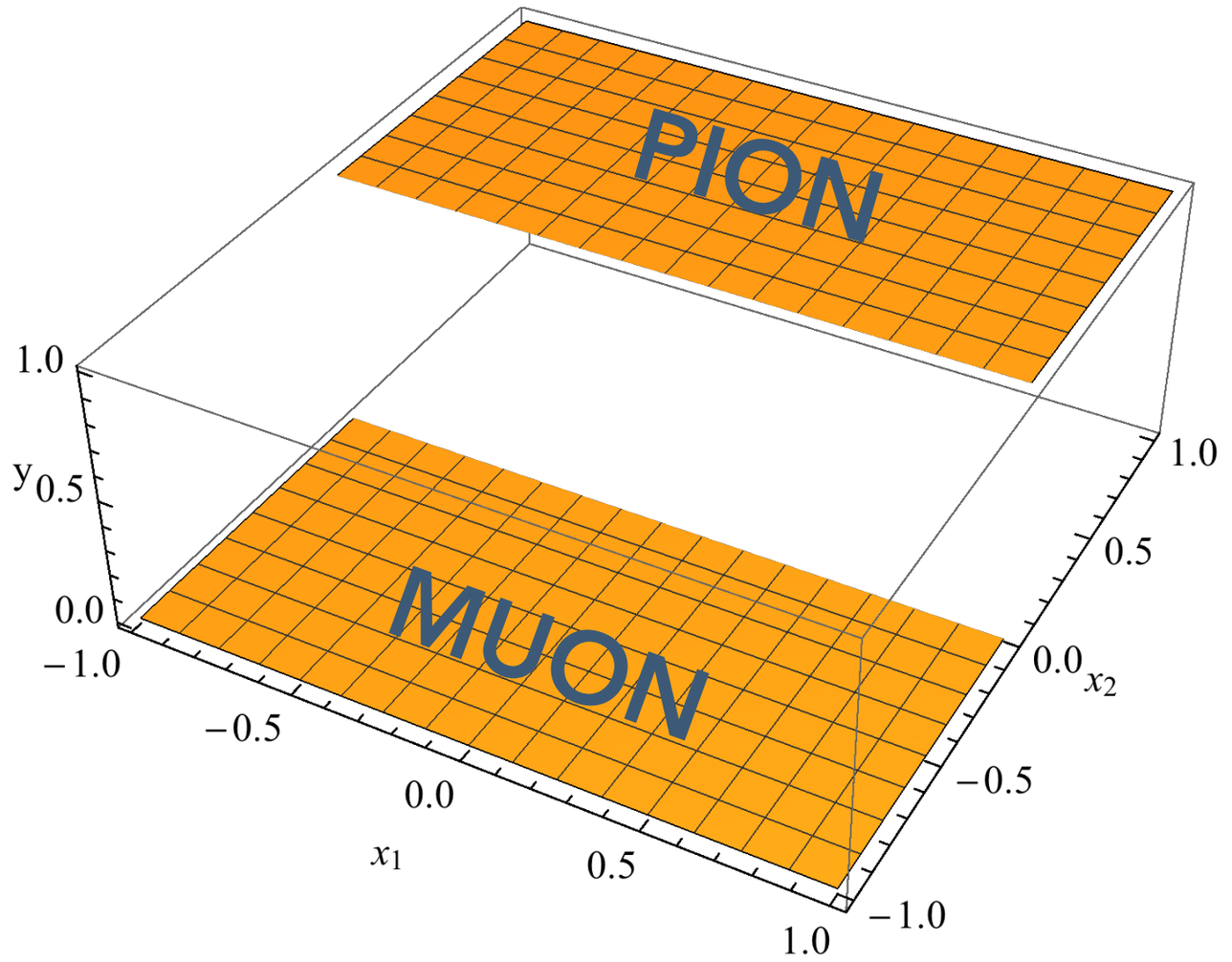


Weight choice 1: $w_1 = 0, w_2 = 1, \theta = 0$

In particle physics we often use machine learning to identify different types of particle, e.g **pion** vs. **muon** -> **classification**.

Particle candidate 1: $x_1 = 0.2, x_2 = -0.5$

Particle candidate 2: $x_1 = -0.6, x_2 = 0.8$



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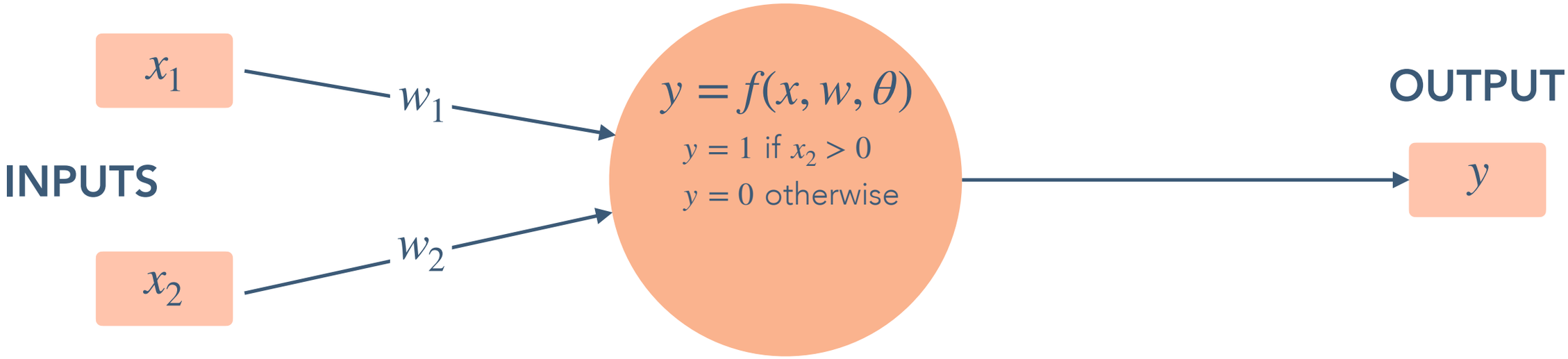

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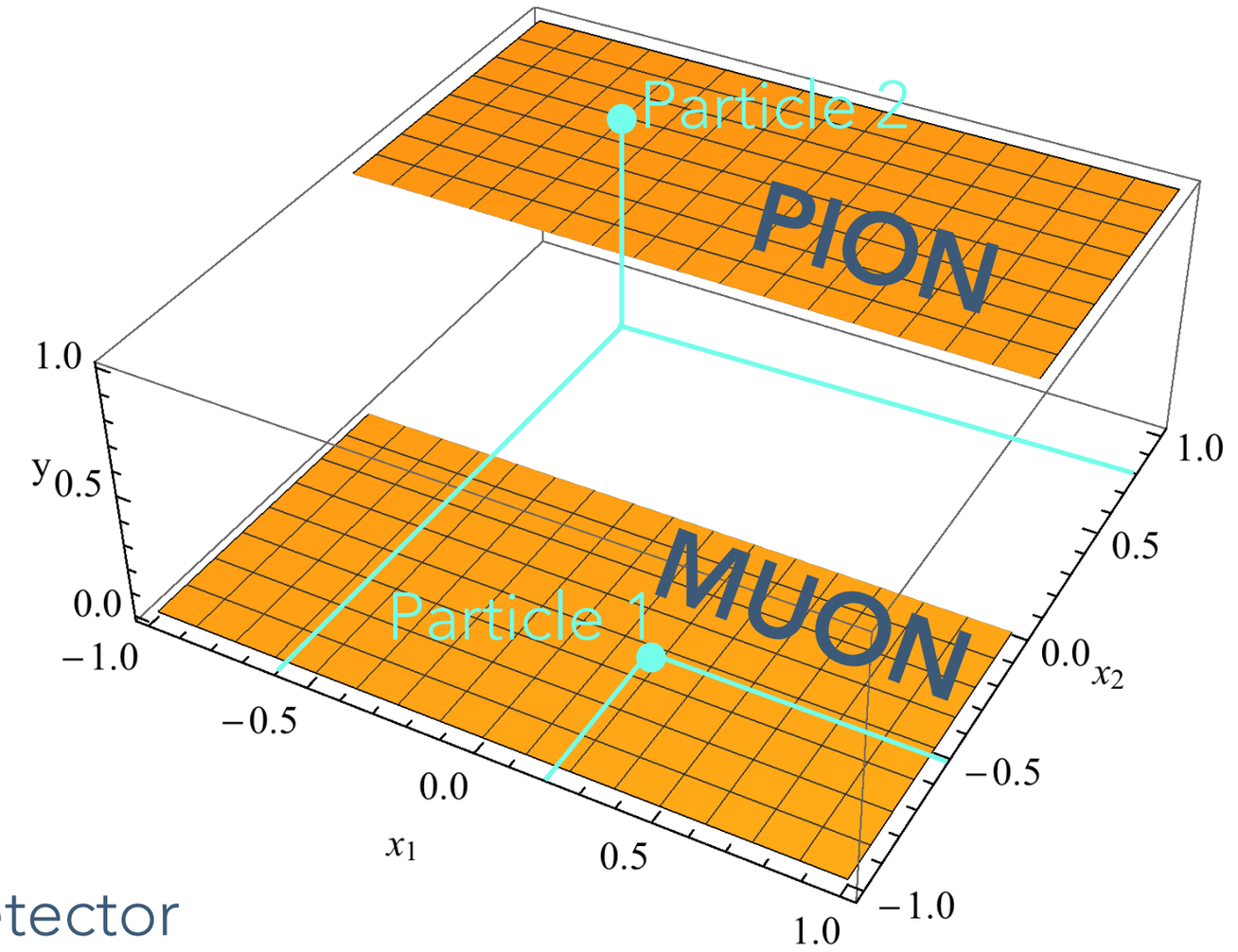
Particle candidate 2: $x_1 = -0.6, x_2 = 0.8$

x_1 ~ momentum x_2 ~ angle in detector



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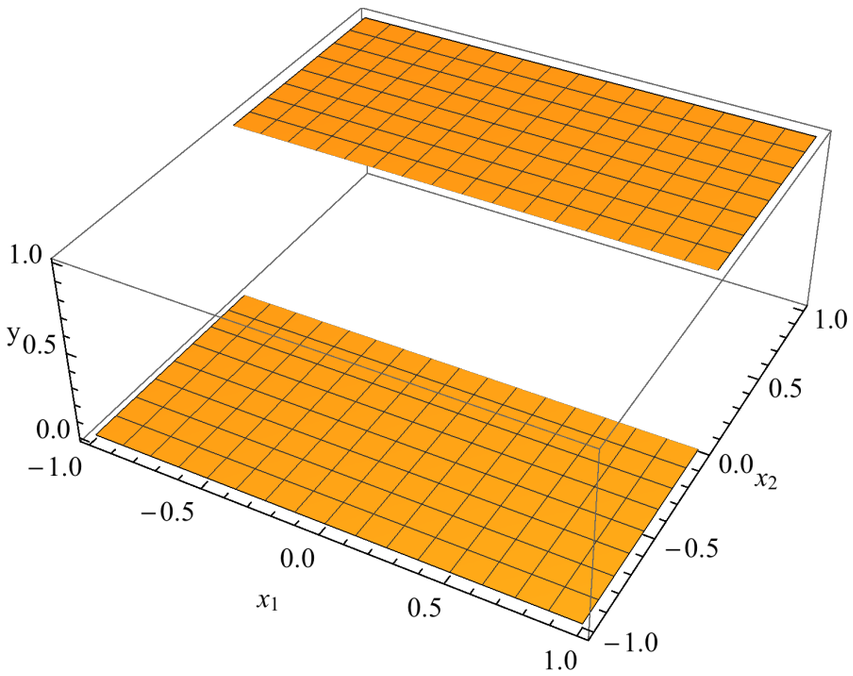

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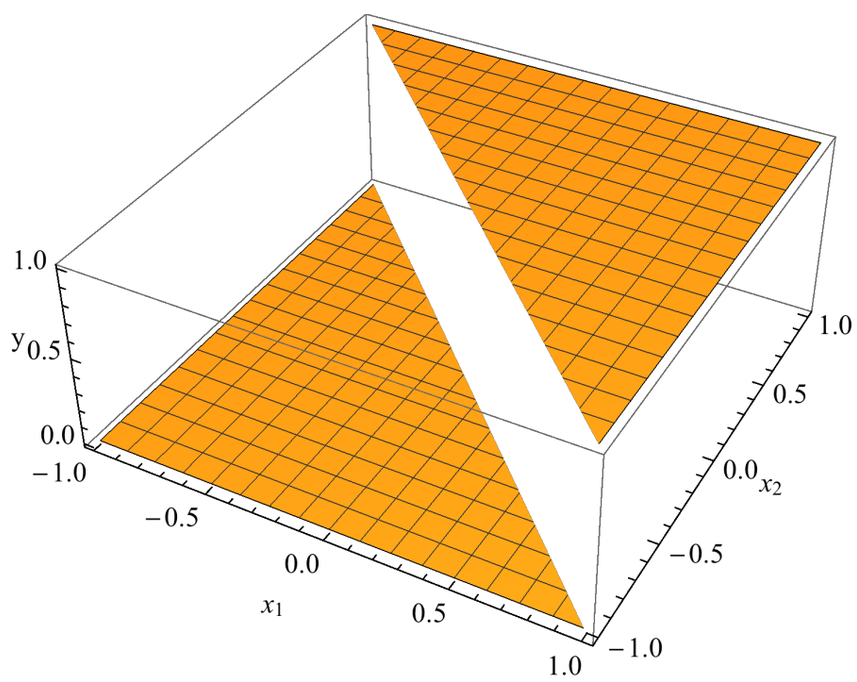
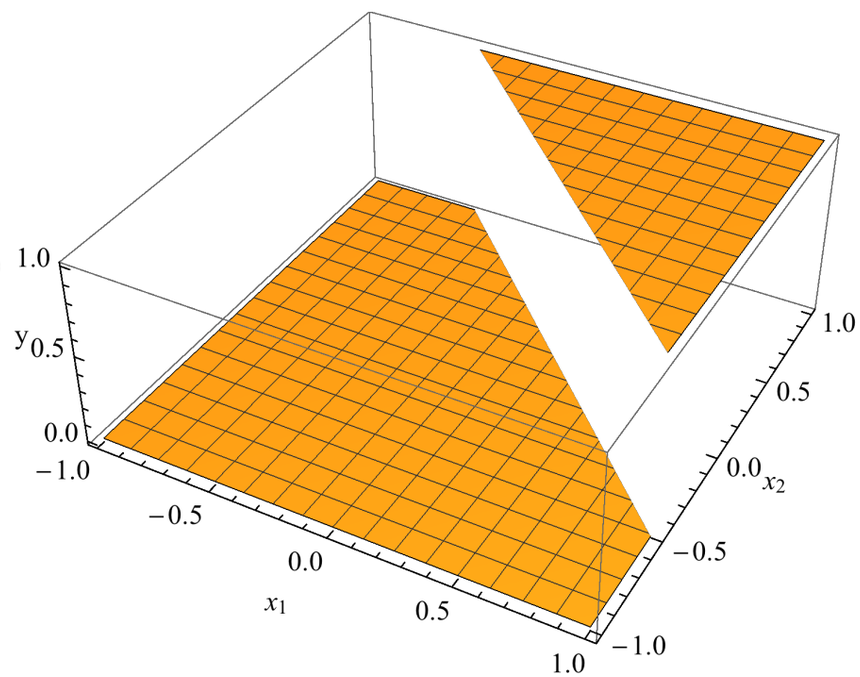
Decision based on x_2 only.



Weight choice 2:

$w_1 = 1,\ w_2 = 1,\ \theta = 0$

Rotate decision plane .



Weight choice 2:

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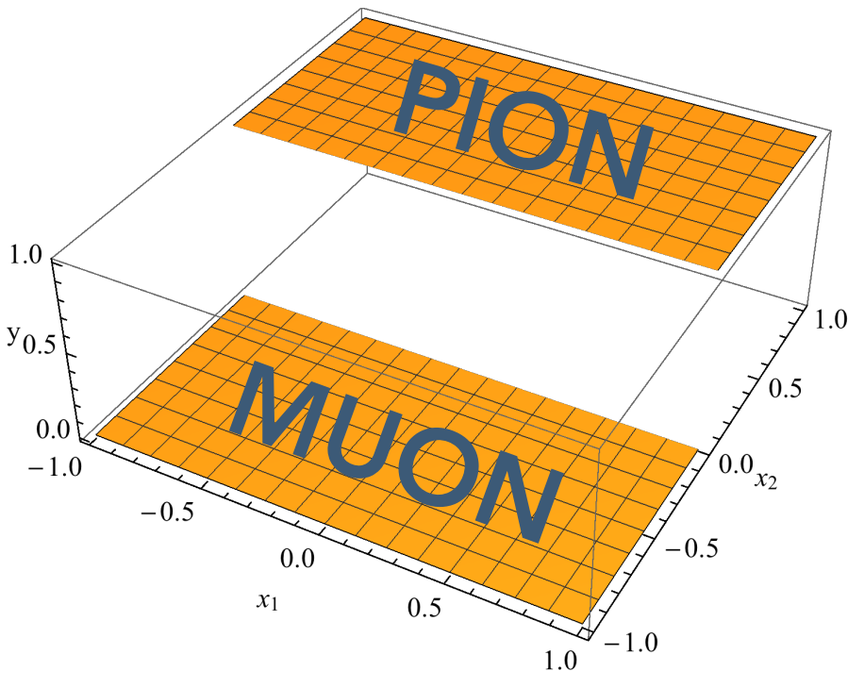
Shift decision plane away from origin.

Choice of weights & bias changes the response of the perceptron.

Perceptrons: Illustrative Example



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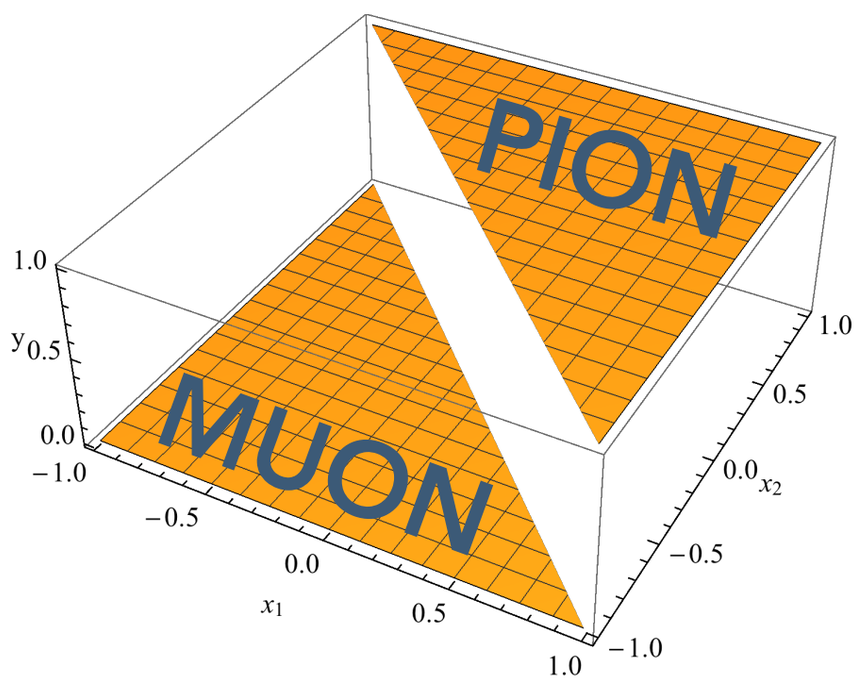

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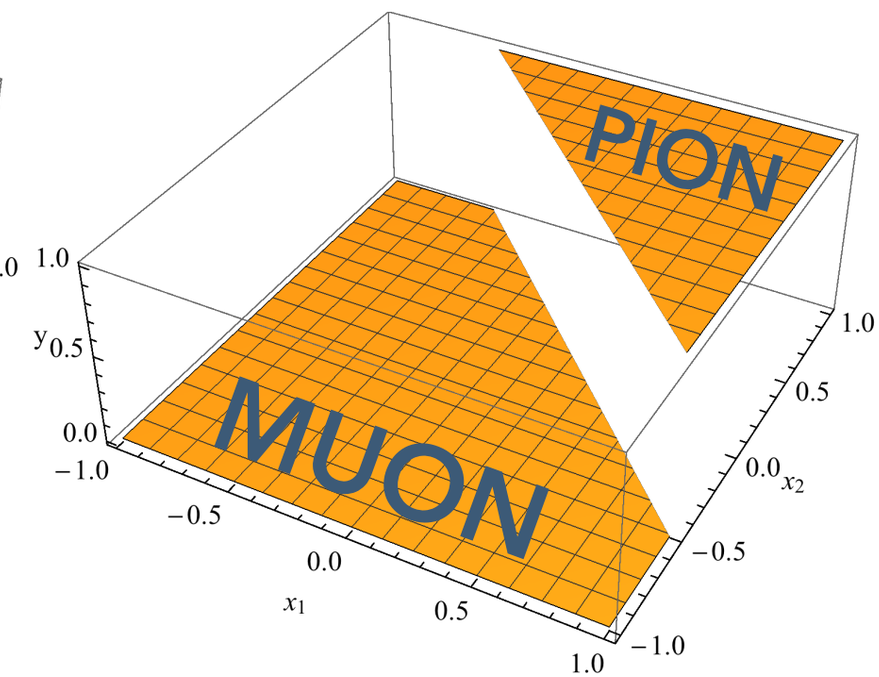


Weight choice 2:

$w_1 = 1, w_2 = 1, \theta = 0.5$

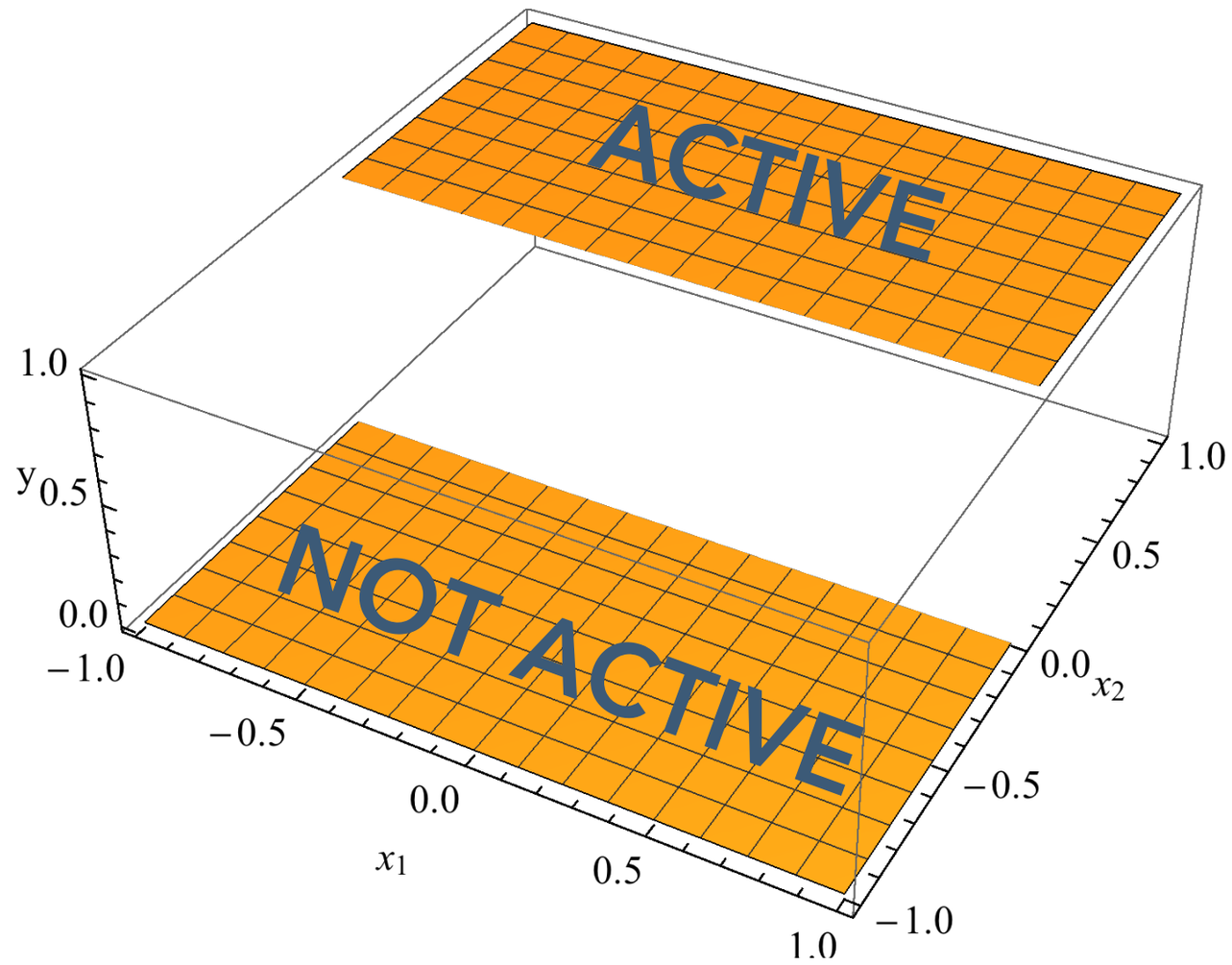
Shift decision plane away from origin.

Optimisation of weights and bias (e.g to give you the best particle classification) is *"training"*.

More Activation Functions

- So far have used **binary activation function**.
  - Gives "all or nothing" response.

- Can be useful to provide an output that is continuous between two extremes.
  - That requires different forms of activation function.



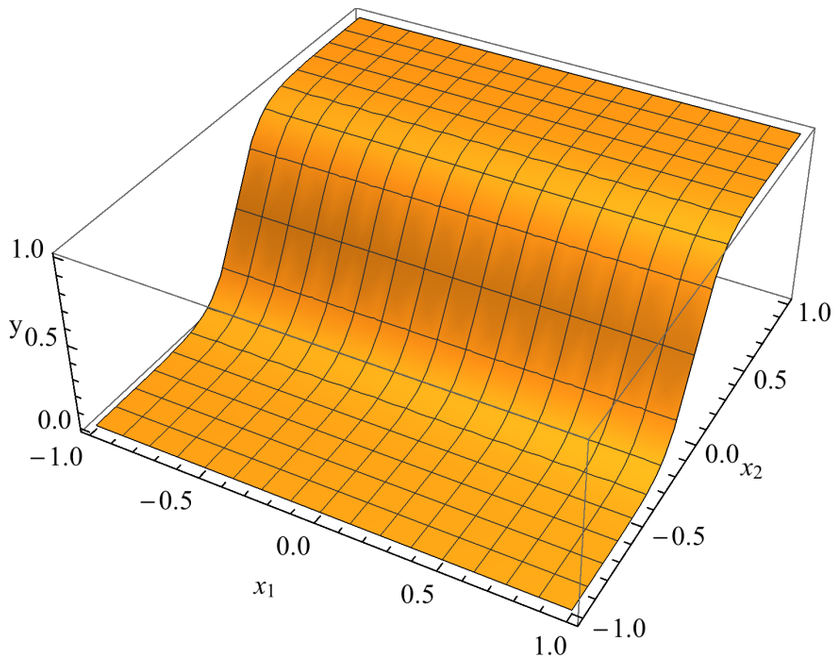
- TensorFlow has the following activation functions (`tf.nn.ACTIVATIONFUNCTION`)
  - relu (covered here)
  - leaky_relu (covered here)
  - relu6
  - crelu
  - elu
  - selu
  - softplus
  - softsign
  - dropout
  - bias_add
  - sigmoid (covered here)
  - tanh

Activation Functions: Logistic (Sigmoid)

A common activation function found in neural networks.

$$y = \frac{1}{1 + e^{w^T x + \theta}}$$

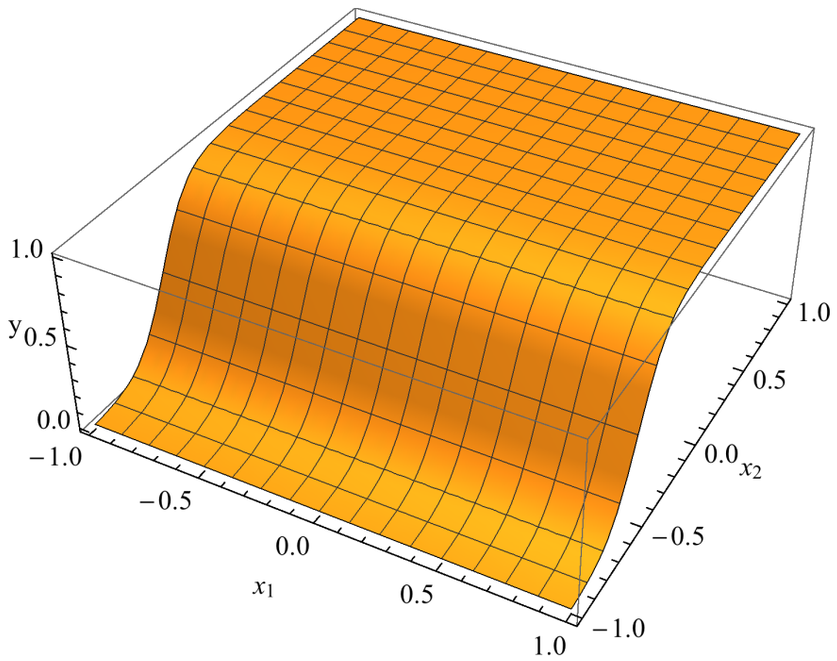
$$= \frac{1}{1 + e^{(w_1 x_1 + w_2 x_2 + \theta)}}$$



$w_1 = 0$

$w_2 = 10$

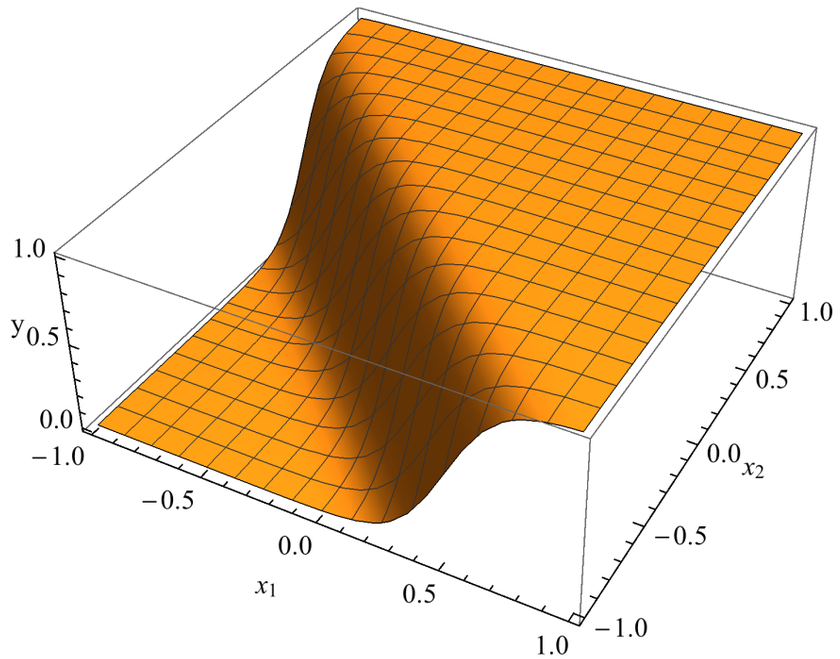
$\theta = 0$



$w_1 = 0$

$w_2 = 10$

$\theta = -5$



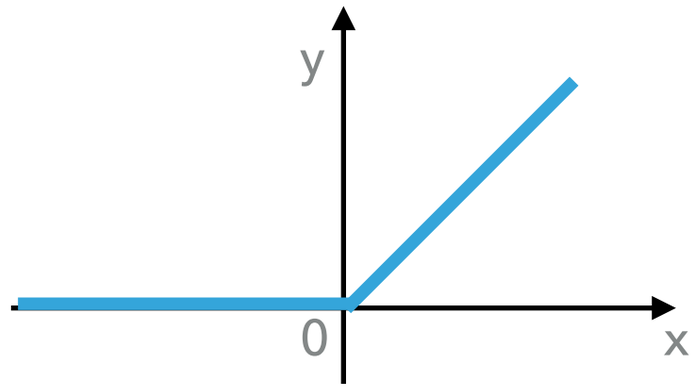
$w_1 = 10$

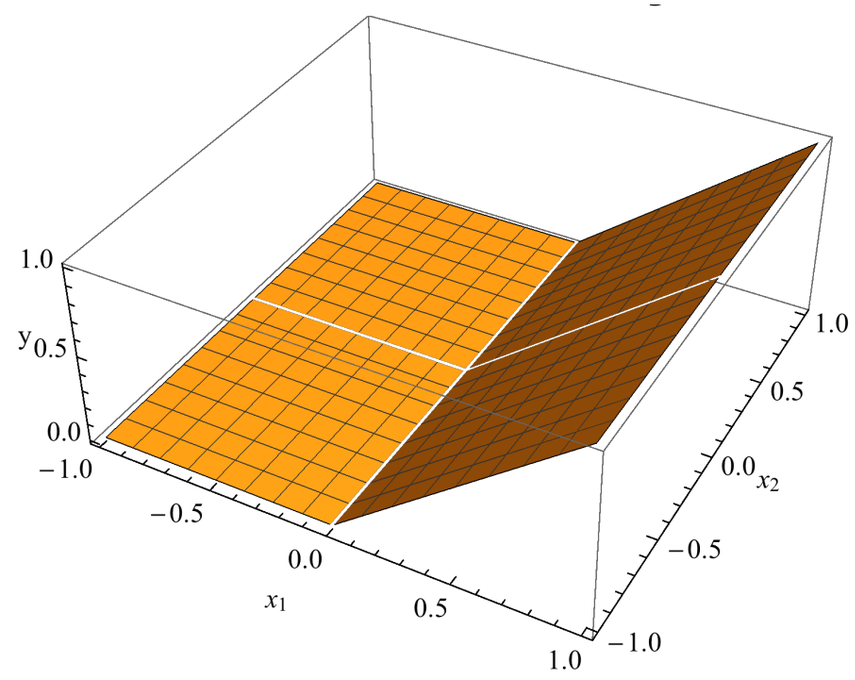
$w_2 = 10$

$\theta = -5$

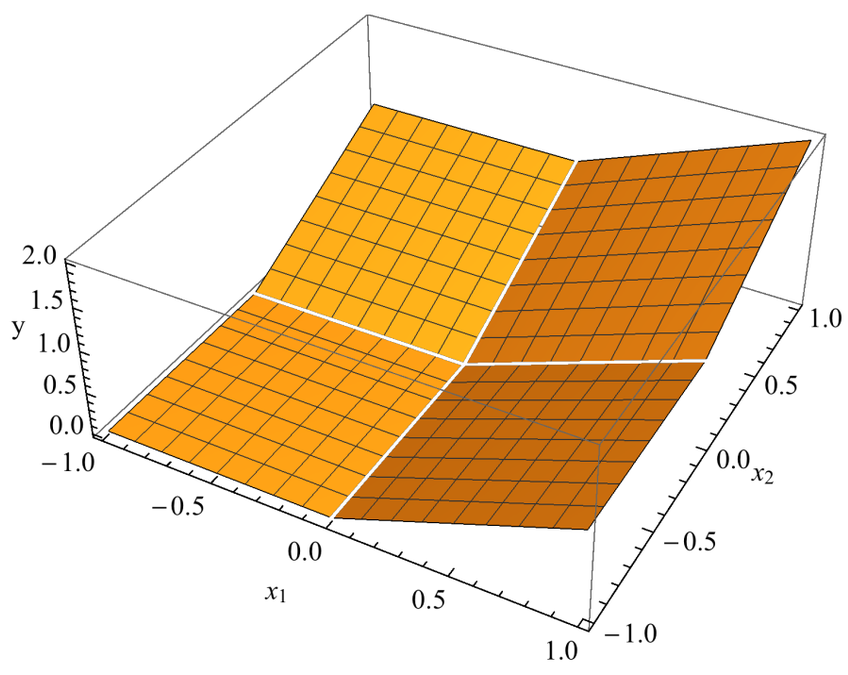
Activation Functions: ReLU

- The **Re**ctified **L**inear **U**nit activation function is commonly used in **convolutional neural networks (CNNs)**.
  - If $x < 0$, $y = 0$
  - Otherwise $y = x$

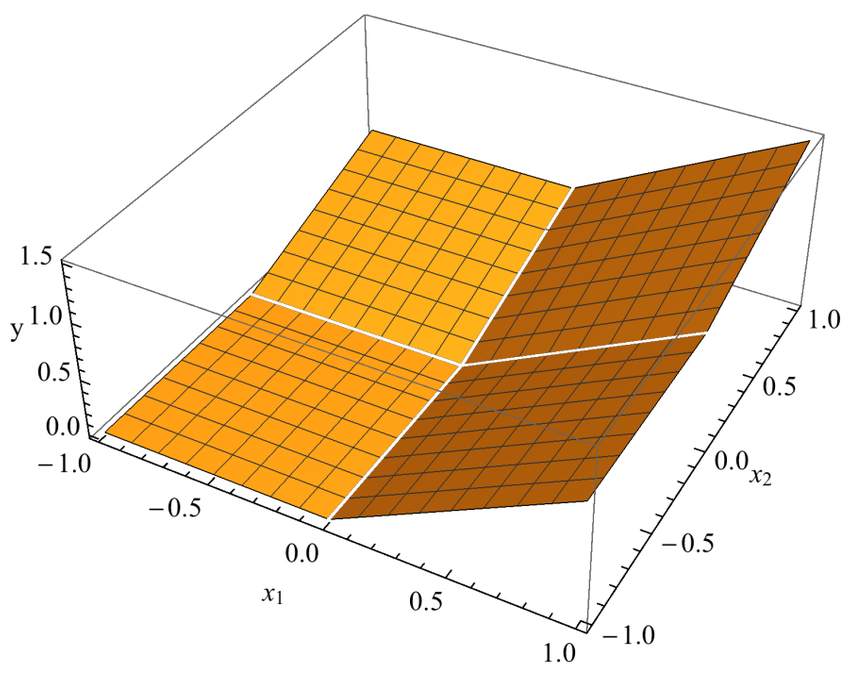




$w_1 = 1, w_2 = 0$



$w_1 = 1, w_2 = 1$

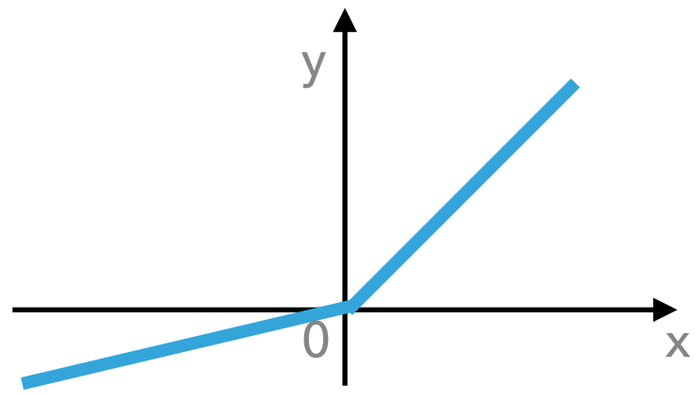


$w_1 = 1, w_2 = 0.5$

Importance of features in the perceptron still depends on weights.

Activation Functions: ReLU Family

- **Leaky ReLU** is a slightly modified version of **ReLU.** For some small constant a:
  - If $x < 0$, $y = ax$
  - Otherwise $y = x$



- **P**arametrised **ReLU**, a is a learnable parameter.

$$f(x) = \max(0, x) + a \min(0, x)$$

Which Activation Function to Use?

It depends!

- **Sigmoid** outputs values between 0 and 1, perfect for probability-based models. Face challenges during training - vanishing and exploding gradient problem.
  - Vanishing gradient: as gradient is **backpropagated**, gets multiplied by the derivative of the activation function at each layer. If derivative is small, repeatedly multiplying causes gradient to diminish -> updates to weights (particularly in early layers) become small -> slow to learn.
  - Exploding gradient: occurs when gradients during **backpropagation** become excessively large, destabilising the model (caused by improper initialisation of parameters or inappropriate learning rate).

- **ReLU** is efficient to calculate with, avoids vanishing / exploding gradient (gradient is 0 or 1) but can lead to inactive neurons.

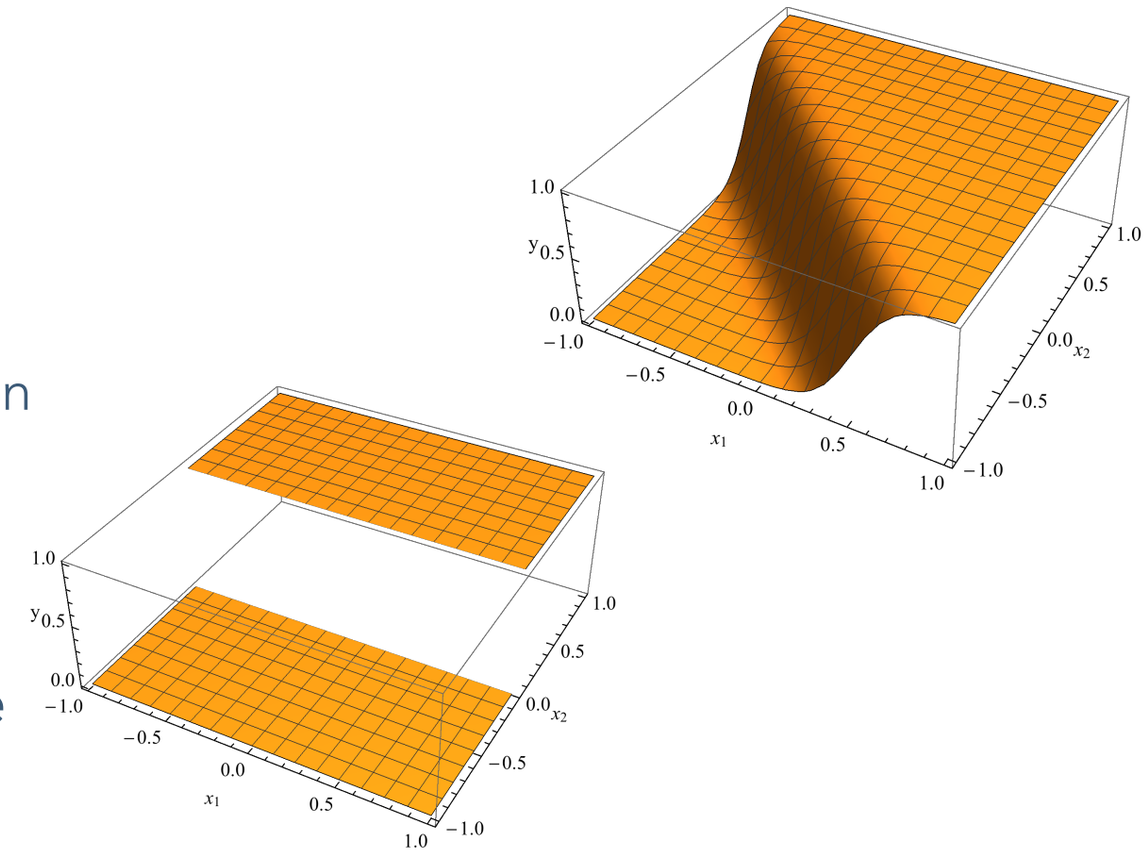
- **Leaky ReLU** less inactive neurons but network can be sensitive to chosen value of a -> inconsistent for different choices.

- **PReLU** enhances model accuracy and convergence but fine-tuning the (learnable) a parameter can be time consuming.

Artificial Neural Networks

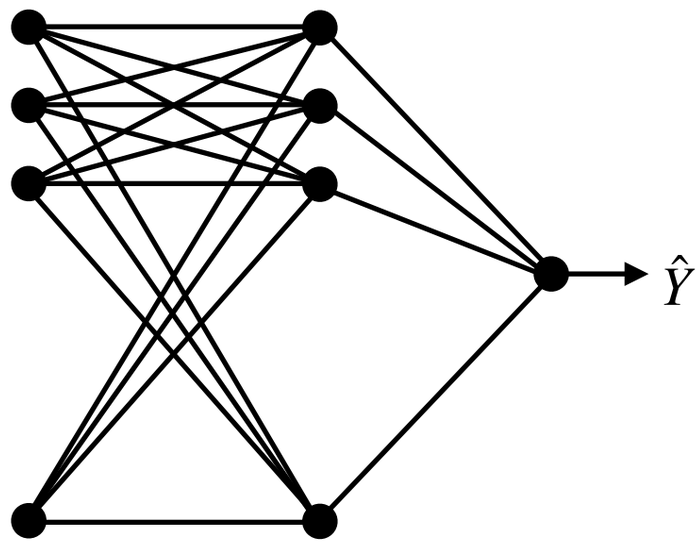
Artificial Neural Networks (ANNs)

- A **single neuron** can be thought of as defining a **hyperplane** that separates the input feature space into two regions.
  - Binary threshold perceptron this is “literally true”.
  - Other perceptrons discussed have a gradual transition from one region to another.



- Can **combine perceptrons** to impose multiple hyperplanes on the input feature space to divide the data into different regions.

- Such a system is an ANN. In HEP, usually synonymous with a **multi-layer perceptron (MLP)**:
  - An MLP has multiple layers of perceptrons.
  - Output of first layer fed into subsequent layer and so on.
  - Ultimately responses of the final layer are brought together to compute an **overall value** $\hat{Y}$ for the network response.



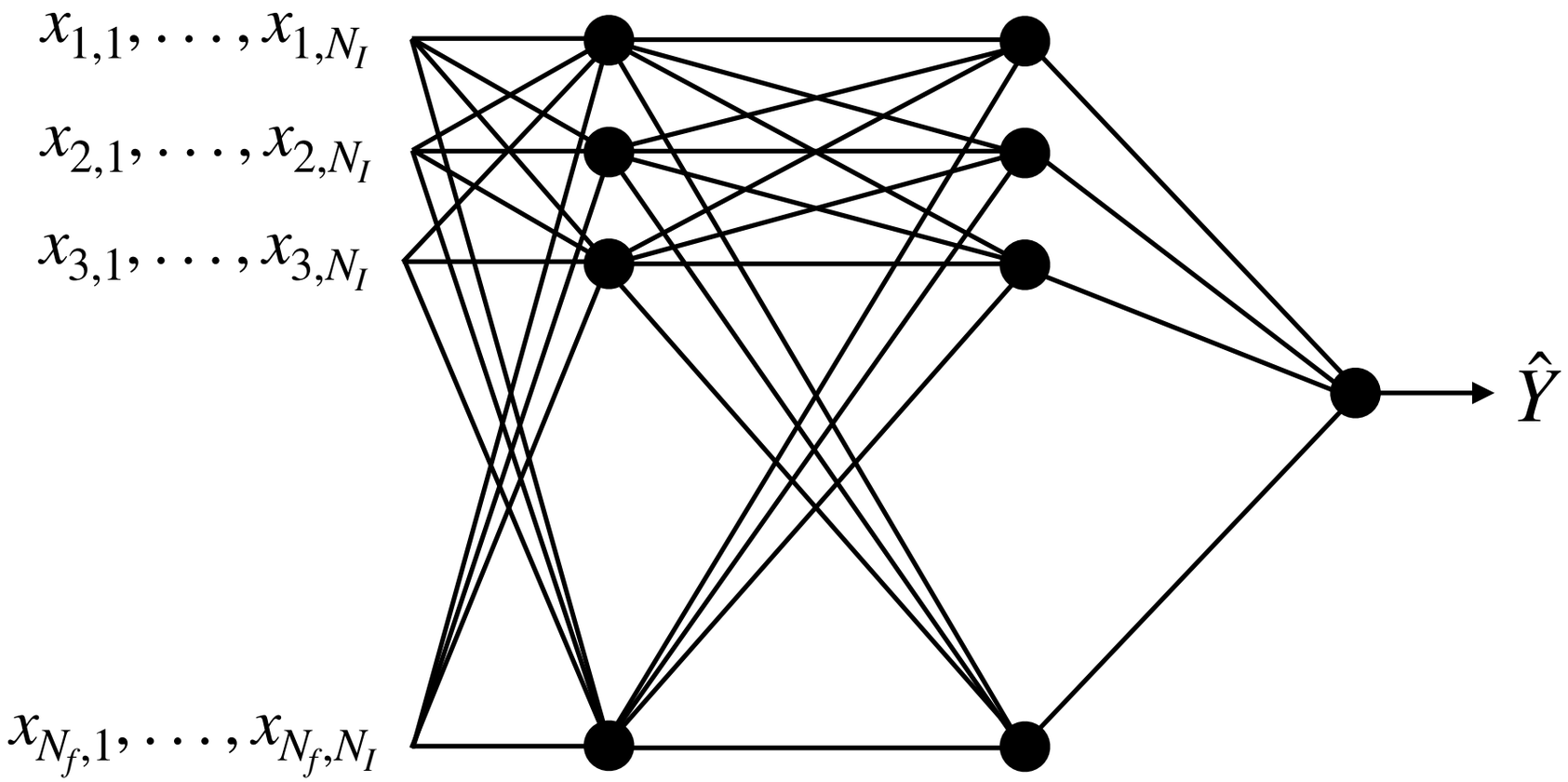
Multi-layer Perceptrons: Illustrative Example

Initial features →

Target feature (to predict)

$$X = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,N_I} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,N_I} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{N_f,1} & x_{N_f,2} & x_{N_f,3} & \cdots & x_{N_f,N_I} \end{bmatrix} \quad \text{Instances} \downarrow$$

$$Y = [y_{I_1}, y_{I_2}, \ldots, y_{I_{N_I}}]$$



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↕ Instances

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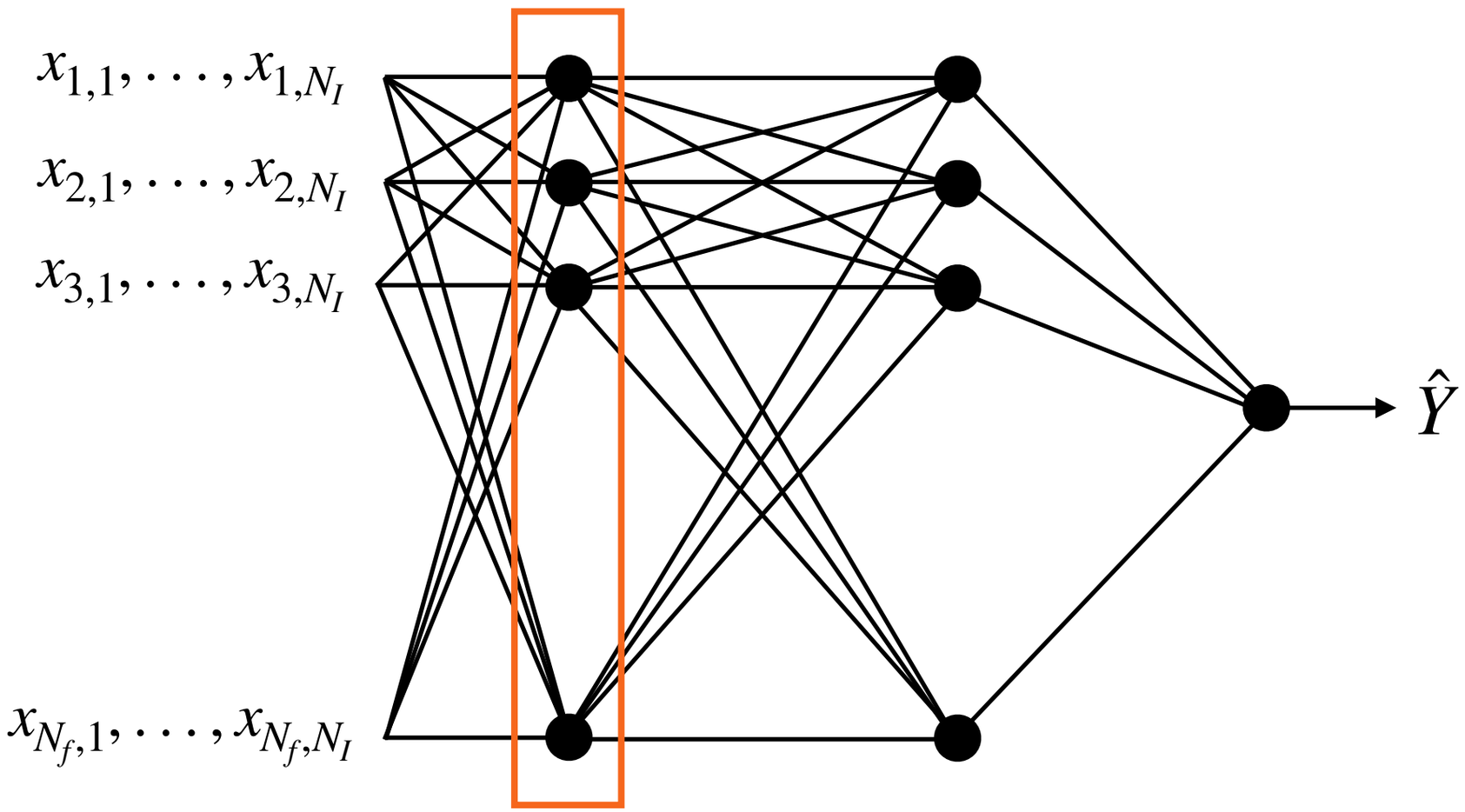
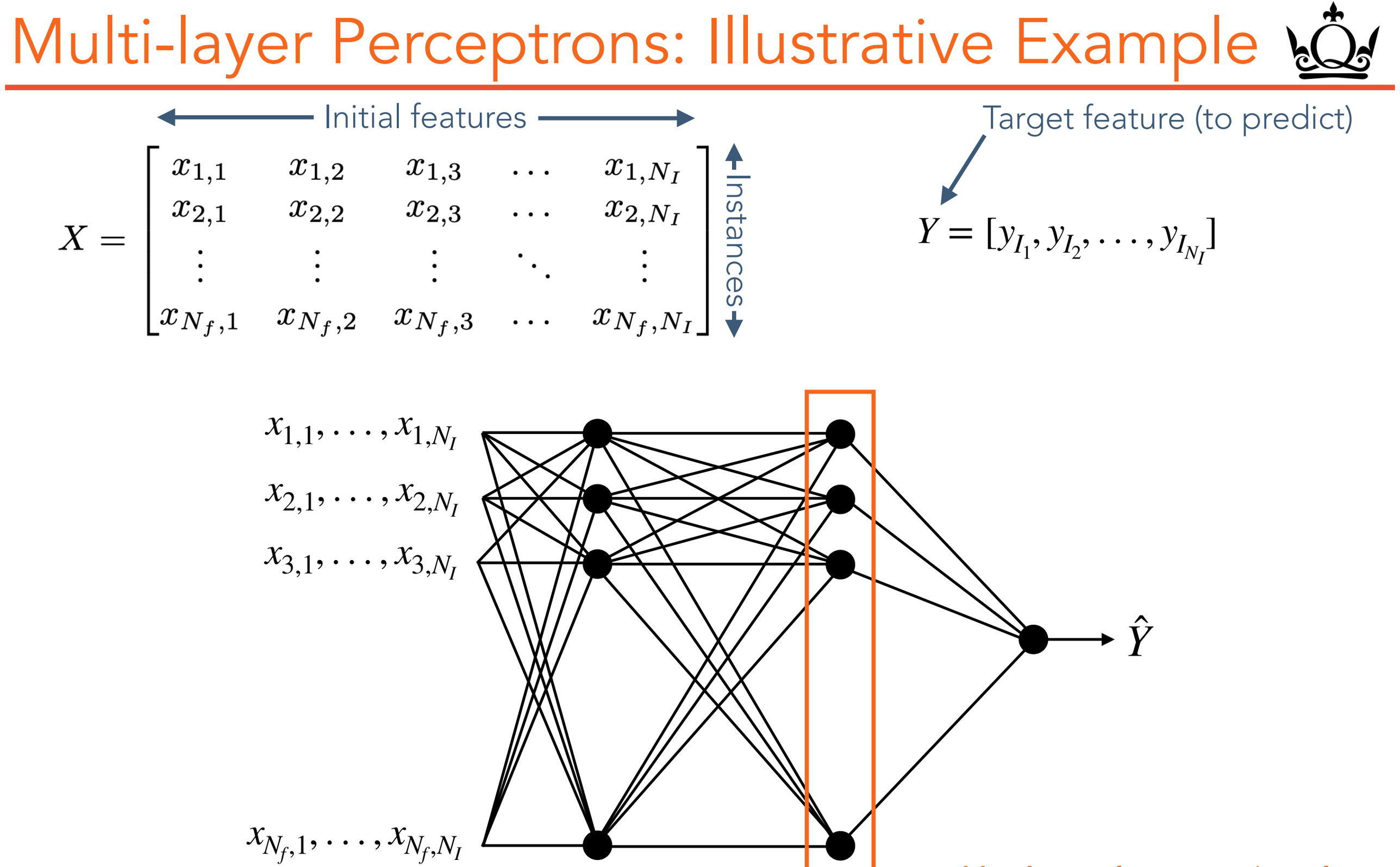


Input layer of N_f perceptrons (one for each dimension of input *feature* space).

Multi-layer Perceptrons: Illustrative Example



This particular layer is **fully connected (dense)** since each node in the layer is connected to every other node in previous layer.

Hidden layer of some number of perceptrons, N_{H_1}; at least one for each dimension of the input feature space.

Multi-layer Perceptrons: Illustrative Example

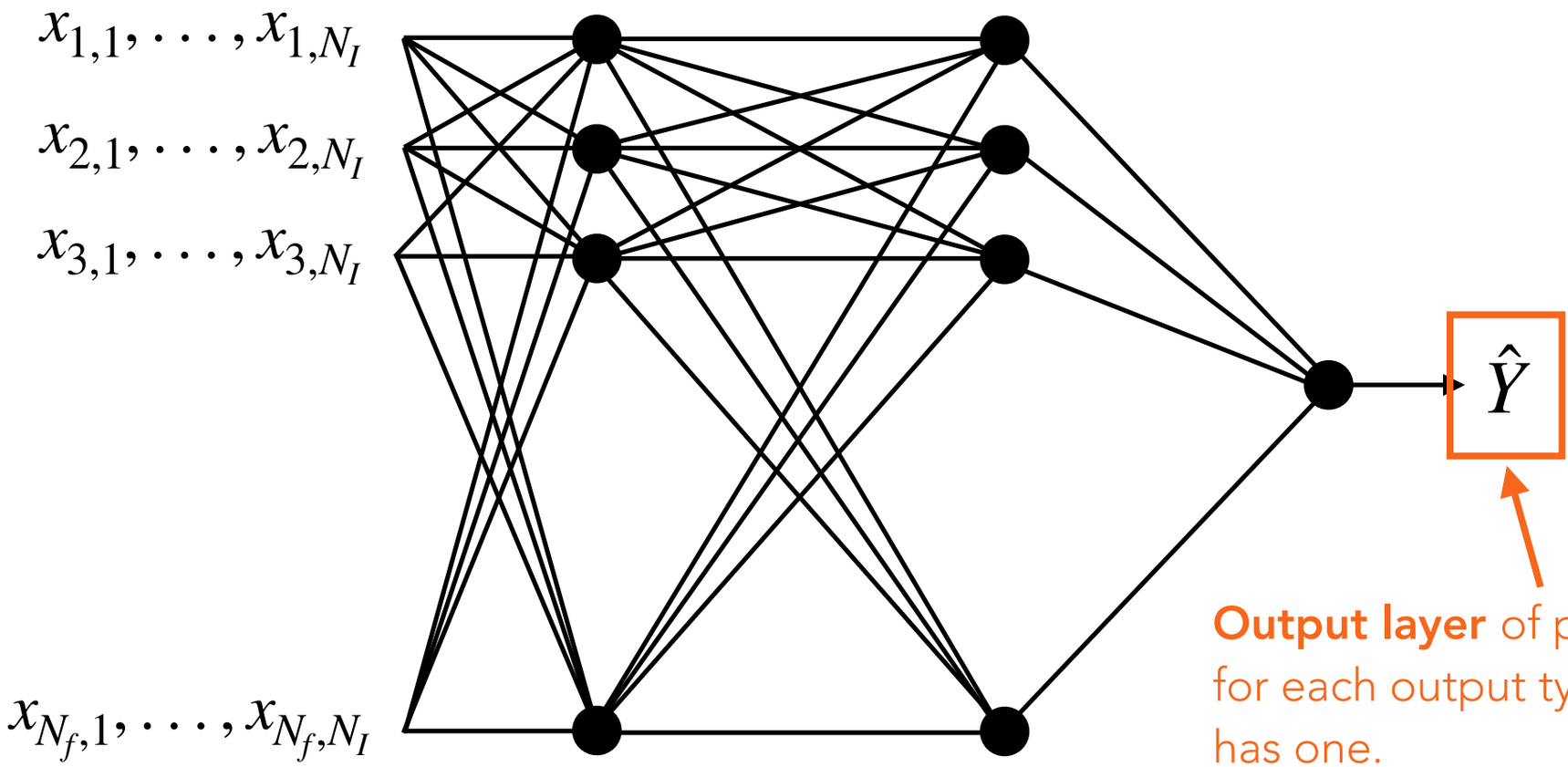
Initial features →

$$X = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,N_I} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,N_I} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{N_f,1} & x_{N_f,2} & x_{N_f,3} & \cdots & x_{N_f,N_I} \end{bmatrix}$$

↕ Instances

Target feature (to predict) ↓

$$Y = [y_{I_1}, y_{I_2}, \ldots, y_{I_{N_I}}]$$



Output layer of perceptrons, one for each output type. This network has one.

Multi-layer Perceptrons: Illustrative Example

Initial features

Instances

$$X = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,N_I} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,N_I} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{N_f,1} & x_{N_f,2} & x_{N_f,3} & \cdots & x_{N_f,N_I} \end{bmatrix}$$

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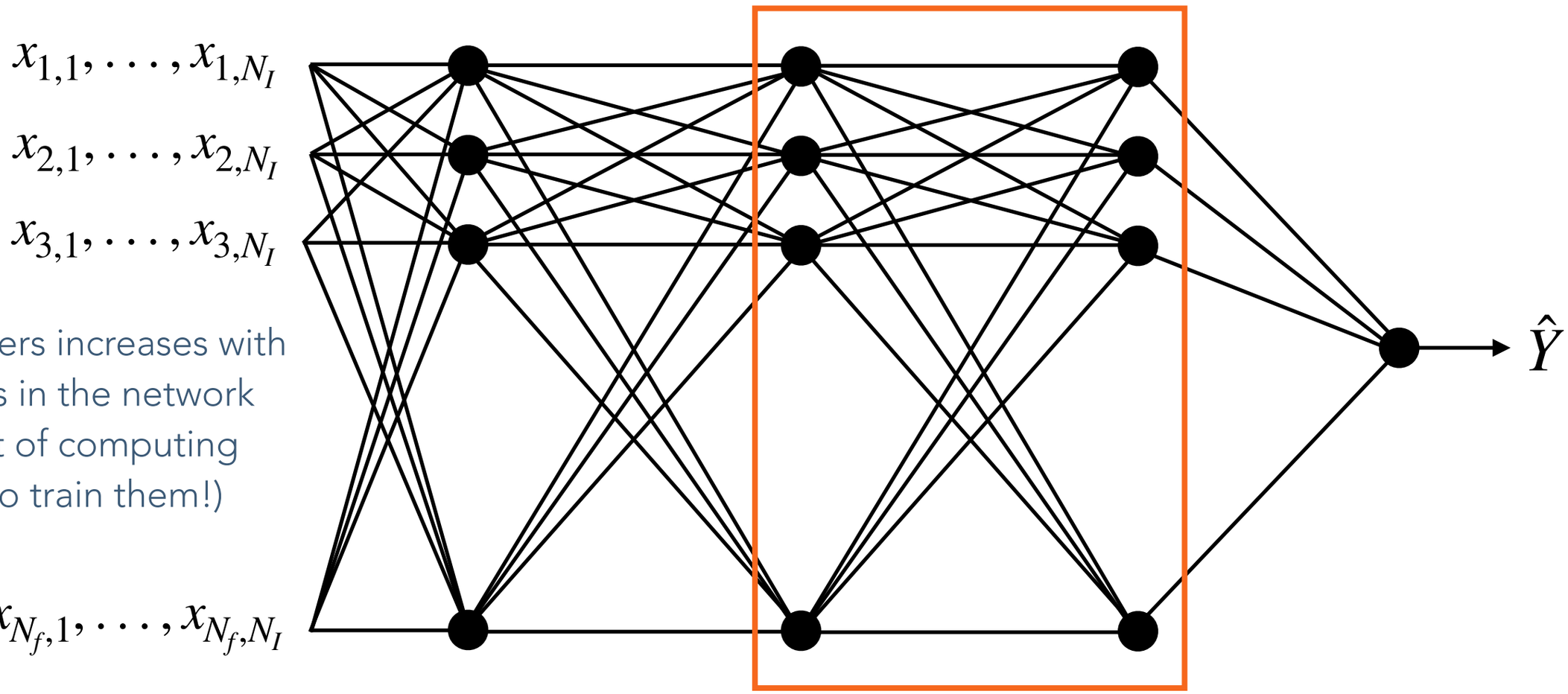


Number of parameters increases with the number of layers in the network (as does the amount of computing resources required to train them!)

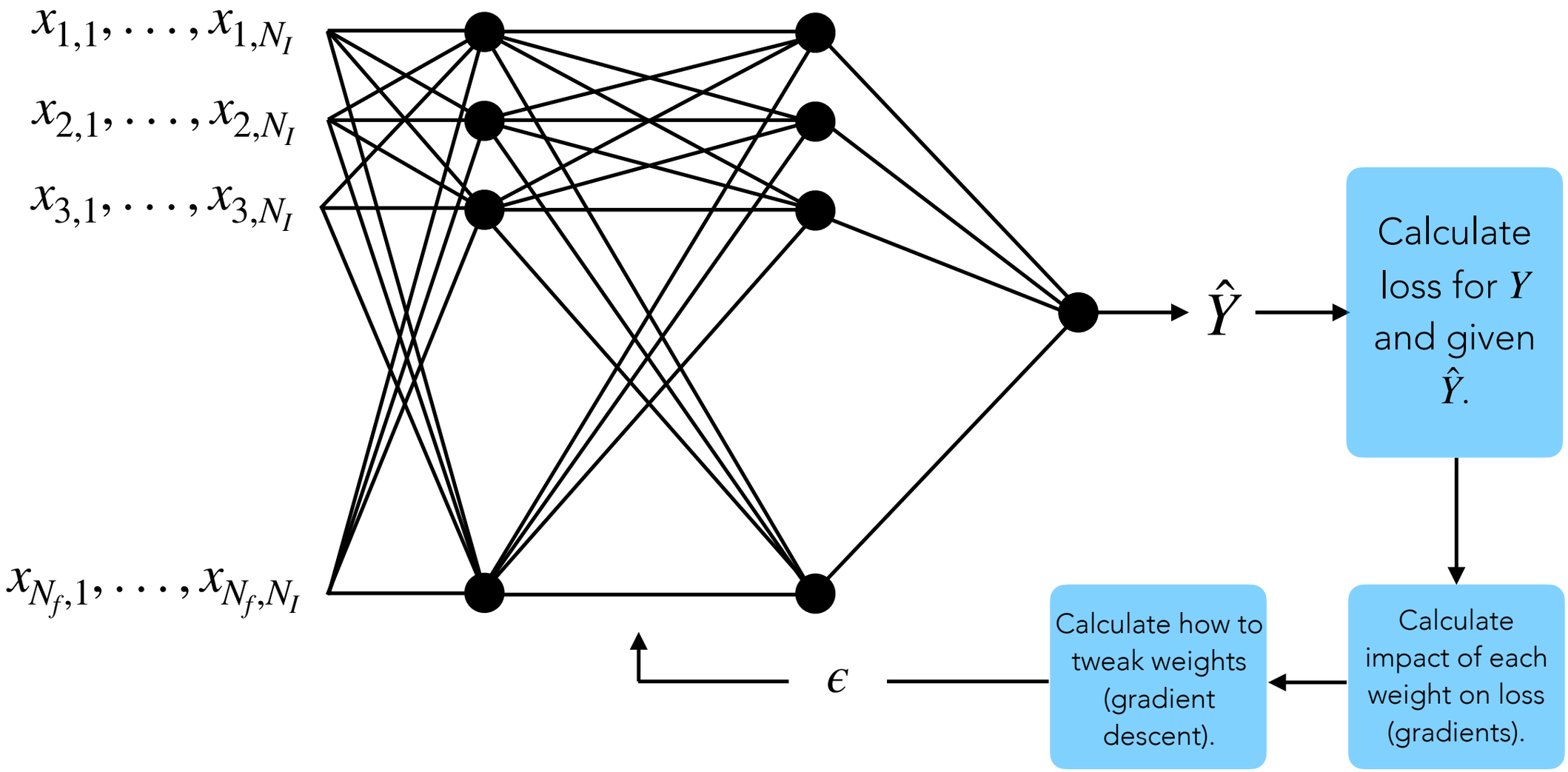
The **depth** of a network relates to the number of hidden layers -> greater than ~ a couple-> **deep NN**.

Training

- Each neuron has its own weights & bias (parameters). The **optimisation / tuning** of these parameters is referred to as **training**.

- Tune based on some metric (figure of merit) called the **loss function**.

- Usually want to **minimise the loss** - usually done by **gradient descent**. Tells us how to **tweak weights to reduce the loss**.



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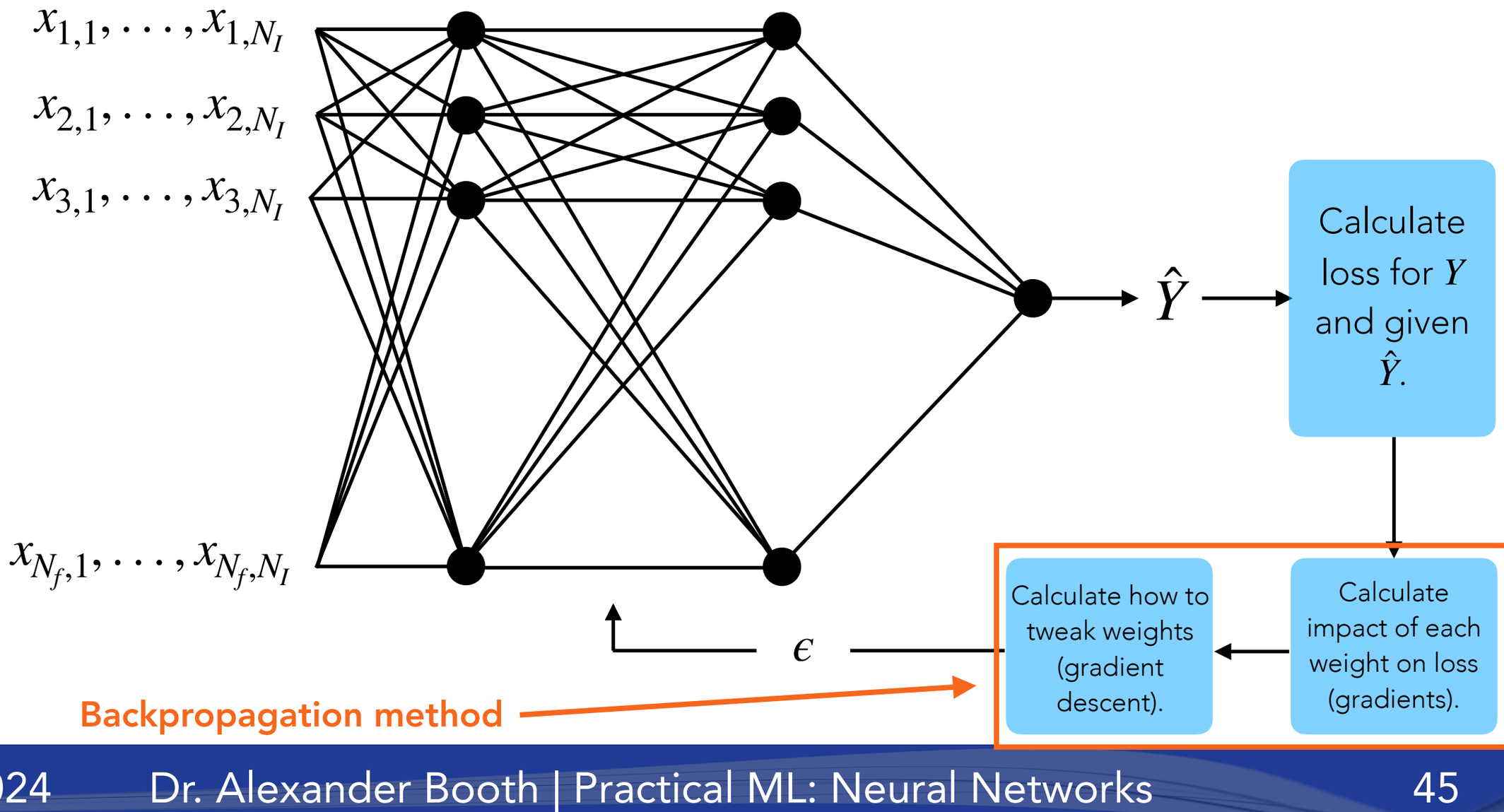
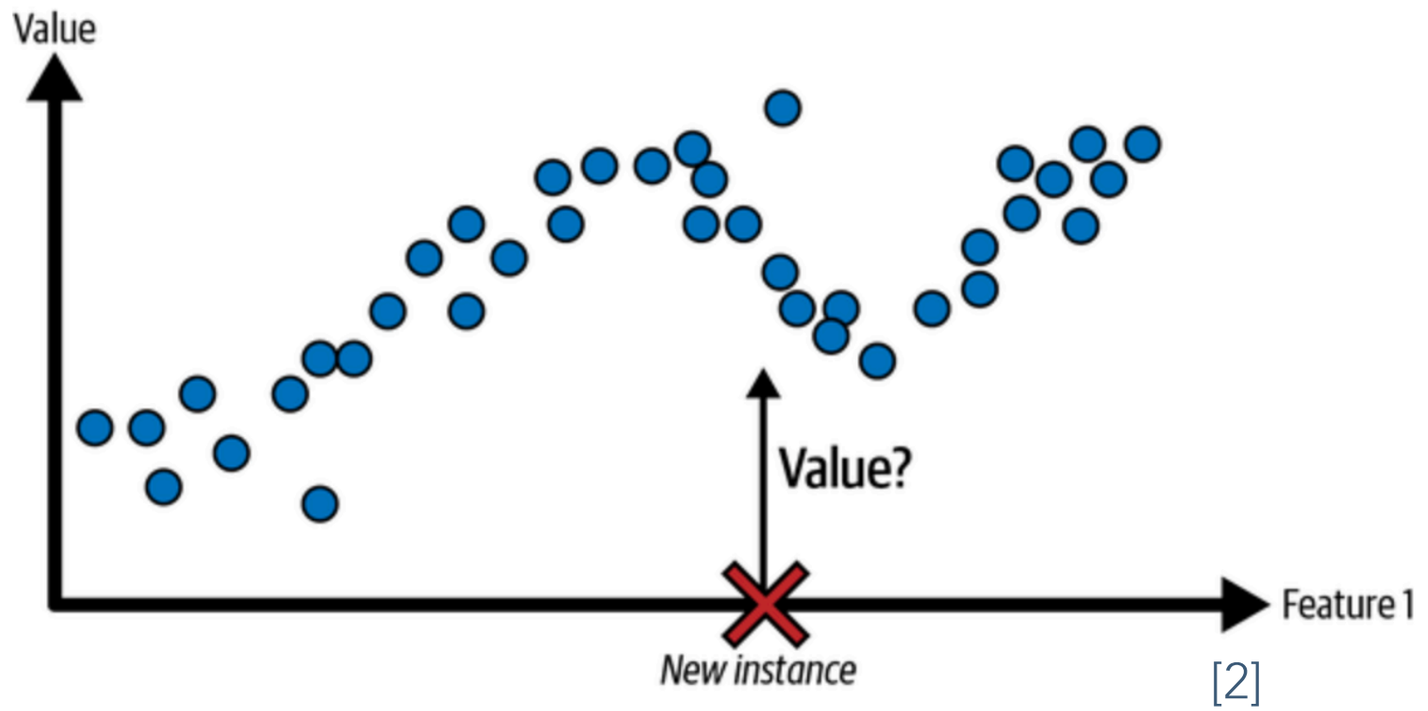


Linear Regression

What is Regression?

- Predicting a target **numeric value** (**response**) given a set of features.
  - House prices given number of bedrooms.
  - Time to run a marathon given resting heart rate and blood pressure.

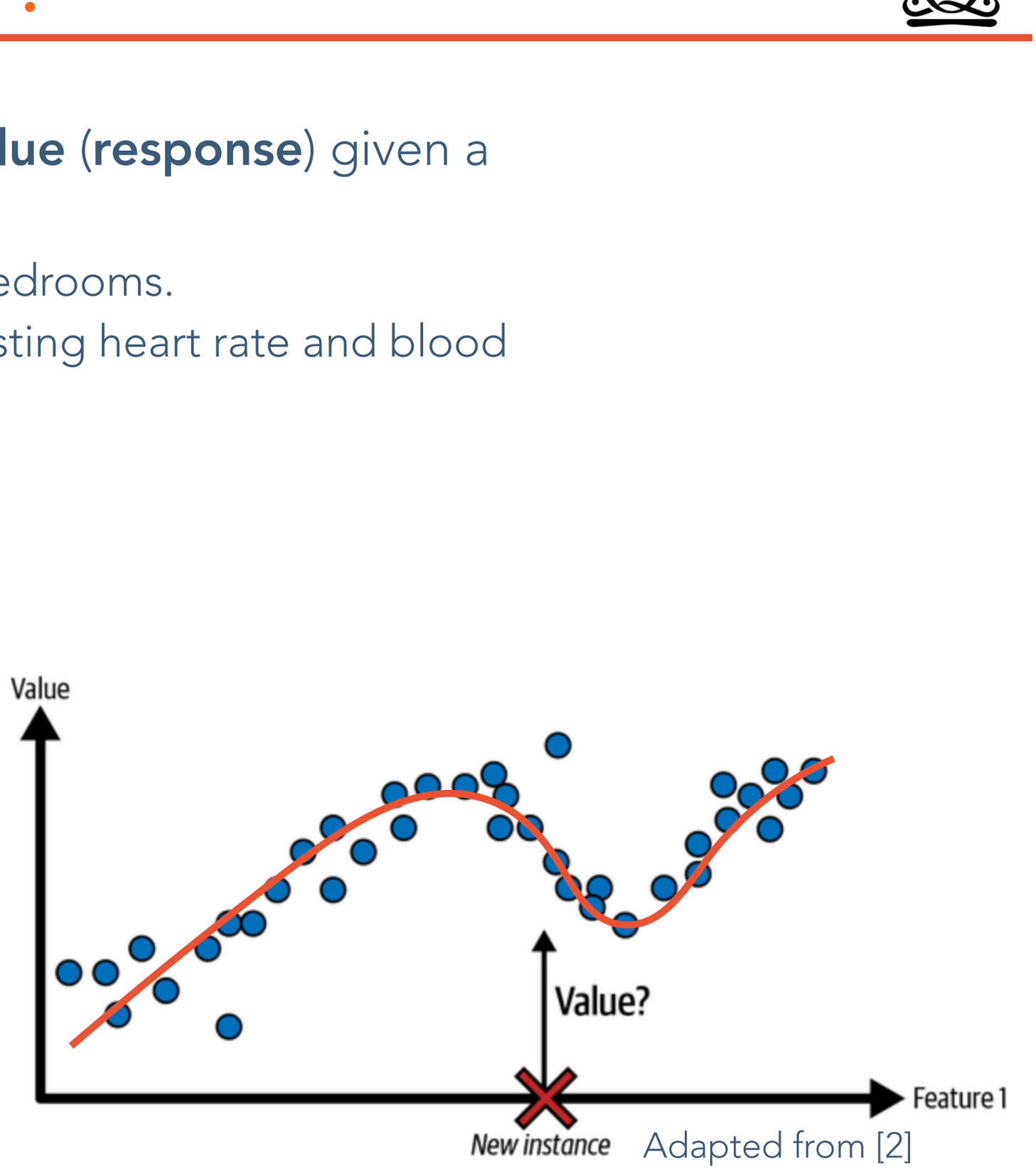


[2]

What is Regression?

- Predicting a target **numeric value** (**response**) given a set of features.
  - House prices given number of bedrooms.
  - Time to run a marathon given resting heart rate and blood pressure.

- "Curve fitting" - parametrising relationship between a set of independent variables and a dependent variable.



Adapted from [2]

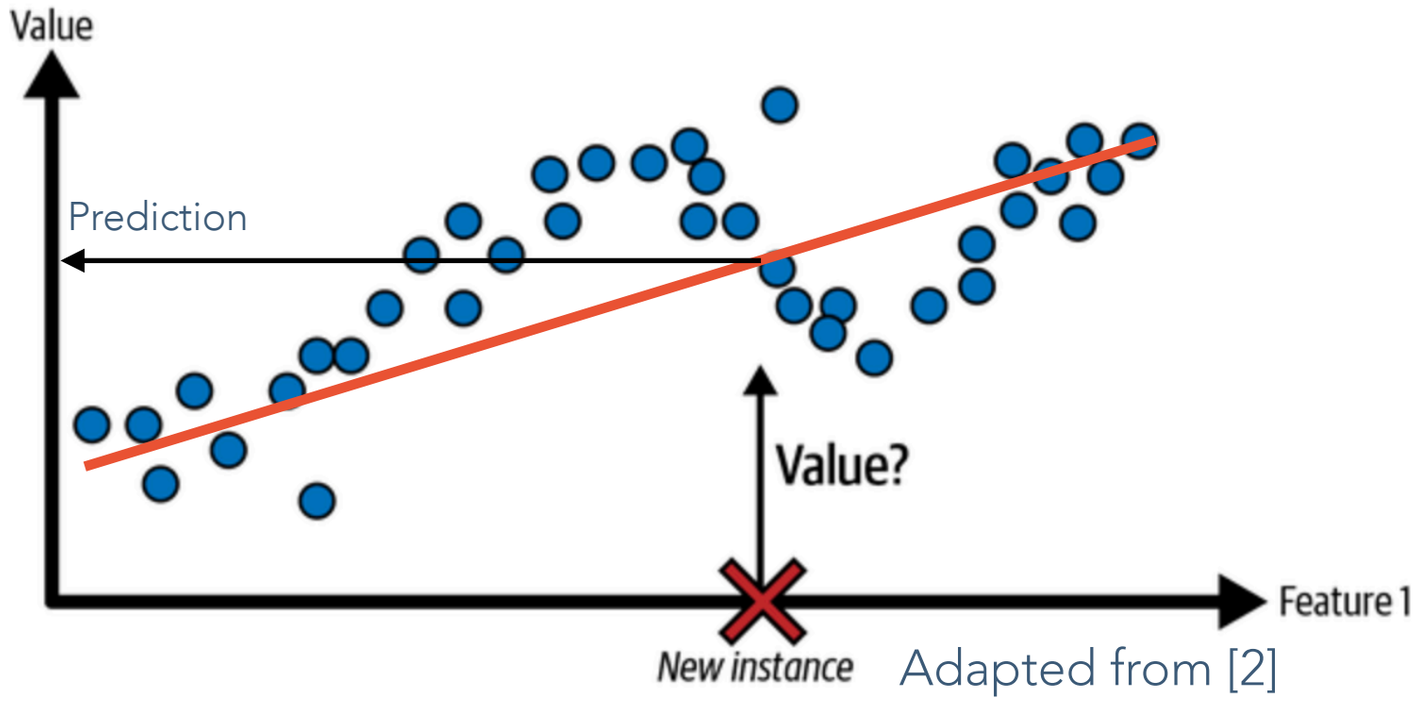
Linear Regression

- Assume the data have a linear relationship -> apply a linear model.

$$y = mx + c$$

- Describes a straight line where:
  - m is the slope of the line
  - c is the constant offset (y value at $x = 0$).

- The problem: selecting the values of m and c in order to obtain the best possible model of the data.



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$$y = mx + c$$

- Describes a straight line where:
  - m is the slope of the line
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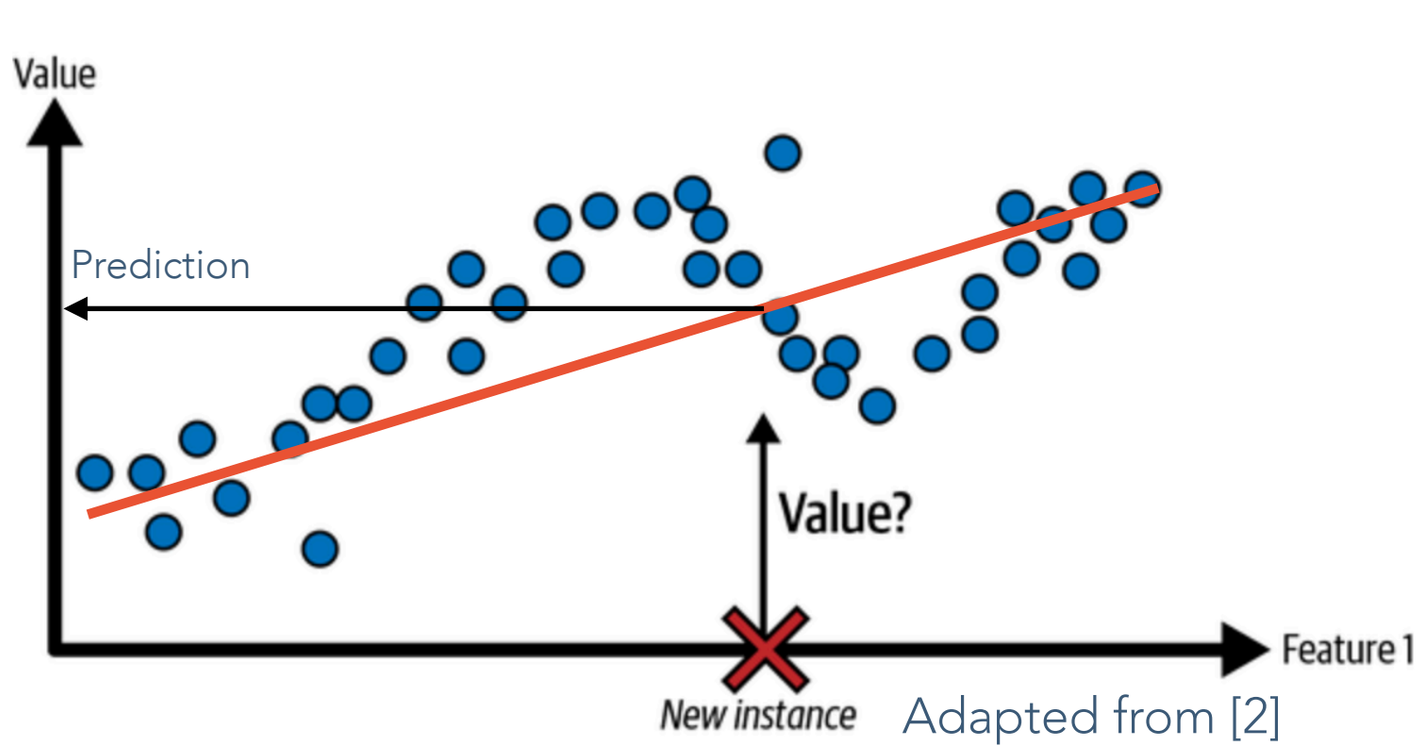
Define a method that can be used to extract optimal values.

- The problem: **selecting the values** of m and c in order to obtain the **best possible model** of the data.

Define a figure of merit.



Adapted from [2]

Linear Regression: Figure of Merit

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - (mx_i + c)}{\sigma_i} \right)^2$$

- χ^2: sum of the normalised square residual of each instance.
  - y_i: y value for the i^{th} instance.
  - x_i: x value for the i^{th} instance.
  - σ_i: error on the value of y for the i^{th} instance.
  - m and c: model parameters to be determined.

Measure of the total "distance" of each point from the line.

- Optimal value of m and c is the pair that produces the smallest χ^2.
  - No guarantee that this choice will result in a good model (overfitting / overtraining discussed tomorrow).

- *Note:* if it's assumed that all data points have a similar error, simplify the problem by neglecting σ_i (setting values to unity).

Linear Regression: Optimisation

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - (mx_i + c)}{\sigma_i} \right)^2$$

- Systematically vary m and c to minimise the χ^2.
  - Conceptually - visualise choosing pairs of m and c, and for each point in this 2D space, compute χ^2.
  - From the ensemble of points in this hyperspace, can select the minimum.

- Algorithmically this is expensive so we use algorithms that approximate the search for the minimum that is more computationally efficient (and adaptable to high dimension parameter spaces - more features).
  - We will use a **gradient descent parameter optimisation** algorithm. For now treat this optimisation process as a black box (revisit in detail in lecture 2).
  - *Note:* this particular problem is solvable analytically.

Linear Regression: Illustrative Example in 1D

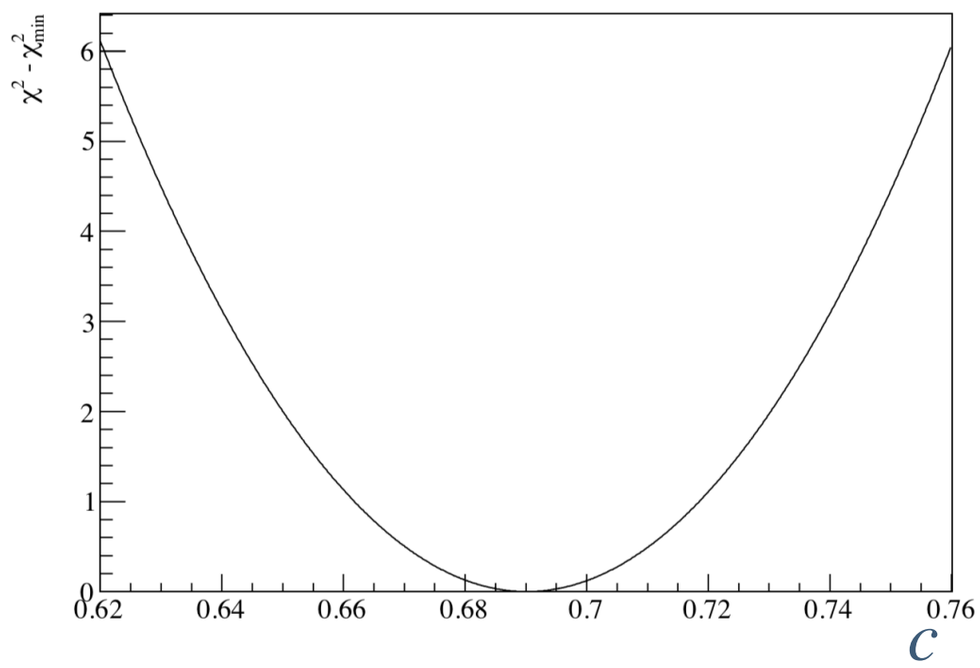
- Take an ensemble of measurements of some quantity S.

i =	1	2	3	4	5	6	7
S	0.662	0.625	0.897	0.614	0.925	0.694	0.601
σ_S	0.039	0.091	0.100	0.160	0.160	0.061	0.239

- "Extract the average value of S from these data" -> fit a line with a gradient of zero -> fitting $y = c$.

$$\chi^2 = \sum_{i=1}^{7} \left(\frac{S_i - c}{\sigma_{S_i}} \right)^2$$

- Optimisation algorithm: choose several sensible values for c, calculate the χ^2 for each one.



Average of S is at the minimum.

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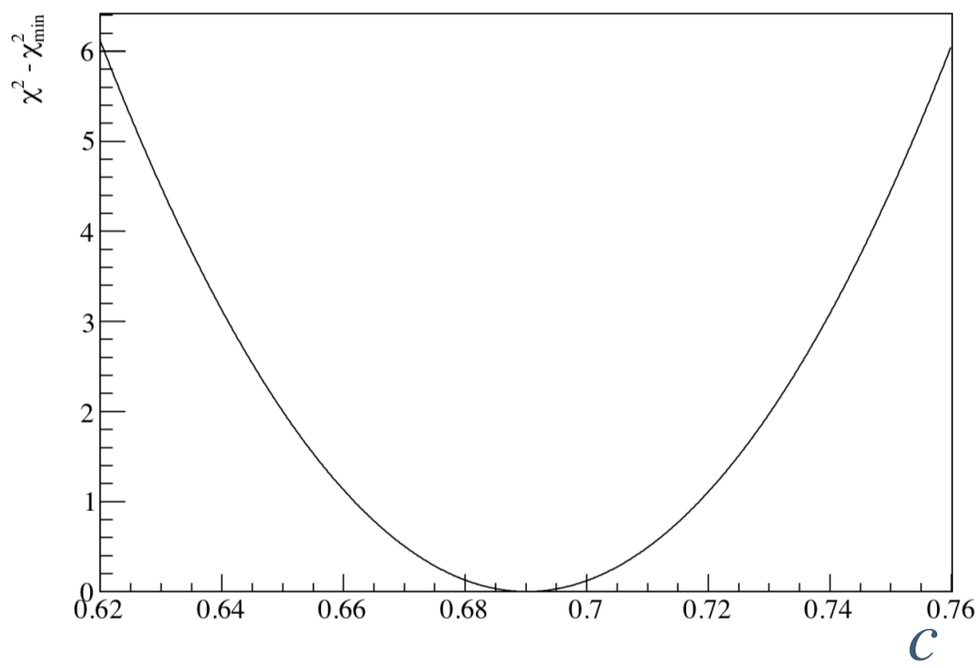


"Grid search"

Average of S is at the minimum.

Linear Regression: Today's Notebook

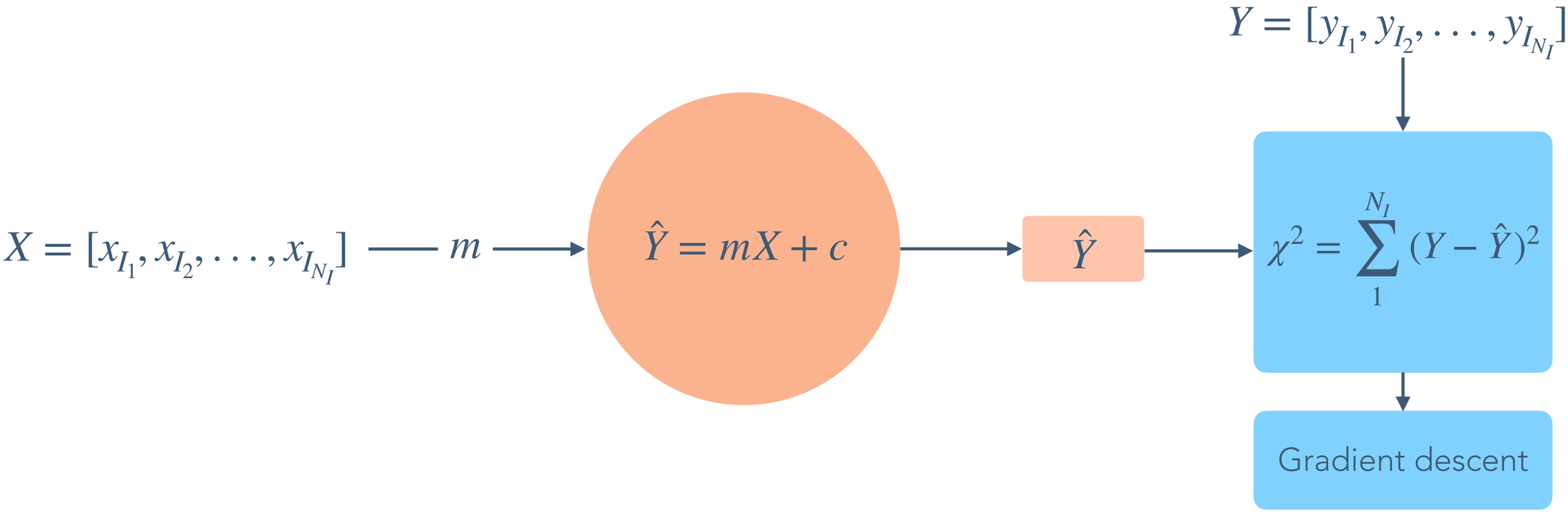
workshop-UCDN_PracticalML/lecture1_1/LinearRegression.ipynb

Perform linear regression using a Keras model.

- Generate "fake" data according to some linear distribution with added noise, ($X = [x_{I_1}, x_{I_2}, \ldots, x_{I_{N_I}}]$, $Y = [y_{I_1}, y_{I_2}, \ldots, y_{I_{N_I}}]$) split into two pieces:
  - **Training set (~90% of total dataset):** dataset used in the optimisation process to create a representative model of the data.
  - **Test set (~10% of total dataset):** dataset unseen in the training process, used to assess generalised performance of the trained model.

- Build model (parameters are a single weight (m) and single bias (c)):
  - Single dense layer with **linear activation function** (nothing done to weighted sum of inputs).
  - Define **loss function** "mean square error" -> χ^2.
  - Define optimisation algorithm (ADAM -> gradient descent) and choose the **learning rate** ("step size").

Linear Regression: Today's Notebook



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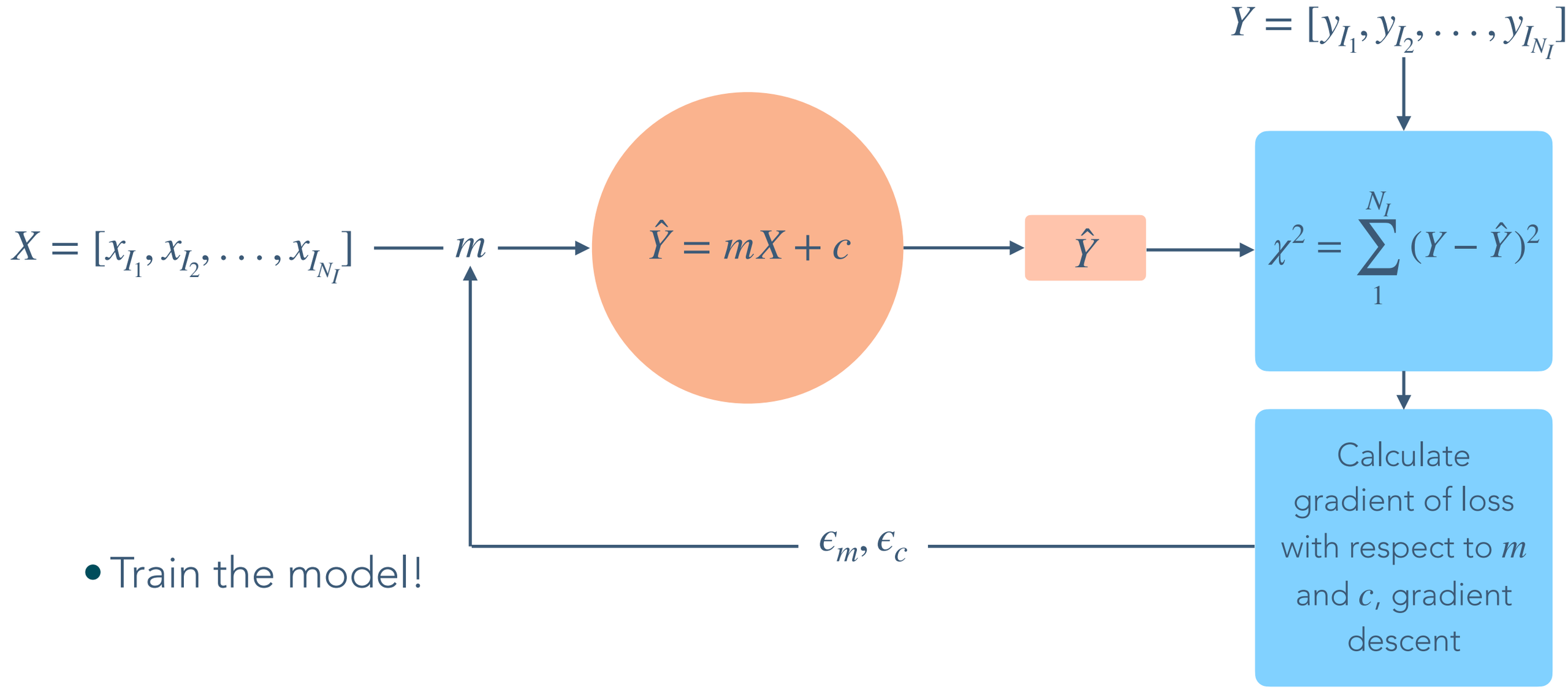
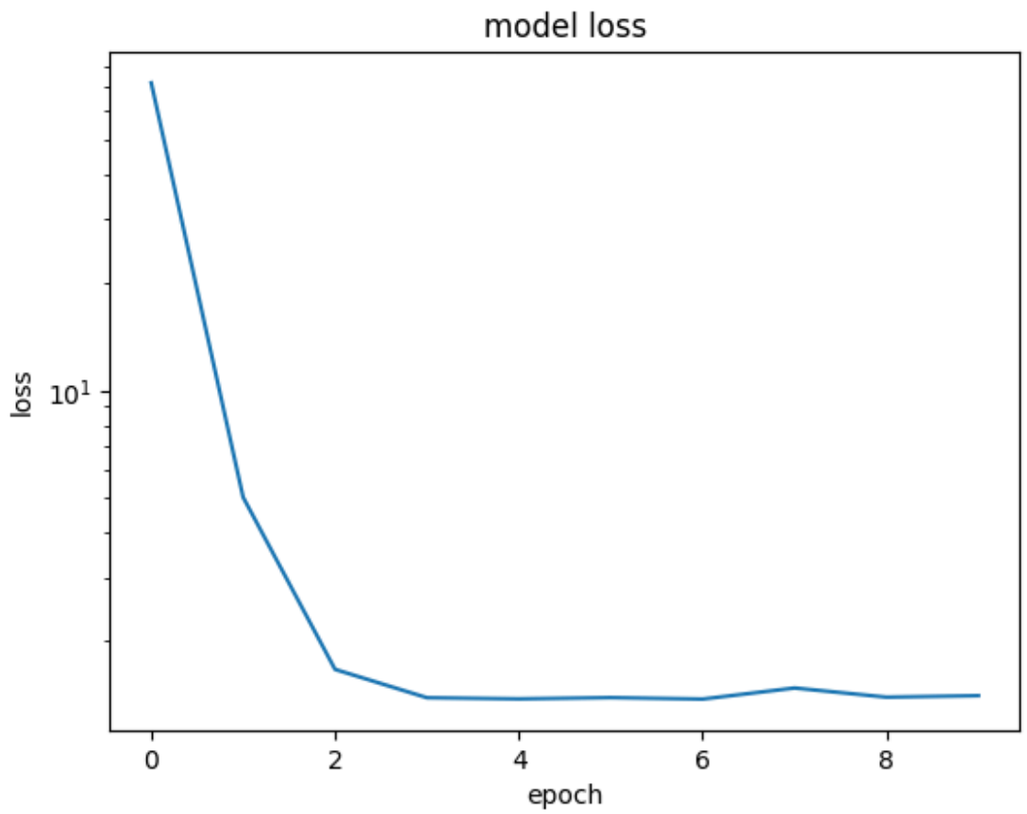


- Train the model!

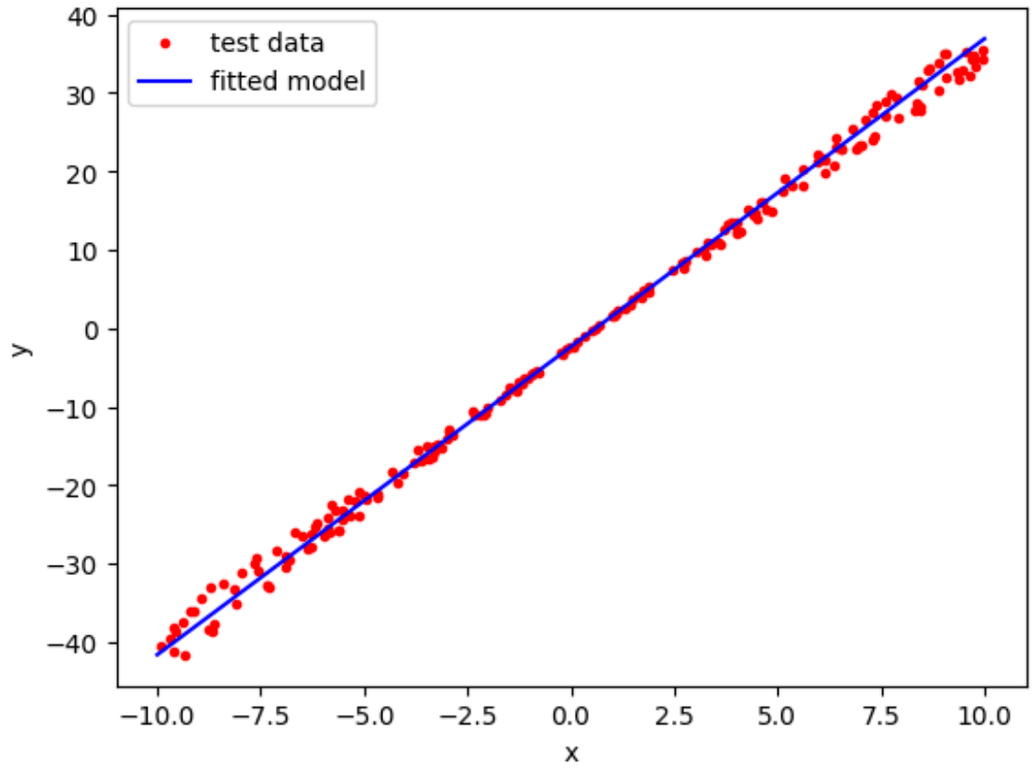
Linear Regression: Today's Notebook

- Study how the solution depends on:
  - The learning rate.
  - The number of **training epochs** (number of times the optimisation is run).

Plotting the loss function evolution as a function of training epoch



Plotting the optimised model and test data

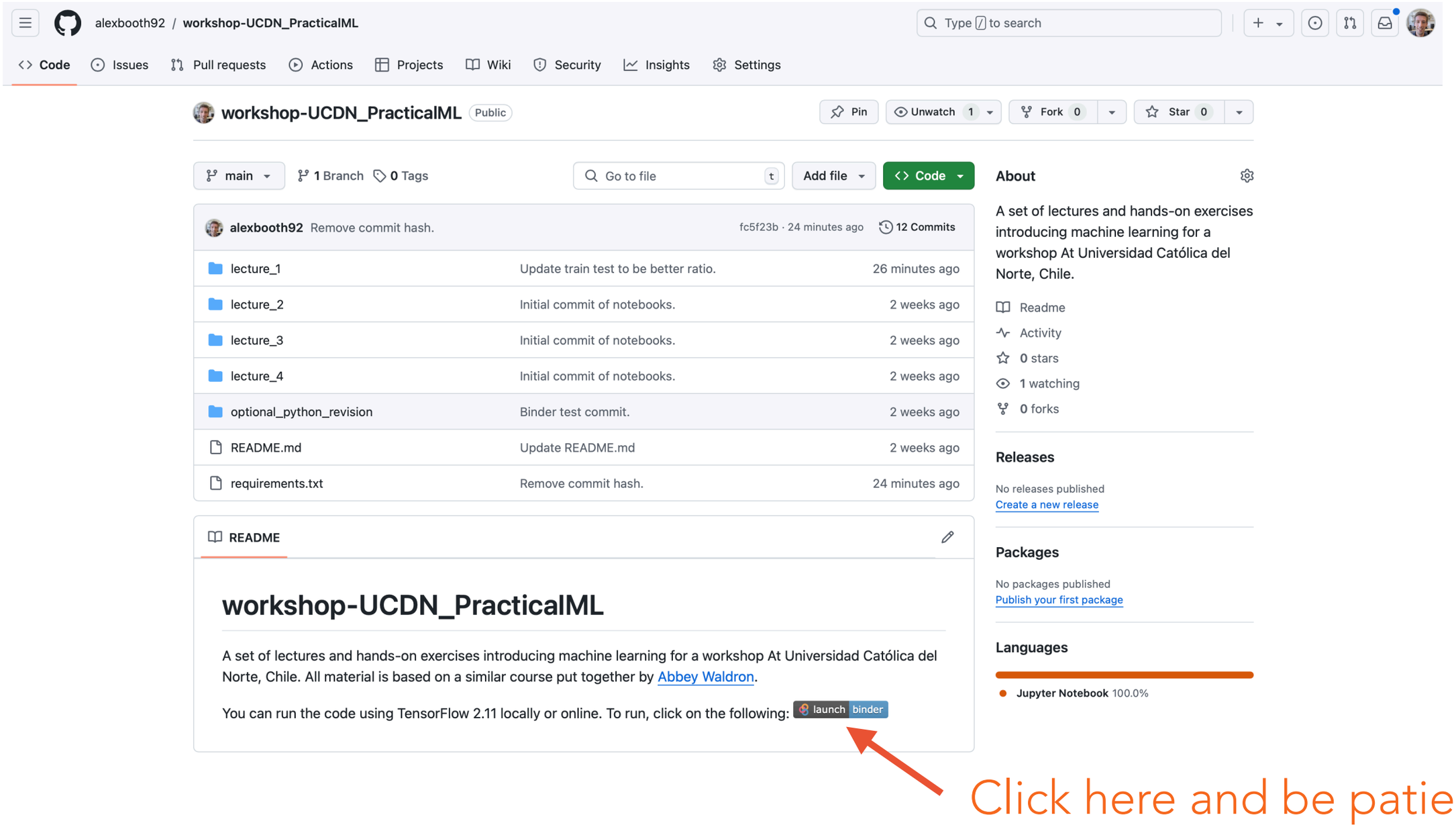



```
m =  3.9265254
c =  -2.354052
MSE loss =
 Fitted line xrange = [-10, 10], y range = [-41.61930561065674, 36.91120147705078]
```

Accessing the Notebooks

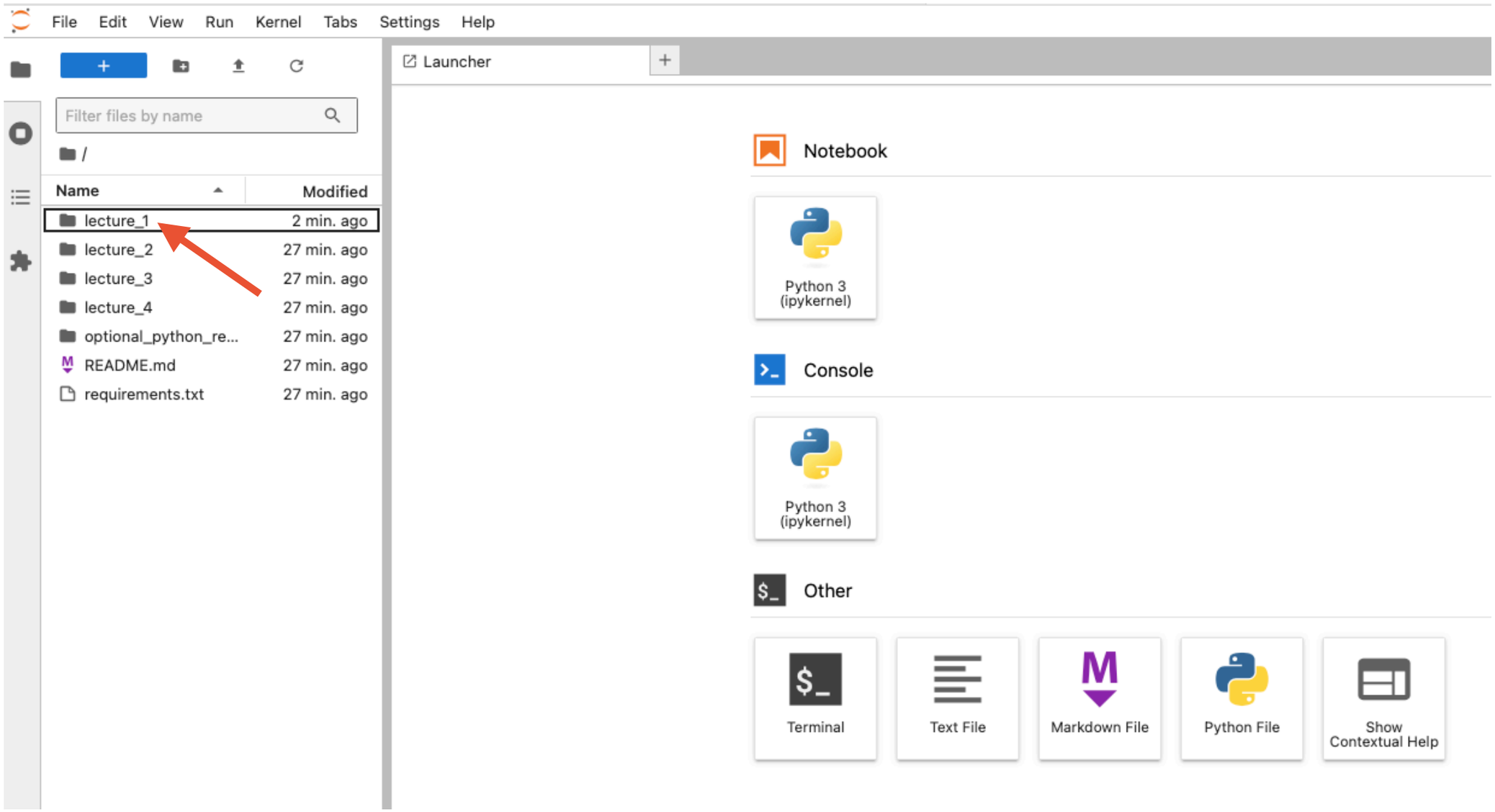
Follow this link:

https://github.com/alexbooth92/workshop-UCDN_PracticalML.git



Click here and be patient!

Accessing the Notebooks



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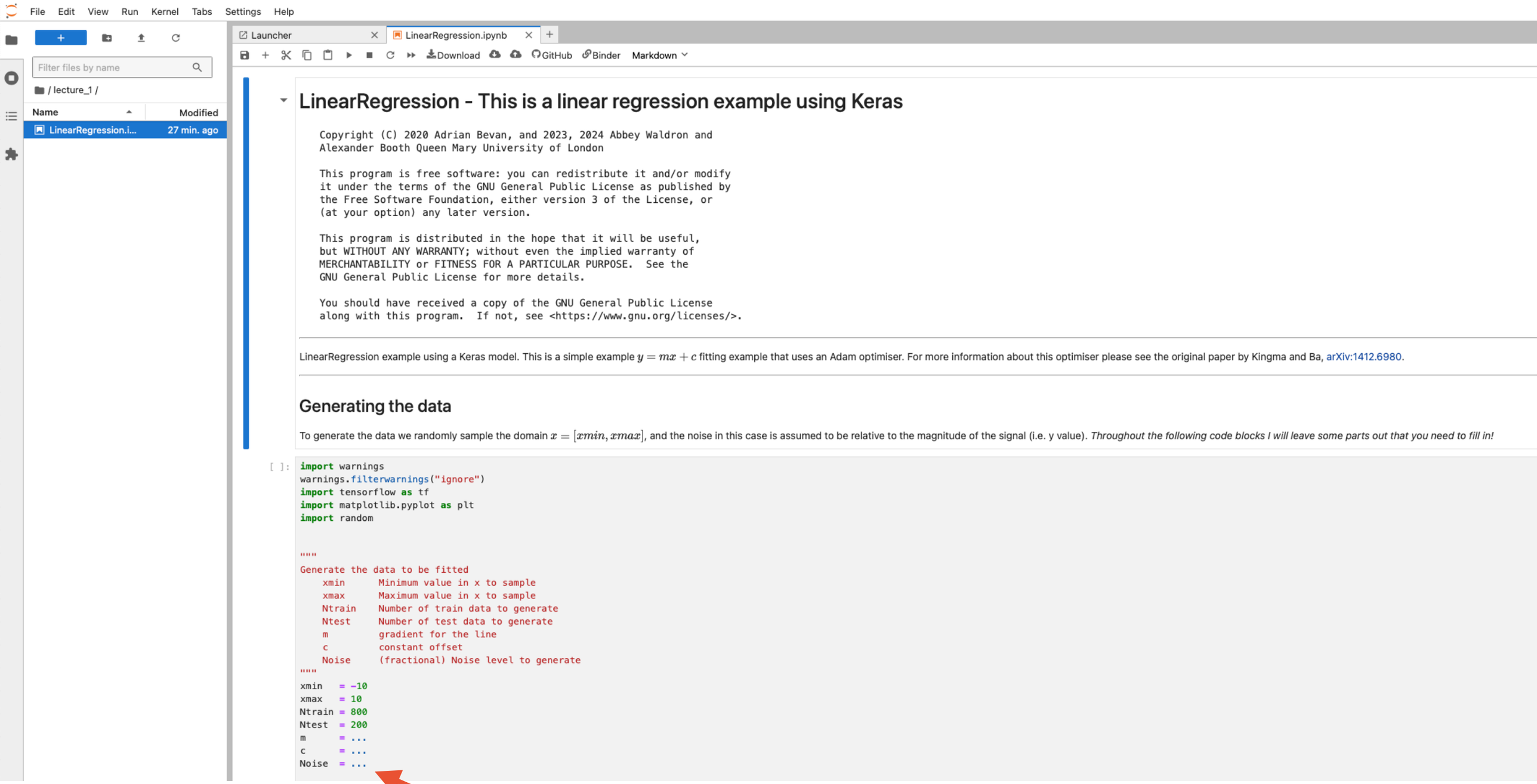

Three dots mean you have to fill this in yourself!

Have Fun!

Queen Mary
University of London

References

[1] https://pixabay.com/vectors/neuron-nerve-cell-axon-dendrite-296581/

[2] A. Géron. Hands on Machine Learning with Scikit-Learn & TensorFlow, 2017.