50.039 Theory and Practice of Deep Learning
Course Introduction

Matthieu De Mari

SINGAPORE UNIVERSITY OF TECHNOLOGY AND DESIGN

A quick word about instructors

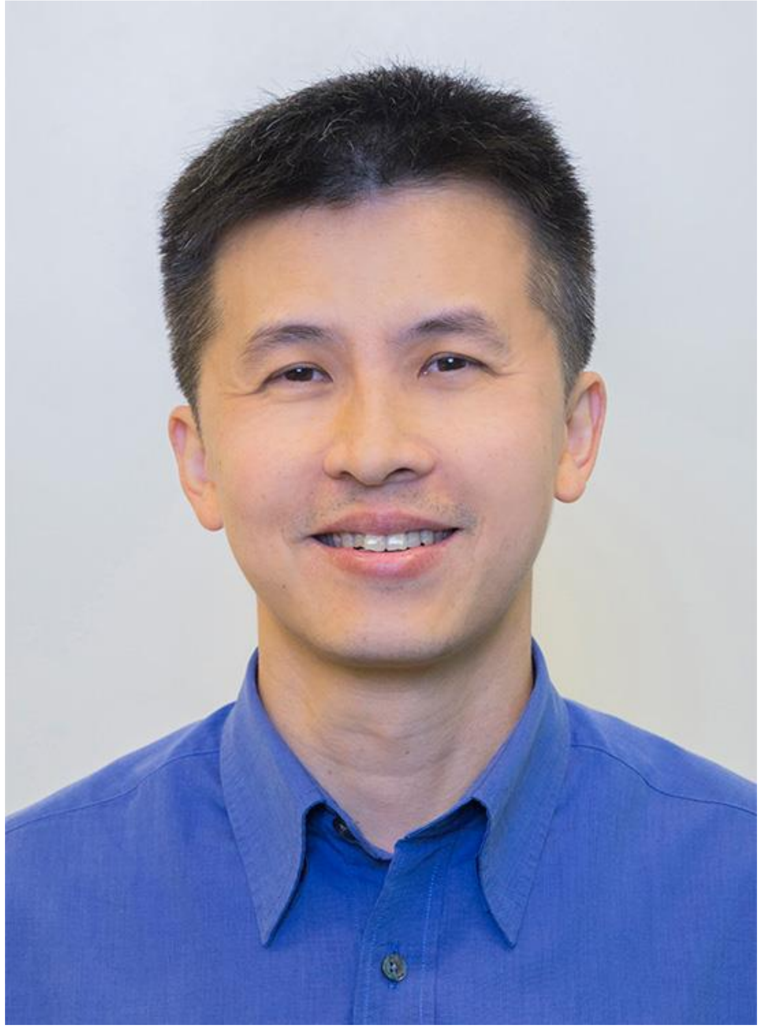
Matthieu (Matt) De Mari

- Lecturer at SUTD (Python, Deep Learning, Prog. Language Concepts, Capstone, etc.)
- Information Systems Technology and Design (ISTD) and Computer Science and Design (CSD) pillar/faculty
- PhD from CentraleSupelec (France)
- Email: matthieu_demari@sutd.edu.sg
- Office @ SUTD (in SUTD Academy/AI cluster): 2.401-07.

A quick word about instructors

Ngai-Man (Man) Cheung

- Assistant Professor at SUTD (Deep Learning, Computer Vision, AI for Medical)
- Information Systems Technology and Design (ISTD) and Computer Science and Design (CSD) pillar/faculty
- PhD from University of Southern California
- Email: ngaiman_cheung@sutd.edu.sg
- Office @ SUTD (in SUTD Academy/AI cluster): 2.401-26.



A quick word about TAs

Nirmalendu Prakash (TA)

Currently, he is working towards the Ph.D. degree in ISTD at SUTD.
His research focus is analysis and mitigation of social biases in language models.

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Hazel Hee (TA)

SUTD ISTD Alumni 2022 graduate. Currently working as a Research Assistant. Has TA various subjects for ISTD since 2020.

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Objectives of 50.039 DL

- Introduce the technical aspects related to the **implementation of Deep Neural Networks from scratch**.
- Teach the students about the **most popular framework** for implementing Deep Neural Networks (as of Jan 2023): **PyTorch.**
- Discuss the **mathematical foundations and intuitions** behind the Deep Learning framework, layers and some techniques.
- Give the students a **global overview of the advanced techniques** related to Deep Learning and Deep Neural Networks.
- Describe **examples of practical applications** of Deep Learning, showing how some key AIs were implemented using Deep Learning.

Restricted

Objectives of 50.039 DL

- Eventually, **assemble all concepts and tricks of the trade** discussed in this course to produce big architecture models that are close to the current state-of-the-art ones (e.g. ChatGPT, Dall-E, etc.).
- Discuss **ethical aspects** related to some of the concepts discussed.
- Give students **an understanding of the current state of research in the Deep Learning community**, and more specifically **pointers** as to where the most up-to-date information can be found.
- This includes **tracking big names** in the field, identifying **key scientific papers** that have changed the field, but also **newsletters**, **websites** or **magazines** that disclose information in Layman terms.

Skills needed for this course

- **Must-have CS:** Python, Numpy, Matplotlib.
- **Must-have Math:** Linear Algebra, multiple variables calculus, derivatives, optimization probability and statistics.
- **Good-to-have CS:** Machine Learning, Data Processing, Scipy, Sklearn.
- **Good-to-have Math:** Graph Theory, Game theory.

Need to revise? No homeworks for the first few weeks…!

Use this time to revise your 10.014 CTD, 10.013 M&A, 10.018 MS&S, 10.022 MU, 10.020 DDW, and 50.007 ML!
(Look at extra slides for details)

The way we teach things

An expert is not someone who

- Took a 6h-long online course,
- Implements Neural Networks by randomly connecting basic layers (typically Linear and Conv),
- Uses a random framework he/she does not understand (or autoML!),
- Cannot obtain more than 80% accuracy on a simple dataset like MNIST or CIFAR-10.

An expert is someone who

- Understands how Neural Networks operate and the mathematical intuition behind typical (advanced) operations used in layers,
- Understands how the frameworks have been built and what they do behind the scenes,
- Knows AI is a fast-evolving field and knows how to stay up to date when it comes to AI.

The way we teach things

- **One topic per week** (or so) and hopefully, we will cover all the important concepts and important directions of DL these days.
- **Lectures slides**, along with **supporting notebooks**.
- **Mathematical aspects** discussed in class (to show what is happening behind the scenes of Neural Networks/Deep Learning).
- **Made a choice:** providing lots of code to demonstrate concepts, but <u>**need you to play with them autonomously**</u> to explore concepts!
- **Extra reading**, for curiosity (supporting papers, articles, etc.) and suggestions of pointers to follow to stay up to date.
- Suggestions for **continuing your learning**, after this course.

The way we teach things

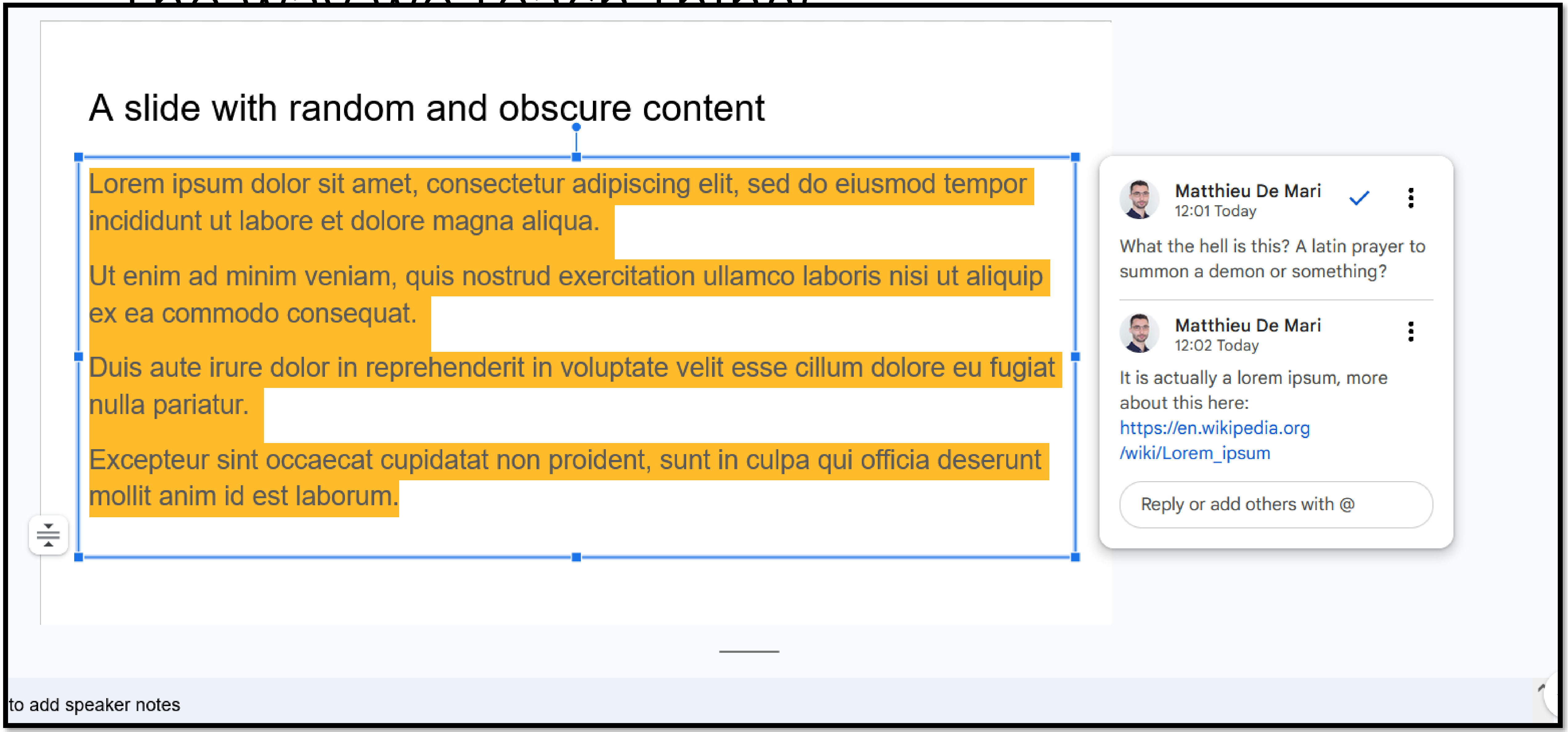
I will upload materials on both **eDimension** and **Google Slides** (everything referenced on eDimension).

- **eDimension slides:** Read-only, reference slides from Prof.

New, this year!

- **Google slides:** shared and can be modified/commented by everyone who has link to slides.
- **Feeling like there is a notion rather obscure?** Comment/ask your questions on the Google Slides and other students/Prof can answer!
- (Will also greatly help me identify parts/materials that need clarifications/improvements for future generations!)

The way we teach things



Syllabus (Detailed syllabus on eDimension)

- **Week 1:** Introduction to course. Some ML jargon reminders, including linear and polynomial regression, generalization, ridge regression and regularization, overfitting/underfitting, logistic regression, neurons objects and how they relate to biology. Building our first shallow neural network in Numpy, gradient descent reminders, training and testing procedure.

- **Week 2:** Introduction to PyTorch framework, tensors and dataloaders. Implementing a shallow neural network in PyTorch, using backpropagation in PyTorch with AutoGrad, advanced optimizers. Multi-label classification with shallow neural networks, moving from shallow to deep neural networks.

Syllabus

- **Week 3:** Guided project and good practices for Deep Learning projects (train/test/dev, bias/variance, advanced regularization, dropout, normalizing inputs/outputs/layers, trainer functions, savers/loader functions for reproducibility and transfer learning). Discussion about the project assessment component.

- **Week 4:** The image data type, image processing techniques and typical computer vision operations, the convolution operation and layers, Convolutional Neural Networks, advanced CNNs and SotA. Preparing transition to the 50.035 Computer Vision course.

Syllabus

- **Week 5:** Continuation of Week 4, and more advanced concepts of Computer Vision. Adversarial machine learning, attacking a Neural Network with basic gradient-based attacks, fundamental limits of Neural Networks, defence mechanisms and state-of-the-art of some advanced attacks techniques.

- **Week 6:** Sequential data (times series, text, etc.), vanilla Recurrent Neural Networks, Gated Recurrent Units, Long-Short Term Memory cells, advanced RNN networks, mixing models for advanced architectures. Recap before MidTerm.

Syllabus

- **Week 8:** The embedding problem, more advanced concepts on RNNs, introduction to Natural Language Processing (NLP) and Word Embeddings for NLP, brief state-of-the-art on NLP, attention and transformers architectures. Preparing transition to the 50.040 Natural Language Processing course.
  MidTerm exam (based on W1-6). One lecture might move to Week 6.

- **Week 9:** Quick introduction to Graph Theory and typical graph datasets and problems, basics of Graph Convolutional Networks, brief state-of-the-art of advanced Graph Convolutional Networks.

Syllabus

- **Week 10:** Generative Models, Autoencoders and Variational Autoencoders, Generative Adversarial Networks (GANs), Advanced concepts on Generative Adversarial Networks, why is it so difficult to train GANs in practice. Basic introduction to diffusion models (more details to be covered in the 50.035 Computer Vision course). If time allows, practice on GANs.

- **Week 11:** Topics for curiosity. Introduction to Physics-Informed Neural Networks. Introduction to deep belief models and diffusion models. Introduction to Explainability/Interpretability and open questions in research about Neural Networks. What will be the next revolution in AI? (a word on ChatGPT, Dall-E, etc.).

Syllabus

- **Week 12:** Brief introduction to reinforcement learning, and state-action-rewards systems, multi-armed bandit problem and the exploration/exploitation trade-off, Q-learning and Deep Q-Learning. Brief state-of-the-art discussion about further works in Reinforcement Learning.

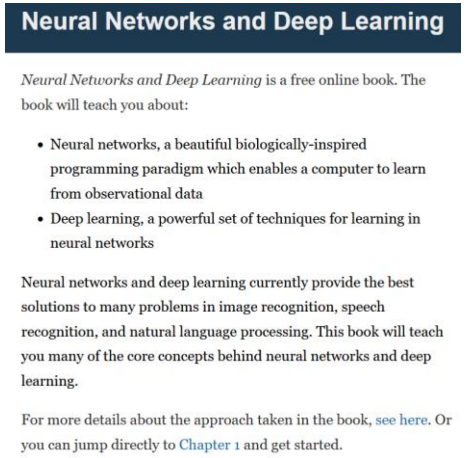
- **Week 13:** Recap. Closing and future directions for studying Deep Learning. Project presentations and guest conferences (TBA).

- **Week 14:** Final exam (probably on content from W1-13).

Supporting Textbooks

Supporting textbooks, for your curiosity (not needed to understand this course).

- Michael A. Nielsen, “Neural networks and deep learning”, 2015. (http://neuralnetworksanddeeplearning.com/)
- Ian Goodfellow, Yoshua Bengio and Aaron Courville, “Deep learning”, 2016. (https://www.deeplearningbook.org/)
- Stevens et al., “Deep Learning with PyTorch”, 2020. (https://www.manning.com/books/deep-learning-with-pytorch)

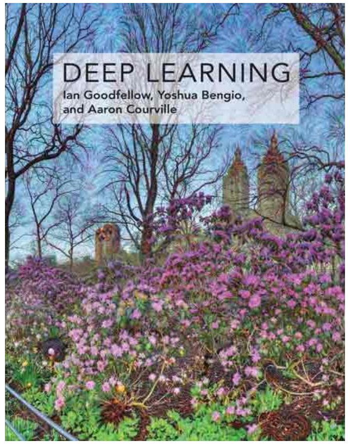

Neural Networks and Deep Learning

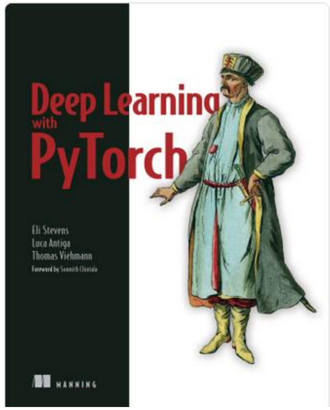
Neural Networks and Deep Learning is a free online book. The book will teach you about:

- Neural networks, a beautiful biologically-inspired programming paradigm which enables a computer to learn from observational data
- Deep learning, a powerful set of techniques for learning in neural networks

Neural networks and deep learning currently provide the best solutions to many problems in image recognition, speech recognition, and natural language processing. This book will teach you many of the core concepts behind neural networks and deep learning.

For more details about the approach taken in the book, see here. Or you can jump directly to Chapter 1 and get started.





Evaluation and grading

- **Homeworks (20%):** Given on Weeks 3, 5, 8, 10 (tentative)
  Usually come in the form of a Jupyter Notebook, containing explanations, code snippets and questions.
  Submissions on eDimension, two weeks later or so, as a small PDF report containing code, figures and answers to questions.
  When time allows, debrief of homeworks in class.

- **MidTerm Exam (20%):** Given on Week 8, March 13th 2024, 2.30pm.
  Theoretical, paper exam, notions of Week 1-6 to be tested.
  More details about venue and exam to be announced closer to the exam date.

Evaluation and grading

- **Final Exam (25%):** Given on Week 14, April 24th 2024, 9am. Theoretical, paper exam, notions of Week 1-13 to be tested. More details about venue and exam to be announced.

- **Project (31%):** Groups of 2-3 students. Submission for project (code, report, presentation) expected on Week 13. More details about the project will be given on Week 3.

- **Participation (2%):** To our discretion.
- **Student Feedback Survey (2%):** As per usual.

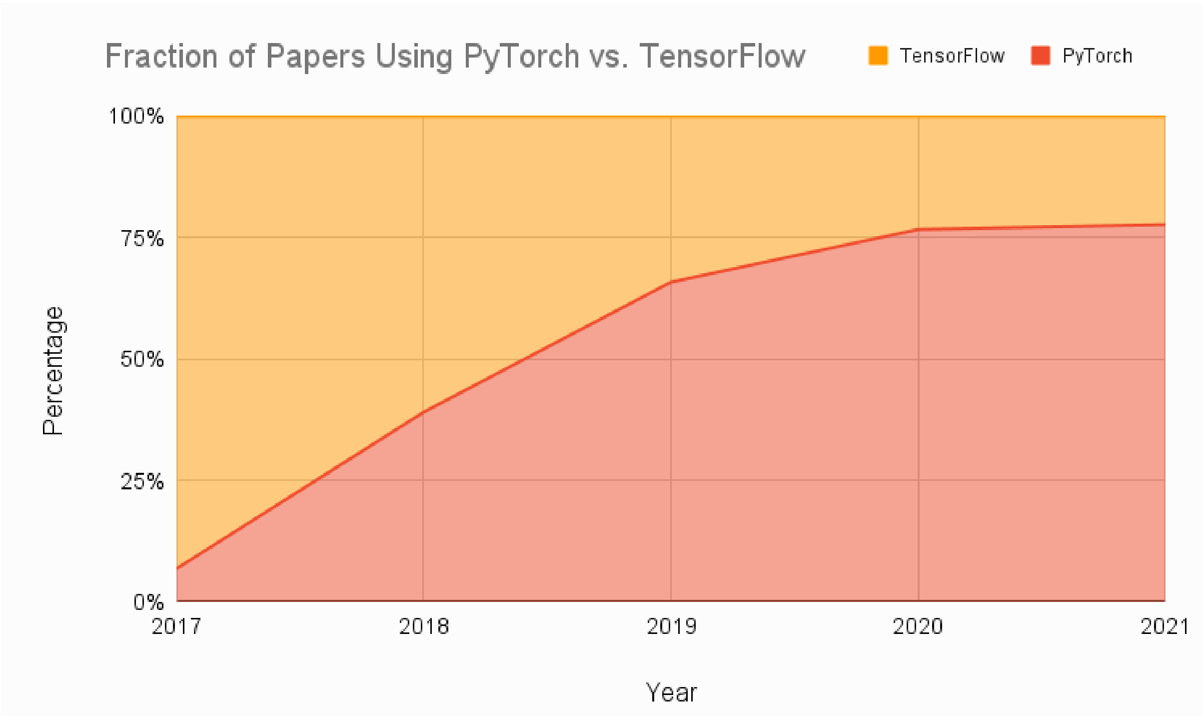
Technical pre-requisites

- Install **Python 3**, if you have not done so already (this course does not cover C++/Java).
- **Libraries needed (maybe more based on projects/homeworks):** numpy, matplotlib, scipy, sklearn, networkx, pillow, gym.
- **Jupyter notebooks** for demos of code, along with the slides.
- In doubt, you can always use **Google Colab** to run the codes.

Technical pre-requisites

- Framework of choice will be **PyTorch!** (not Tensorflow, not Keras, not MXNet, etc.)
- Increasing popularity and preferred to Google's Tensorflow these days for many reasons.
- Learn more, if curious: https://www.assemblyai.com/blog/pytorch-vs-tensorflow-in-2022/

PyTorch



Installing PyTorch and CUDA

- Install PyTorch, by getting the right version from https://pytorch.org/get-started/locally/
- Setting up CUDA/GPU acceleration is always a good idea! (More details in bonus slides).

PyTorch Build	Stable (2.0.1)		Preview (Nightly)	
Your OS	Linux	Mac	Windows	
Package	Conda	Pip	LibTorch	Source
Language	Python		C++ / Java	
Compute Platform	CUDA 11.7	CUDA 11.8	~~ROCm 5.4.2~~	CPU
Run this Command:	`pip3 install torch torchvision torchaudio --index-url https://download.pytorch.org/whl/cu117`			

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W1-S1 Introduction and Machine Learning Reminders

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About this week (Week 1)

1. What are the **typical concepts of Machine Learning** to be used as a starting point for this course?
2. What are the **different families of problems** in Deep Learning?
3. What is the **typical structure of a Deep Learning problem**?
4. What is **linear regression** and how to implement it?
5. What is the **gradient descent algorithm** and how is it used to **train Machine Learning models**?
6. What is **polynomial regression** and how to implement it?
7. What is **regularization** and how to implement it in **Ridge regression**?

About this week (Week 1)

8. What is **overfitting** and why is it bad?
9. What is **underfitting** and why is it bad?
10. What is **generalization** and how to evaluate it?
11. What is a **train-test split** and why is it related to **generalization**?
12. What is a **sigmoid** function? What is a **logistic** function?
13. How to perform **binary classification** using a **logistic regressor** and how is it related to linear regression?

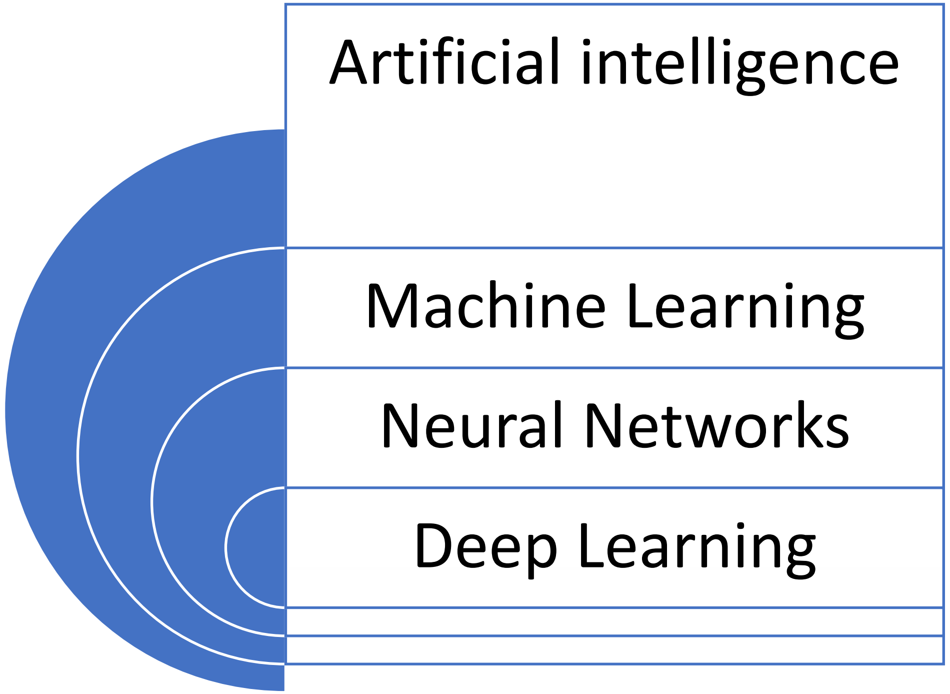
About this week (Week 1)

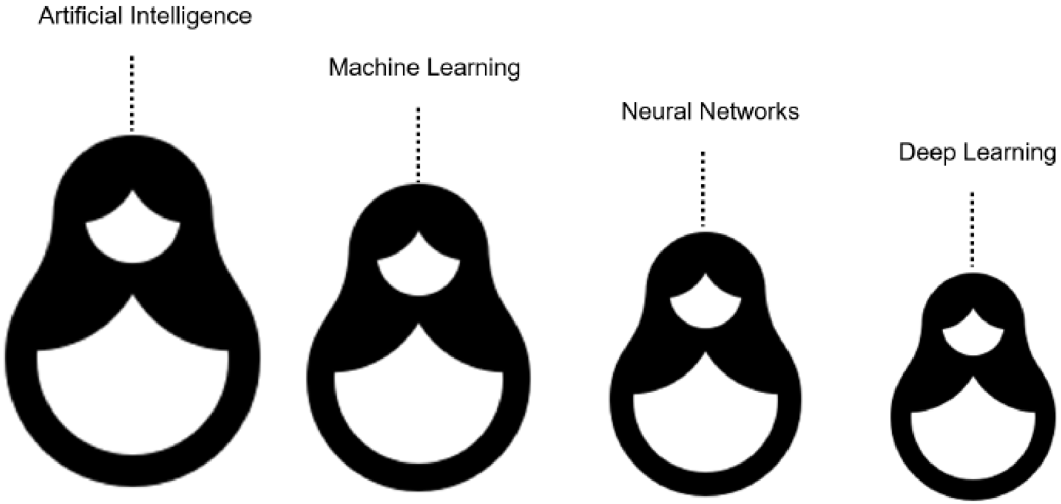
14. What are **Neural Networks** and how do they relate to the **biology of a human brain**?
15. What is a **Neuron** in a Neural Network and how does it relate to linear/logistic regression?
16. What is the **difference** between a **shallow** and a **deep neural network**?
17. How to **implement a shallow Neural Network** manually and define a **forward propagation** method for it?
18. How to **train a shallow Neural Network** using **backpropagation**? How to define **backward propagation** and **trainer** functions?

What is AI/ML/NN/DL?

Definition (Artificial Intelligence):

In Computer Science, **Artificial Intelligence (AI)** refers to the theory and development of computer systems capable to **replicate/emulate the human brain**, more specifically **perform cognitive tasks** that normally require human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages.





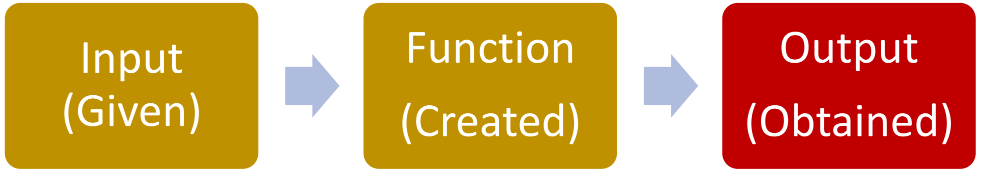
What is AI/ML/NN/DL?

Definition (Machine Learning):

In Computer Science, **Machine Learning (ML)** refers to the field of study that describes **techniques** and **algorithms** that give computers the **ability to learn without being explicitly programmed**.

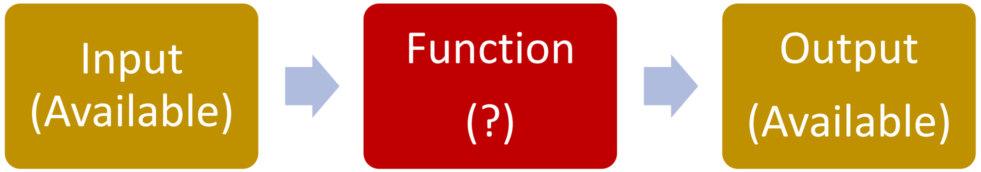
<u>**Some**</u> implementations of machine learning may rely on **data** and **neural networks**.

Conventional programming



VS.

Machine Learning



Restricted

What is AI/ML/NN/DL?

What we have done in programming so far was to design functions,

- which would do **specific operations,**
- and return **outputs,**
- for any **input** we could give it.

Input (Given) → Function (Created) → Output (Obtained)

But sometimes, we can encounter problems where

- we can easily find **inputs** and **expected** outputs,
- but the **function** to be coded is **not simple** to figure out.
- **E.g., what animal in picture?**

Input (Available) → Function (?) → Output (Available)

What is AI/ML/NN/DL?

E.g., what animal is in the picture?

Typical problem in **Computer Vision**, called **Image Recognition**.

Input x (available) → Function f (?) → Output y = f(x) (available)

Very easy for a human…
But, how would we explain the logic of it to a computer?

It's a cat!

What is AI/ML/NN/DL?

Other scenarios have to do with tasks where there is **no easy closed-form expression connecting inputs to outputs.**

- **E.g., what is a good selling price for my appartment?**
- Guessing the selling price of an appartment based on its parameters (size, location, etc.) and previous sales.

S$ 1,680,000 Negotiable

3 🛏 3 🛁 1184 sqft S$ 1,418.92 psf

Details

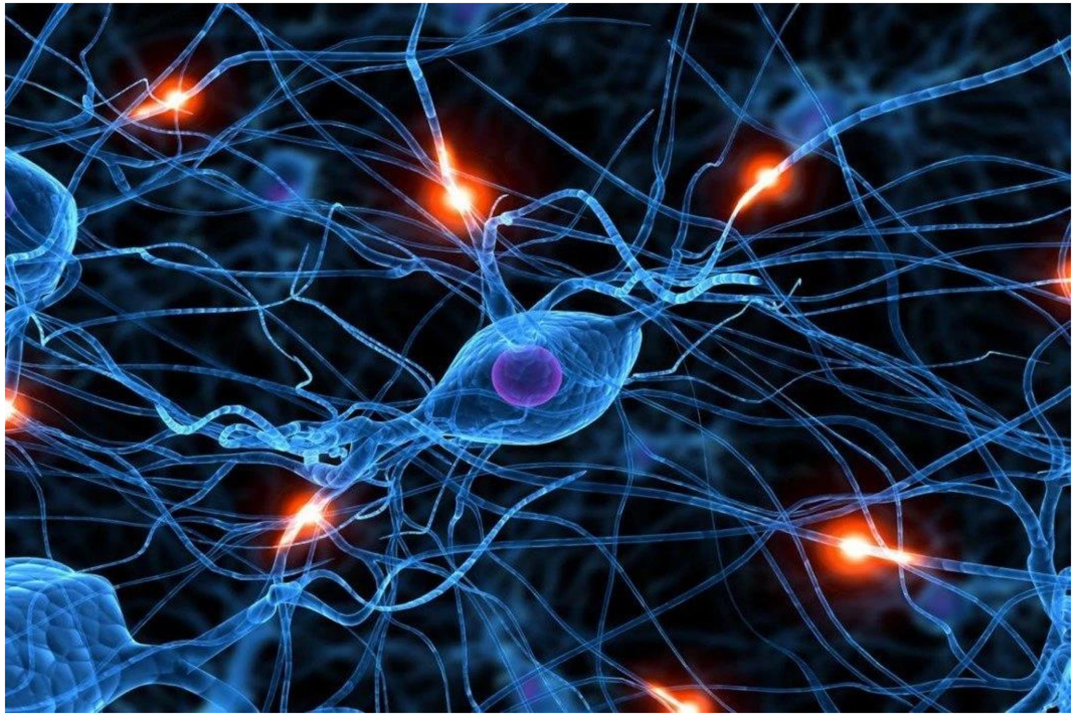
Property Type	Floor Size
Executive Condominium For Sale	1184 sqft
Developer	PSF
Tampines EC Pte Ltd	S$ 1,418.92 psf
Furnishing	Floor Level
Partially Furnished	High Floor
Tenure	TOP
99-year Leasehold	January, 2016

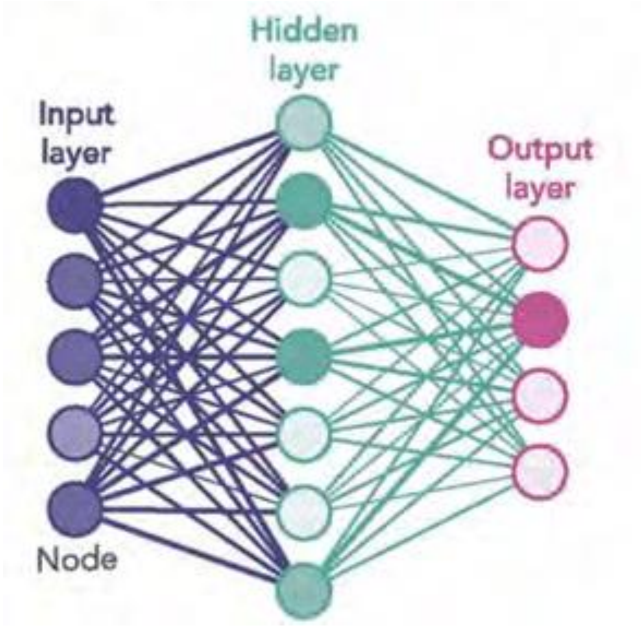
What is AI/ML/NN/DL?

Definition (Neural Networks):

Neural Networks (**NNs**) are computing systems inspired by the biological neural networks that constitute animal brains.

NNs are based on a **collection of connected units (or nodes) called artificial neurons**, which are a (loose) model for the neurons in a biological brain.





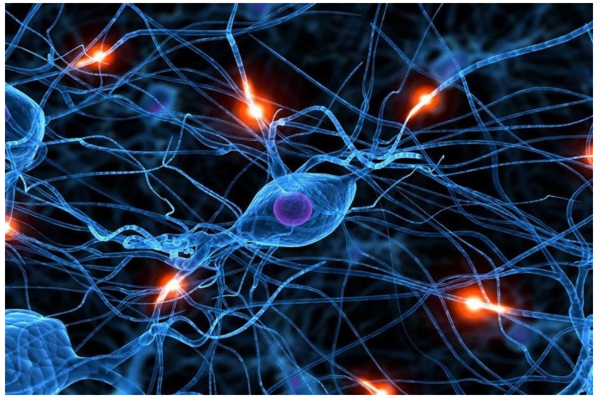
What is AI/ML/NN/DL?

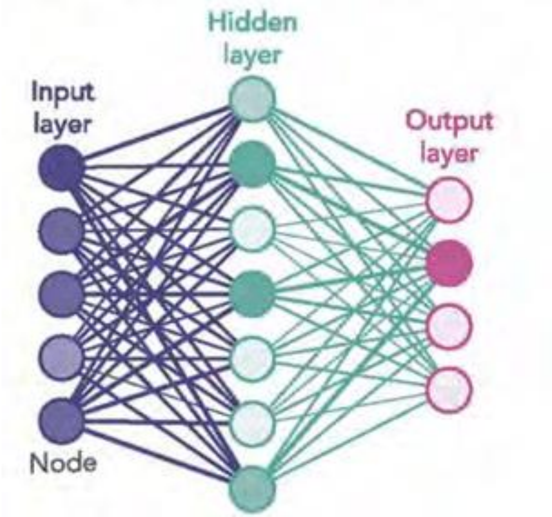
Definition (Neural Networks):

Neural Networks (**NNs**) are computing systems inspired by the biological neural networks that constitute animal brains.

NNs are based on a **collection of connected units (or nodes) called artificial neurons**, which are a (loose) model for the neurons in a biological brain.

Each connection, like the synapses in a biological brain, can transmit a signal to other neurons, therefore **processing any information given as inputs and producing a final signal as output**.



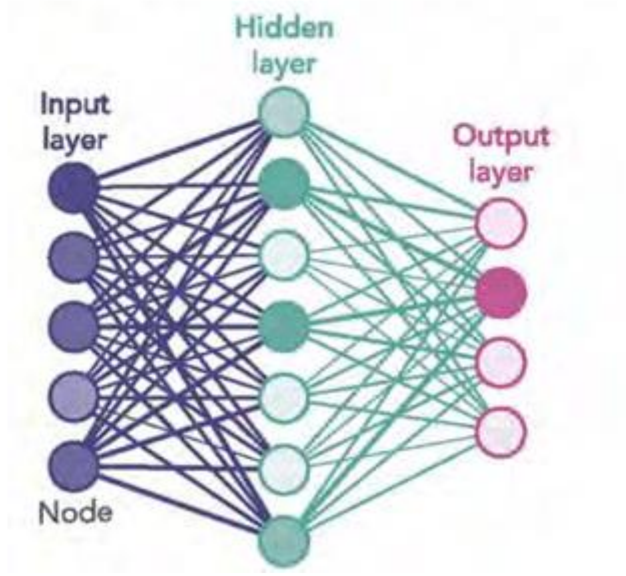


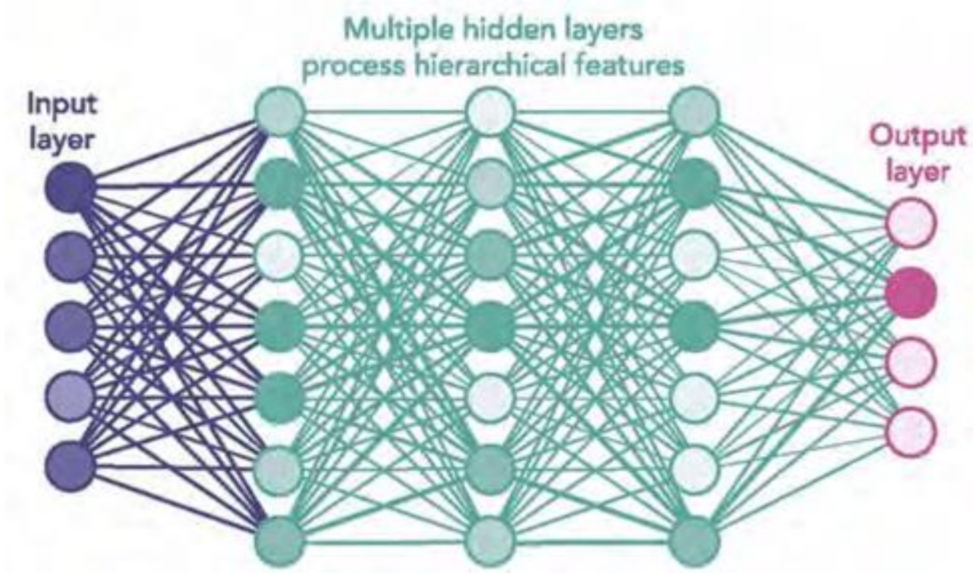
What is AI/ML/NN/DL?

Definition (Deep Learning):

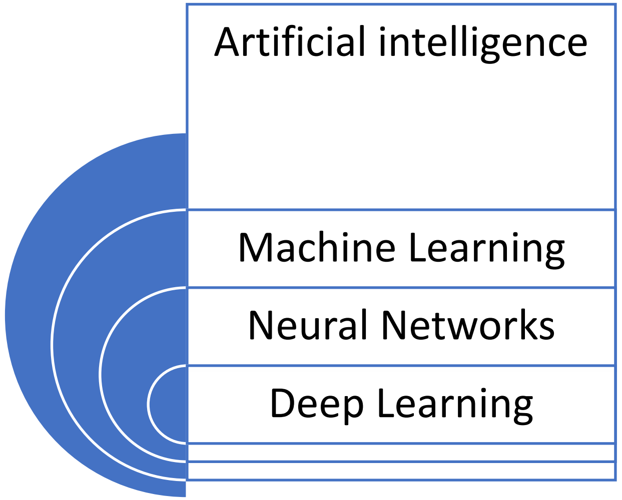
Deep Learning (DL) is a subfield of machine learning, and **deep neural networks** make up the backbone of deep learning algorithms.

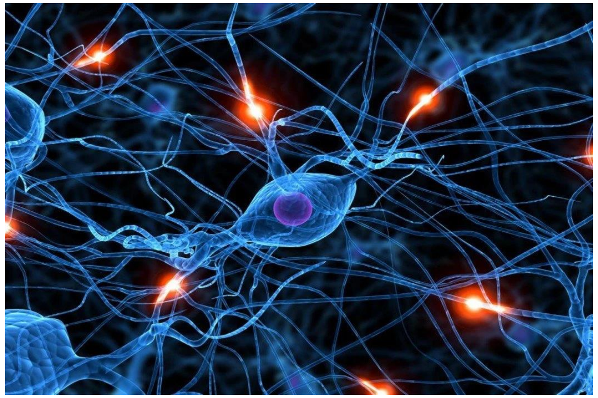
The **number of node layers,** or **depth**, of neural networks is what distinguishes a **shallow neural network** from a **deep neural network**, which must have more than three.

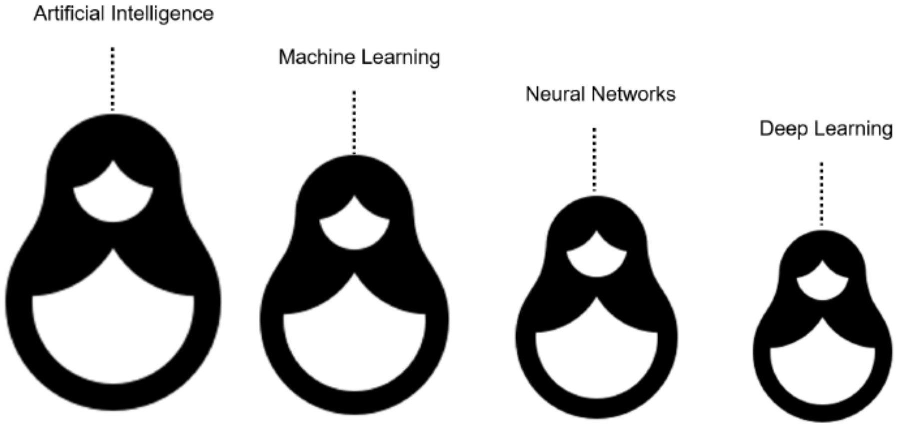


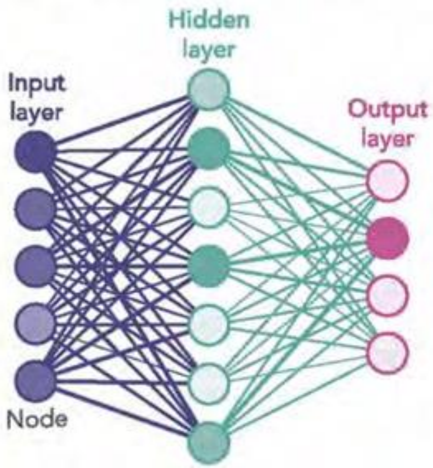


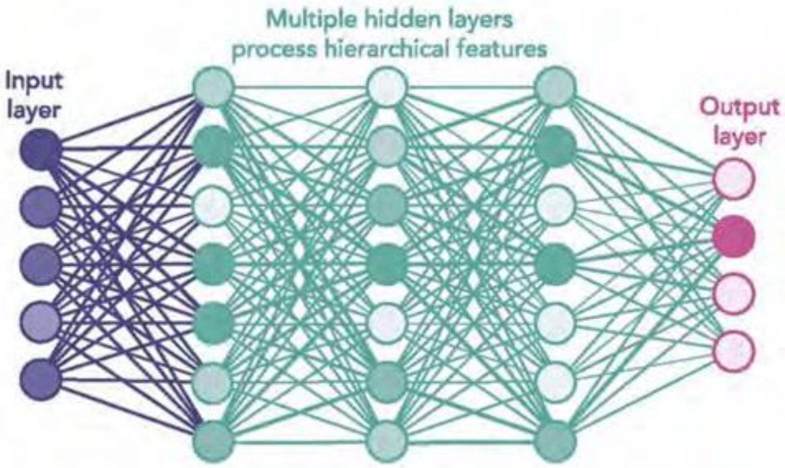
What is AI/ML/NN/DL?











Restricted

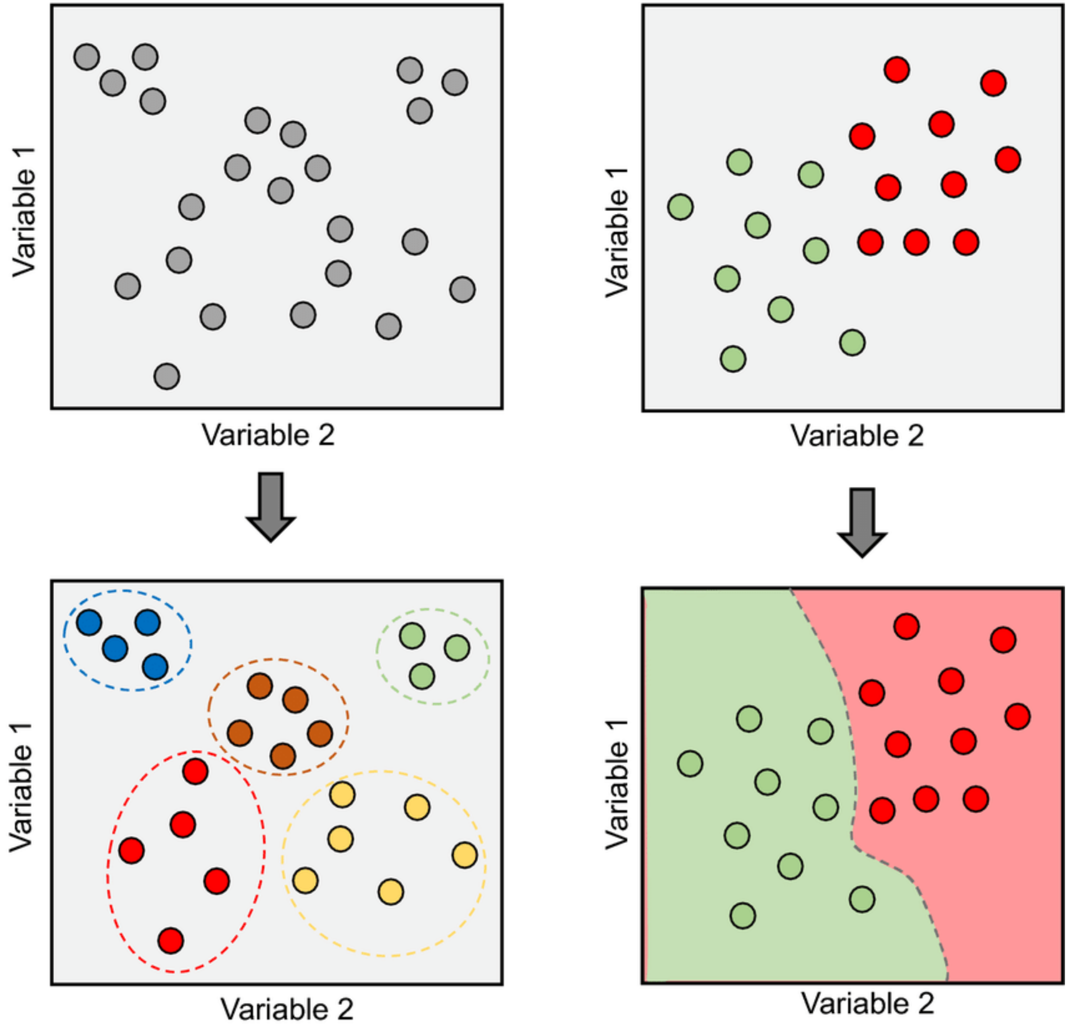
Supervised vs Unsupervised Learning

Definition (Supervised vs. Unsupervised Learning):

Supervised and Unsupervised Learning are the two techniques of ML.

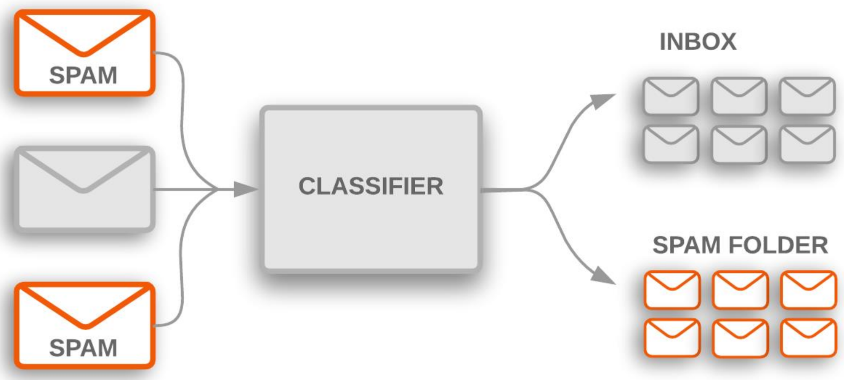
The main difference is **the need for labelled training data**:

- Supervised machine learning relies on labelled input and output data to learn and make predictions,
- while **unsupervised learning does not require labelled data.**



Supervised Learning Examples

- Examples of **supervised learning:** spam detection, text classification, predicting the stock market, etc.



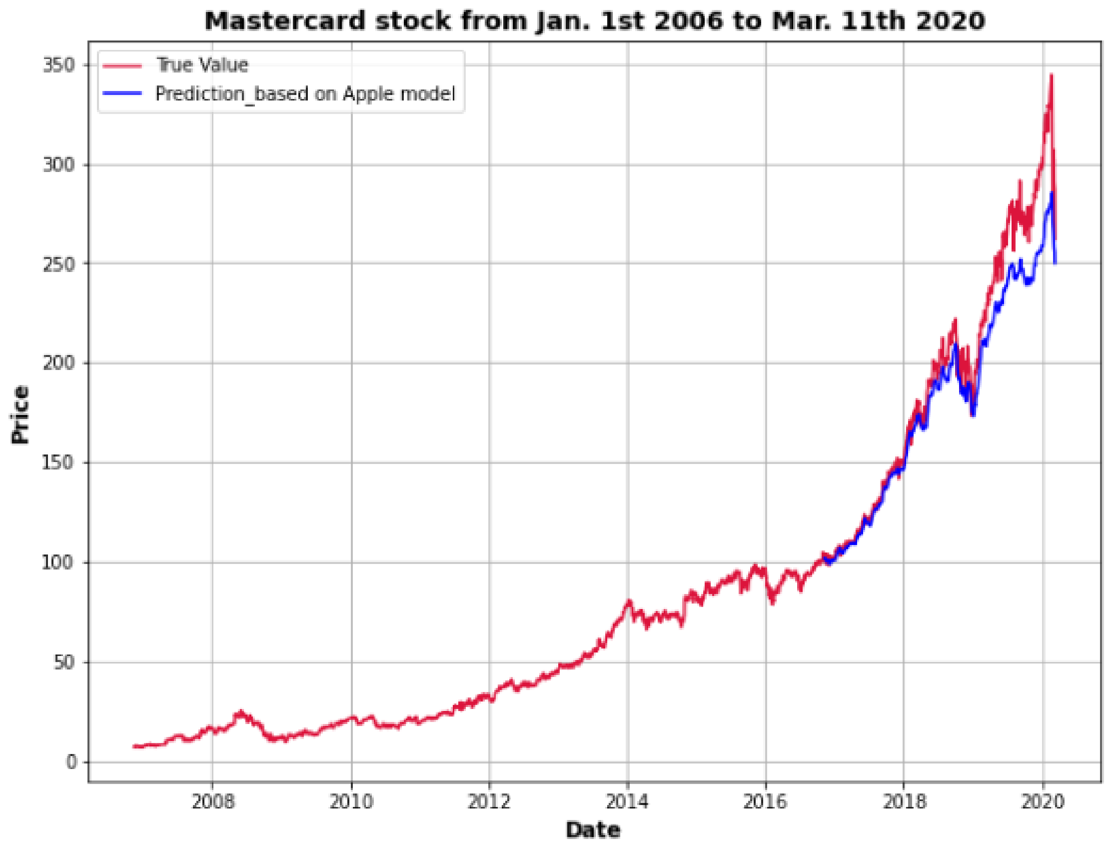


Figure 7. MAST stock price predictions using LSTM trained on AAPL

Regression vs. Classification

Definition (Regression):

Regression models are used to identify the relationships between the input and output variables.

Regression algorithms are used to **predict continuous values** such as price, salary, age, etc.

In regression, the outputs are often **continuous numerical values**.

S$ 1,680,000 Negotiable

3 3 1184 sqft S$ 1,418.92 psf

Details

Property Type Executive Condominium For Sale	Floor Size 1184 sqft
Developer Tampines EC Pte Ltd	PSF S$ 1,418.92 psf
Furnishing Partially Furnished	Floor Level High Floor
Tenure 99-year Leasehold	TOP January, 2016

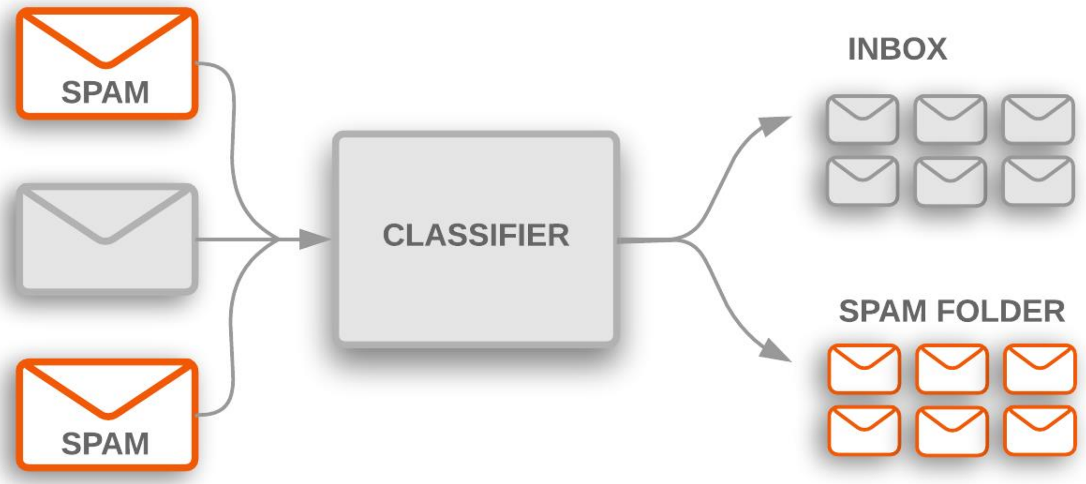
Regression vs. Classification (Supervised)

Definition (Classification):

Classification models are used to divide the samples in the dataset into different **classes**.

Classification algorithms are then used to predict/classify **discrete values**, such as Male or Female, True or False, Spam or Not Spam, etc.

In Classification, the outputs are **discrete** or **categorical values**.



Supervised Learning Examples

Example: predicting the market.

Question: is it a **regression** or a **classification** task?

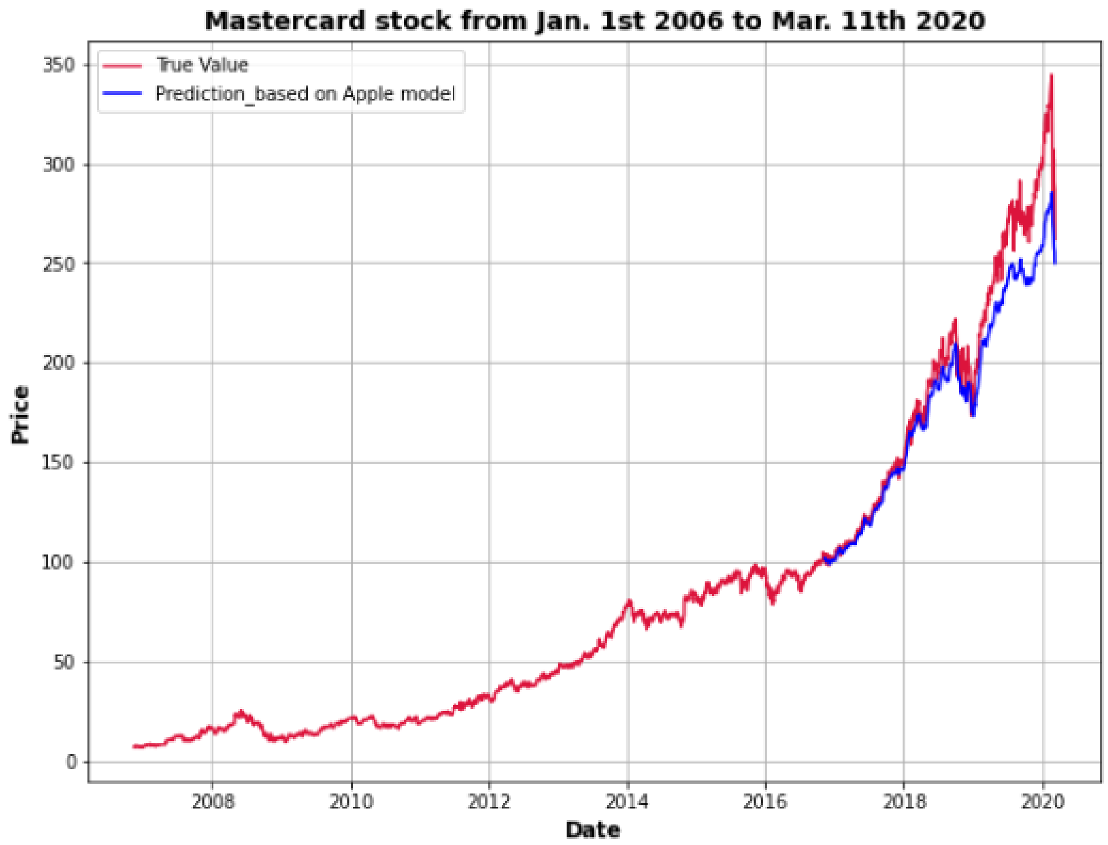


Figure 7. MAST stock price predictions using LSTM trained on AAPL

Supervised Learning Examples

Example: predicting the market.

Question: is it a **regression** or a **classification** task?

Depends.

If the output we are predicting is **the value of the stock in the future**, then probably **regression**.

If the plan is to **predict whether we should buy, sell or hold**, then probably **classification**.

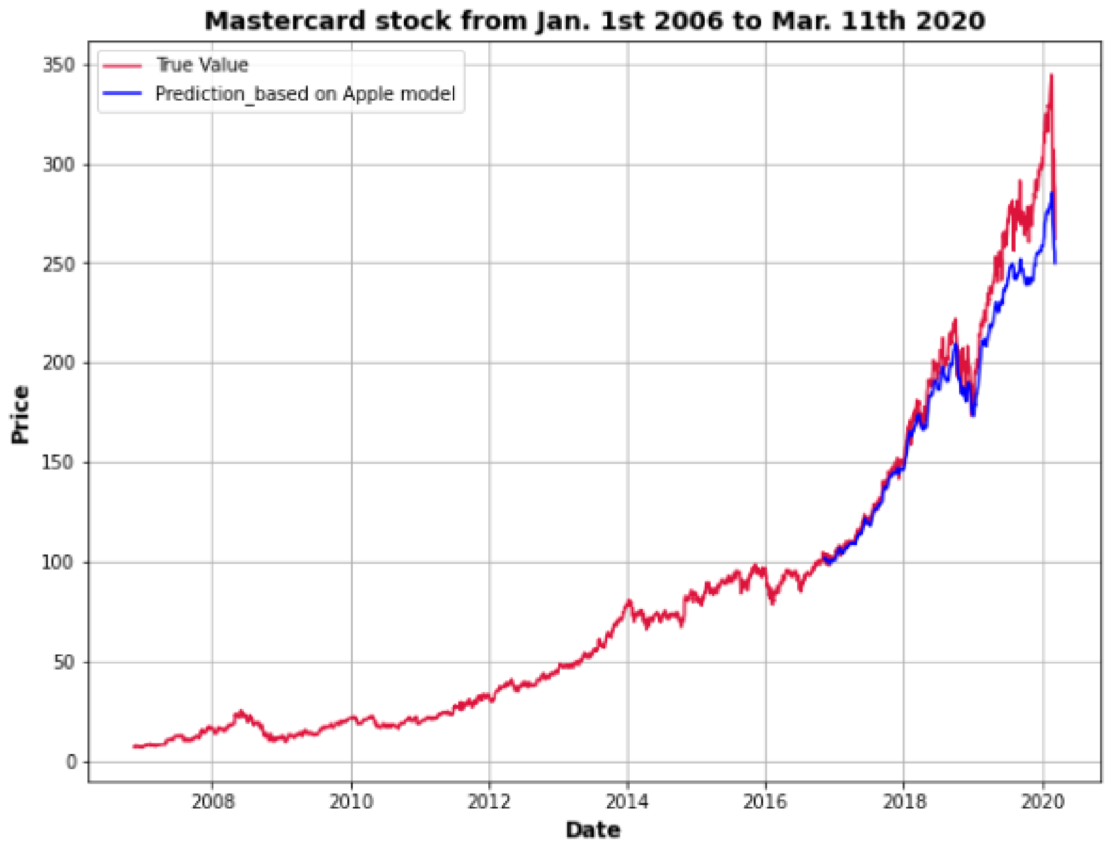


Figure 7. MAST stock price predictions using LSTM trained on AAPL

Deep Learning and Supervised/Unsupervised

While it is possible to use Deep Learning models and Neural Networks to perform both Supervised and Unsupervised tasks…

The vast majority of DL/NN tasks fall in the category of **supervised learning**.

(And we will therefore mostly focus on that)

Elements of a ML problem

Definition (Elements of a ML problem):

Machine learning problems should be well-defined, i.e. the following elements must be clearly identified:

1. **Task (T)** at hand,
2. **Inputs (I)** and **Outputs (O)**,
3. **Model (M)** definition and its **trainable parameters (P)**,
4. **Loss (L)** function to measure the performance of current model on said task and dataset.

S$ 1,680,000 Negotiable

3 bedrooms 3 bathrooms 1184 sqft S$ 1,418.92 psf

Details

Property Type	Floor Size
Executive Condominium For Sale	1184 sqft
Developer	PSF
Tampines EC Pte Ltd	S$ 1,418.92 psf
Furnishing	Floor Level
Partially Furnished	High Floor
Tenure	TOP
99-year Leasehold	January, 2016

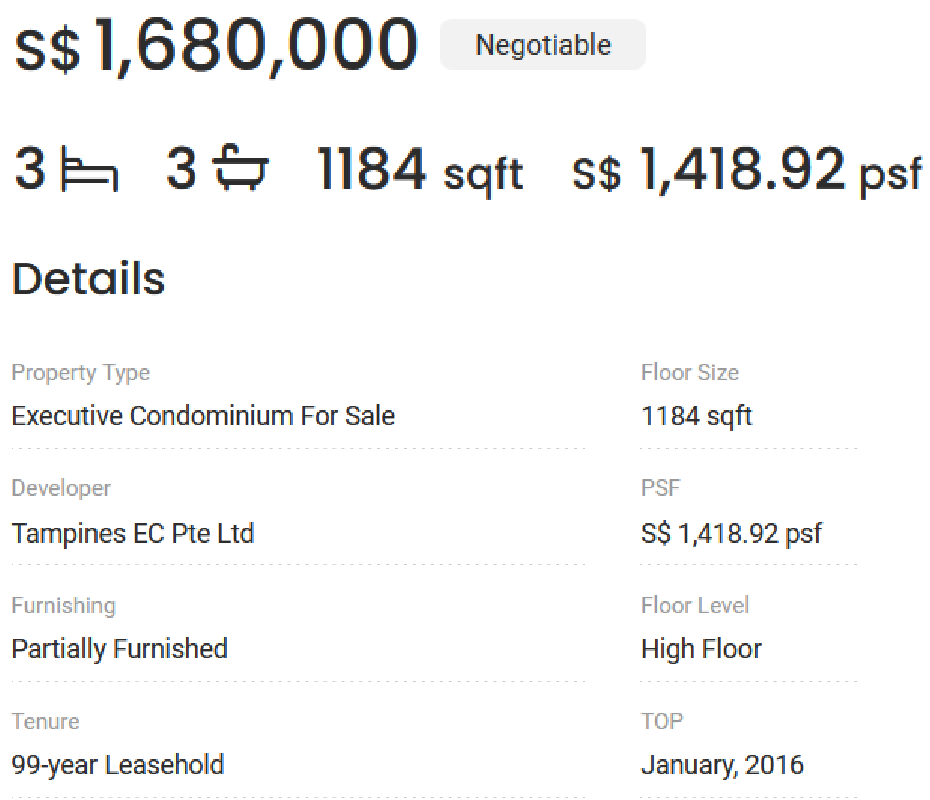
Restricted

Our first toy example

Our first toy example: simplified version of the apartment price prediction.

1. **Task (T)** at hand:

- **Predict price of an apartment based on the apartment features.**
- We will generate a “fake” dataset consisting of apartments with features and selling prices.
- It is a **supervised regression task**.



Our first toy example

Our first toy example: simplified version of the apartment price prediction.

2. Inputs (I) and **Outputs (O):**

- **Inputs** will be a **list of apartment features**, which here will only consist of the **surface of the apartment**, in square meters (sqm).
- **Output** will be the **selling price** in millions of SGD (mSGD).

S$ 1,680,000 Negotiable

3 3 1184 sqft S$ 1,418.92 psf

Details

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Furnishing Partially Furnished	Floor Level High Floor
Tenure 99-year Leasehold	TOP January, 2016

Our first toy example (mock dataset)

Have a look at Week 1, Notebook 1.

We will create a dataset, which uses surfaces as inputs, with values drawn randomly between 40 and 150 sqm.

We will assume that the price is randomly generated, using a uniform distribution, with:

- Average price being 100000 + 14373 times the surface in sqm,
- and a random "variation" of +/- 10% around the average value.

Our first toy example (mock dataset)

```python
# Two random generator functions to generate a mock dataset.
# 1. Surfaces randomly generated as uniform between min_surf and max_surf
def surface(min_surf, max_surf):
    return round(np.random.uniform(min_surf, max_surf), 2)
```

```python
# 2. Price is 100000 + 14373 times the surface in sqm, +/- 10%
# (randomly shifted to give the dataset some diversity).
def price(surface):
    # Note: this will return the price in millions of SGD.
    return round((100000 + 14373*surface)*(1 + np.random.uniform(-0.1, 0.1)))/1000000
```

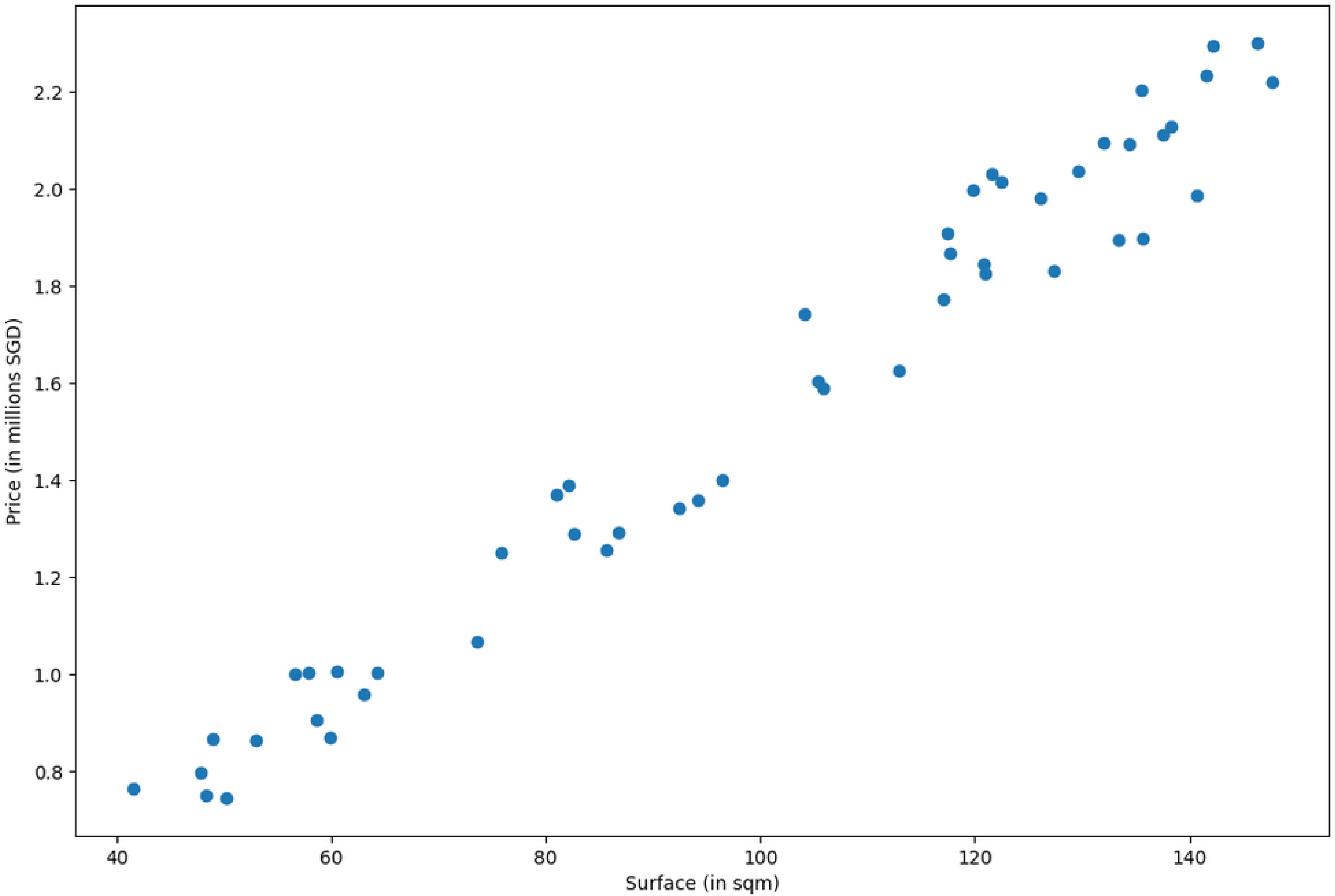
```python
# 3. Generate dataset function
def generate_datasets(n_points, min_surf, max_surf):
    x = np.array([surface(min_surf, max_surf) for _ in range(n_points)])
    y = np.array([price(i) for i in x])
    return x, y
```

Our first toy example (mock dataset)

```python
# 4. Dataset generation (n_points points will be generated).
# Surfaces randomly generated as uniform between 40sqm and 150sqm.
# We will use a seed for reproducibility.
min_surf = 40
max_surf = 150
np.random.seed(27)
n_points = 50
inputs, outputs = generate_datasets(n_points, min_surf, max_surf)
print(inputs)
print(outputs)
```

```
[ 86.83 129.6  120.89 135.48  82.17 147.74 138.25  63.07 121.6  112.95
 137.55 134.38 122.42 135.72  60.54  75.81  81.02 127.31  56.62  58.69
  48.93  73.57 126.16  57.92  47.77 117.12  59.91 105.88  85.68  96.49
  64.27 119.81 133.44 142.18 120.95  92.42  94.22 105.4   48.36  52.92
 146.31 104.17  50.17  41.5  132.06 140.63 117.5   82.57 117.63 141.56]
[1.290893 2.034977 1.84501  2.201767 1.389632 2.218678 2.127228 0.959054
 2.029469 1.623609 2.111638 2.09194  2.012386 1.89553  1.004256 1.250228
 1.368325 1.830127 1.000719 0.906513 0.867629 1.065907 1.979544 1.001403
 0.796199 1.771816 0.867878 1.587176 1.25434  1.40047  1.002361 1.9972
 1.894479 2.293443 1.823577 1.340533 1.358613 1.602167 0.750759 0.863093
 2.30035  1.741468 0.7448   0.763732 2.093772 1.986868 1.90702  1.289541
 1.86578  2.231851]
```

```python
# Display dataset and see that there is a rather clear linear trend.
plt.figure(figsize = (12, 8))
plt.scatter(inputs, outputs)
plt.xlabel("Surface (in sqm)")
plt.ylabel("Price (in millions SGD)")
plt.show()
```



Our first toy example

Our first toy example: simplified version of the apartment price prediction.

3. **Model (M)** definition and its **trainable parameters (P):**

- Here, our model will consist of a **linear regression model**.

S$ 1,680,000 Negotiable

3 3 1184 sqft S$ 1,418.92 psf

Details

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Our first model, the linear regression

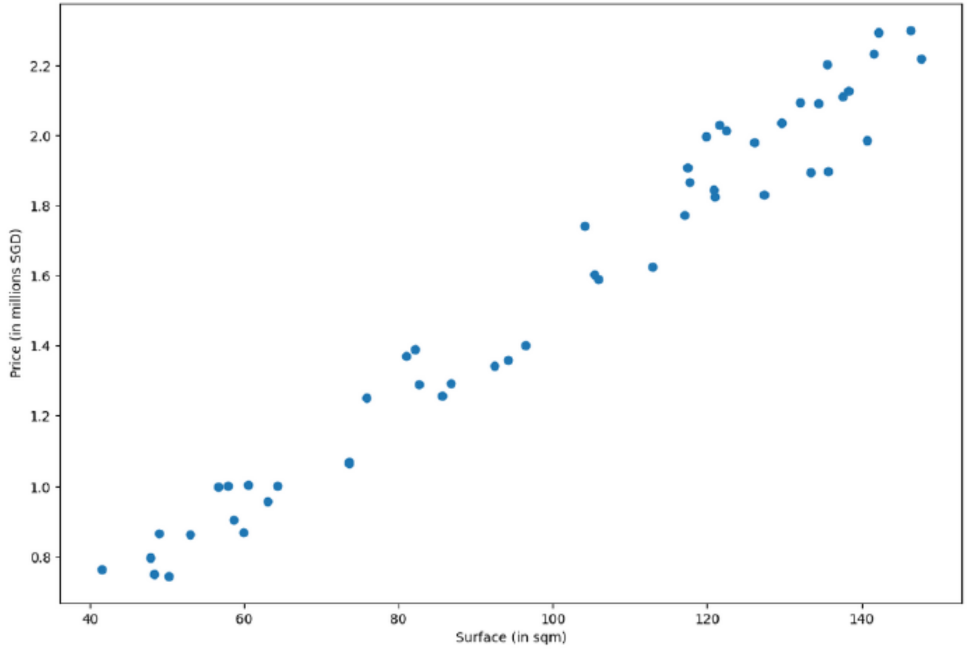
Definition (Linear Regression):

Linear Regression is a model, which **assumes that there is a linear relationship between inputs and outputs.**

It therefore consists of **two trainable parameters** $(\boldsymbol{a}, \boldsymbol{b})$, to be freely chosen.

These will connect any **input** x_i to its respective **output** y_i, with the following equation:

$$y_i \approx \; a\, x_i \; + \; b$$




```python
# Linear regression has two trainable parameters (a and b).
# Other parameters, like min_surf, max_surf, n_points will
# help get points for the upcoming matplotlib displays.
def linreg_matplotlib(a, b, min_surf, max_surf, n_points = 50):
    x = np.linspace(min_surf, max_surf, n_points)
    y = a*x + b
    return x, y
```

Let us try different values of (a, b)

```
# Display dataset
plt.figure(figsize = (12, 8))
plt.scatter(inputs, outputs)
plt.xlabel("Surface (in sqm)")
plt.ylabel("Price (in millions SGD)")

# Add some linreg (model 1)
a1 = 25000/1000000
b1 = 0
linreg_dataset1_inputs, linreg_dataset1_outputs = linreg_matplotlib(a1, b1, min_surf, max_surf, n_points)
plt.plot(linreg_dataset1_inputs, linreg_dataset1_outputs, 'r', label = "Model 1")

# Another linreg (model 2)
a2 = 17000/1000000
b2 = 50000/1000000
linreg_dataset2_inputs, linreg_dataset2_outputs = linreg_matplotlib(a2, b2, min_surf, max_surf, n_points)
plt.plot(linreg_dataset2_inputs, linreg_dataset2_outputs, 'g', label = "Model 2")

# A final linreg (model 3)
a3 = 14500/1000000
b3 = 95000/1000000
linreg_dataset3_inputs, linreg_dataset3_outputs = linreg_matplotlib(a3, b3, min_surf, max_surf, n_points)
plt.plot(linreg_dataset3_inputs, linreg_dataset3_outputs, 'k', label = "Model 3")

# Display
plt.legend(loc = 'best')
plt.show()
```

Model 1 (red)

Model 2 (green)

Model 3 (black)


Model 1
Model 2
Model 3
Which model is the best fit for this task in your opinion? (red, green or black?)
Why is one better than another?
Price (in millions SGD)
Surface (in sqm)
3.5
3.0
2.5
2.0
1.5
1.0
40
60
80
100
120
140

The need for a loss function

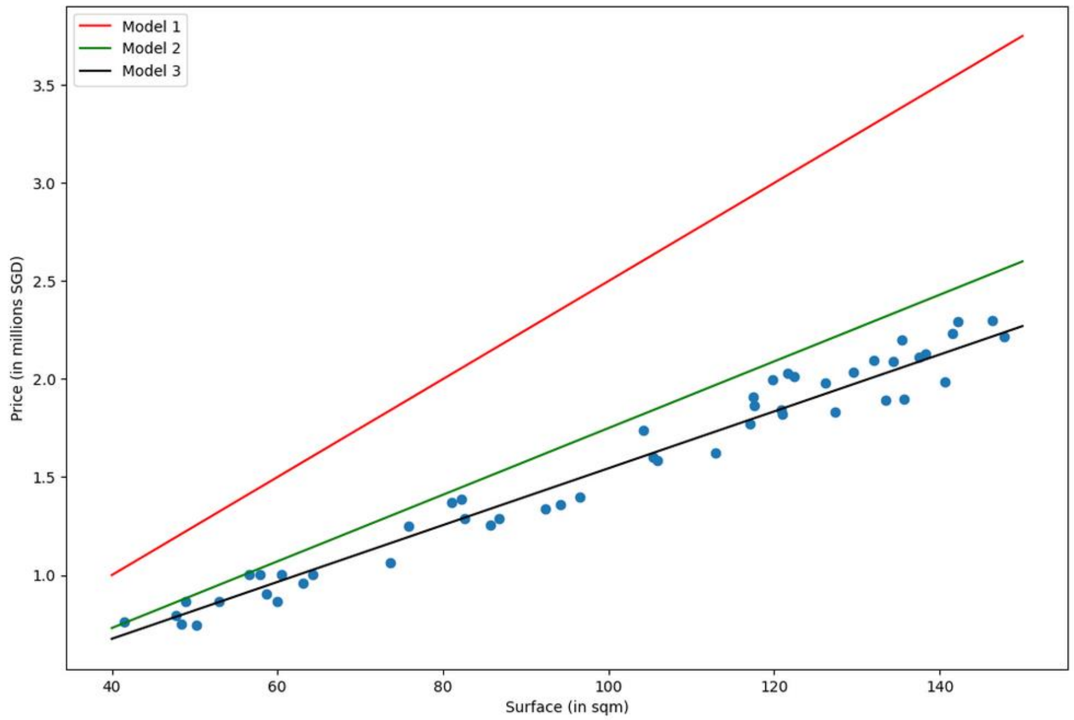
Which model is the best fit for this task in your opinion? (red, green or black?)

Why is one better than another?

Telling which model is best at a given ML task can prove difficult, especially for close values of its trainable parameters, here (a, b).

Good news, there is one last element we have not used.

4. **Loss (L)** function to measure the performance of the current model and its current parameters on said task and dataset.



The need for a loss function

Definition (Loss function):

A **loss function** (also known as a **cost function**) is a mathematical function that measures the difference between the predicted output of a model and the true output we should be matching.

It is used to

- **evaluate the performance of the model,**
- And more specifically **evaluate how good our choice of trainable parameters** (here, the parameters are a and b) are at fitting the data.

It is used to guide the optimization process during **training**.

The need for a loss function

Definition (The Mean Square Error loss function):

In our linear model, a good loss function we could use consists of the **Mean Square Error (MSE) loss function**.

The MSE is calculated by calculating the square difference between:

- The **prediction** $\boldsymbol{p_i(x_i, a, b) = ax_i + b}$ formed by the model for some given inputs x_i,
- The **true value** $\boldsymbol{y_i}$ that we should be matching.

We then repeat this operation for every sample i, and average those errors together, i.e.

$$L(a, b, x, y) = \frac{1}{N}\sum_{i=1}^{N}(p(x_i, a, b) - y_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(ax_i + b - y_i)^2$$

The need for a loss function

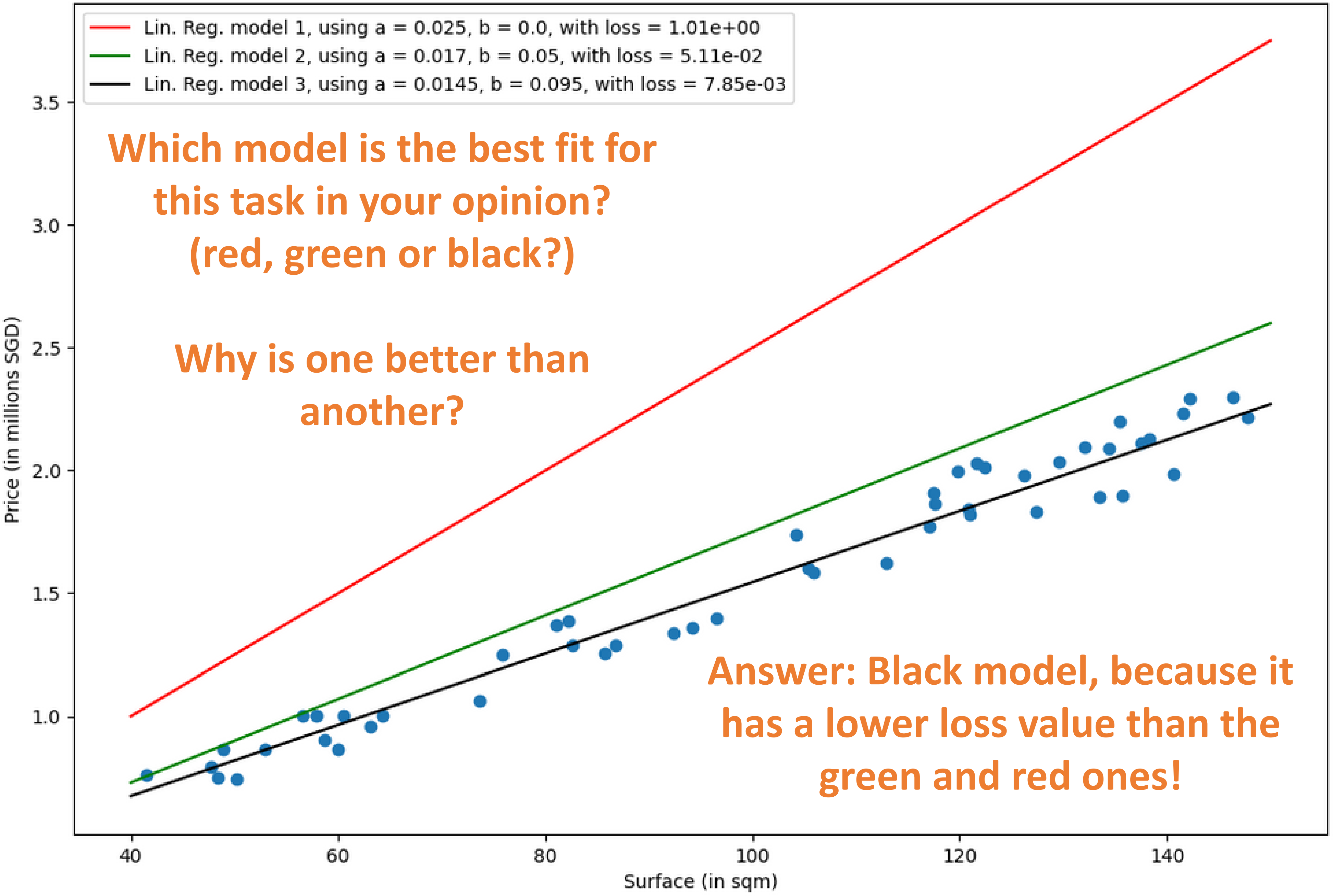
Recall the definition of the MSE loss function

$$L(a, b, x, y) = \frac{1}{N}\sum_{i=1}^{N}(ax_i + b - y_i)^2$$

In [9]:
```
# Mean square error as a loss function
# Displaying Loss using exponential notation (XXXe-YYY)
def loss_mse(a, b, x, y):
    val =  np.sum((y - (a*x + b))**2)/x.shape[0]
    return '{:.2e}'.format(val)
```

In [10]:
```
# The lower the loss function, the better the linear regression values (a, b) fit the dataset.
loss1 = loss_mse(a1, b1, inputs, outputs)
loss2 = loss_mse(a2, b2, inputs, outputs)
loss3 = loss_mse(a3, b3, inputs, outputs)
print(loss1, loss2, loss3)
```

```
1.01e+00 5.11e-02 7.85e-03
```



Which model is the best fit for this task in your opinion? (red, green or black?)

Why is one better than another?

Answer: Black model, because it has a lower loss value than the green and red ones!

Training a model

Definition (Training a model):

Training a model consists of **finding the best values for the trainable parameters of the chosen model**, for the given task and dataset.

By best values for the trainable parameters, we mean the values that **minimize the chosen loss function**. It is therefore an optimization problem of some sort!

Once a minimal value is obtained on the loss function, then we can claim that the "optimal" trainable parameters have been found.

Or in other words, that the model has been trained.

Training a linear regression model

In the case of linear regression, training the model consists of solving the following optimization problem.

$$(a^*, b^*) = \underset{a,b}{\operatorname{argmin}} \, [L(a, b, x, y)]$$

That is, using the explicit formula of the loss function,

$$(a^*, b^*) = \underset{a,b}{\operatorname{argmin}} \left[\frac{1}{N} \sum_{i=1}^{N} (a x_i + b - y_i)^2 \right]$$

Training a linear regression model

Definition (The normal equation for linear regression):

Solving this optimization problem can be done analytically, as it can be proven that the optimal choice of parameters $W^* = \begin{pmatrix} b^* \\ a^* \end{pmatrix}$ follows the **normal equation**, below.

$$W^* = (X^T X)^{-1} X^T Y$$

(Proof in bonus slides)

With

$$X = \begin{pmatrix} 1 & x_1 \\ \dots & \dots \\ 1 & x_N \end{pmatrix}$$

And

$$Y = \begin{pmatrix} y_1 \\ \dots \\ y_N \end{pmatrix}$$

Finally, X^T denotes the transposed matrix of X and $(X)^{-1}$ its inverse.

Training a linear regression model

Normal Equation: $W^* = (X^T X)^{-1} X^T Y$

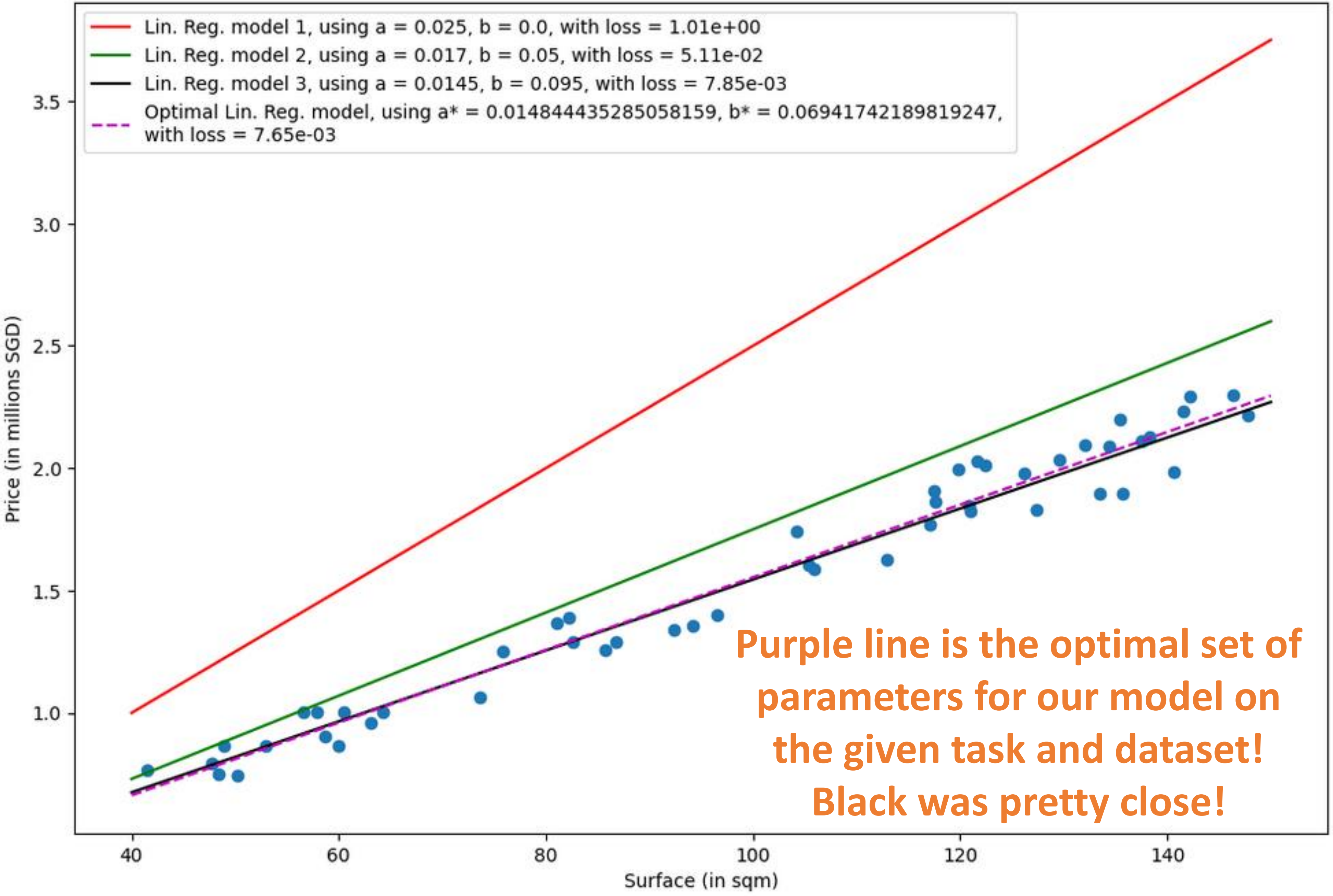
```
# Defining the X matrix, following the notation above, as a numpy array.
X = np.array([[1, x_i] for x_i in inputs])
print(X)
```

```
# While we are at it, let us define the transposed version of X.
XT = np.transpose(X)
print(XT)
```

```
# Defining the Y matrix, following the notation above, as a numpy array.
Y = np.array([[y_i] for y_i in outputs])
print(Y)
```

```
# Defining W_star according to our formula.
W_star = np.matmul(np.linalg.inv(np.matmul(XT,X)), np.matmul(XT,Y))
print(W_star)
# Extracting a_star and b_star values from W_star.
b_star, a_star = W_star[0, 0], W_star[1, 0]
print("Optimal a_star value: ", a_star)
print("The value we used for a in the mock dataset generation: ", 14373/1000000)
print("Optimal b_star value: ", b_star)
print("The value we used for b in the mock dataset generation: ", 100000/1000000)
```

Restricted



Purple line is the optimal set of parameters for our model on the given task and dataset! Black was pretty close!

Restricted

The problem with the normal equation

The normal equation $W^* = (X^T X)^{-1} X^T Y$ immediately gives the optimal set of parameters (a^*, b^*) to use for linear regression.

A few problems when using the normal equation:

- It can become **computationally expensive when the number of samples (or features) in X is large**.
- It might even be **impossible to use when the matrix product of feature variables $\left(X^T X\right)^{-1}$ cannot be calculated ($X^T X$ might not always be invertible)**.

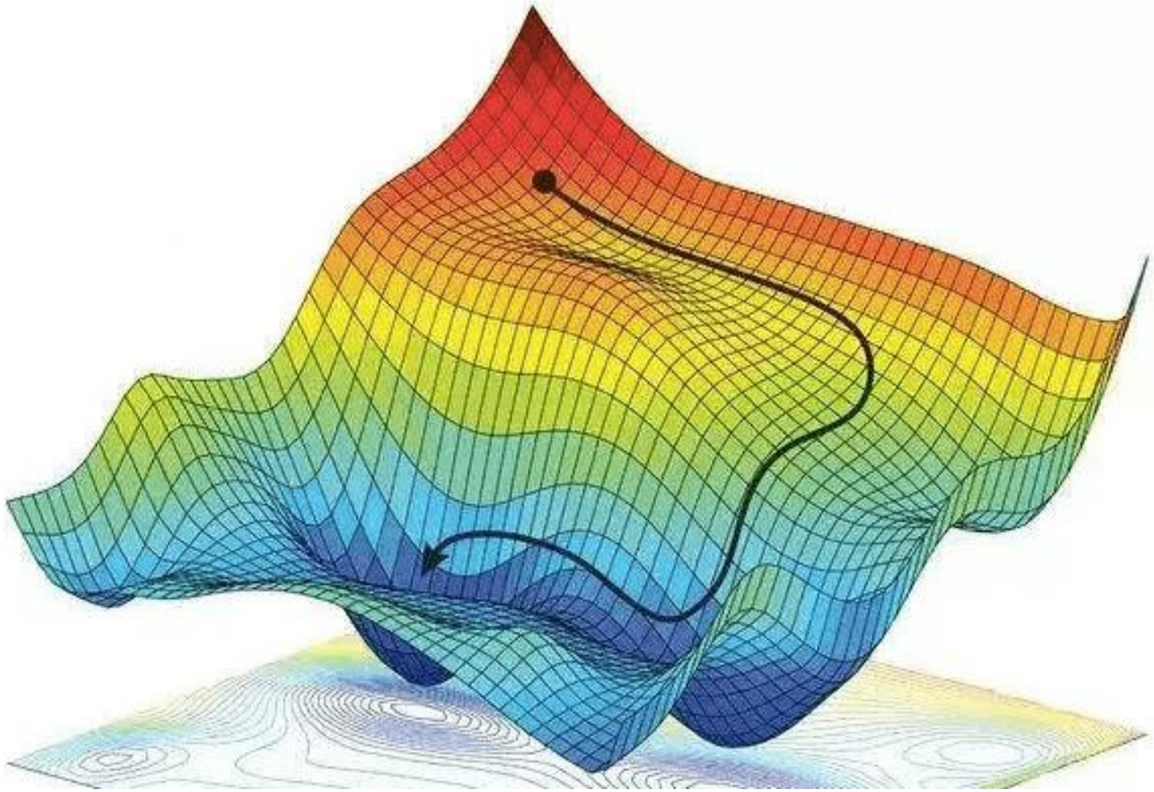
Another problem: More sophisticated models than linear regression will NOT have a normal equation, anyway.

Gradient Descent, to the rescue!

Definition (Gradient Descent):

Gradient Descent (GD) is an iterative algorithm used to solve optimization problems.

- It starts with an initial non-optimal set of parameters for our model.
- It then repeatedly updates the parameters in the direction of the negative gradient of the given cost function, until it converges to a local minimum.



Forgot about GD?
Have a look at your notes from 10.013 M&A!

Gradient Descent, to the rescue!

Definition (Gradient Descent):

Gradient Descent (GD) is an iterative algorithm used to solve optimization problems.

- It starts with an initial non-optimal set of parameters for our model.
- It then repeatedly updates the parameters in the direction of the negative gradient of the given cost function, until it converges to a local minimum.

- The normal equation has many problems…
- But GD, on the other hand can be used to find the optimal solution even when the normal equation is not applicable.
- While sub-optimal, the main advantage of gradient descent is that it can handle very large datasets and it can also be used for non-linear models.

GD in Linear Regression

In the case of Linear Regression, with the MSE loss defined earlier, we have

$$(a^*, b^*) = \underset{a,b}{\operatorname{argmin}} \left[L(a, b, x, y) = \frac{1}{N} \sum_{i=1}^{N} (ax_i + b - y_i)^2 \right]$$

GD in Linear Regression

We can calculate (by hand) the derivatives, with respect to a and b:

$$D_a = \frac{\partial L}{\partial a} = \frac{-2}{N} \sum_{i=1}^{N} x_i \left(y_i - (a\, x_i + b) \right)$$

$$D_b = \frac{\partial L}{\partial b} = \frac{-2}{N} \sum_{i}^{N} y_i - (a\, x_i + b)$$

Restricted

GD in Linear Regression

The gradient descent **update rules** are therefore defined as

$$a \leftarrow a \ - \alpha D_a$$

$$a \leftarrow a + \frac{2\alpha}{N} \sum_{i=1}^{N} x_i \left(y_i \ - \ (a\, x_i \ + \ b)\right)$$

And

$$b \leftarrow b \ - \alpha D_b$$

$$b \leftarrow b + \frac{2\alpha}{N} \sum_{i}^{N} y_i \ - \ (a\, x_i \ + \ b)$$

We call parameter α the **learning rate** for the gradient descent, and this parameter value will have to be decided manually, later.

GD in Linear Regression

Gradient Descent Linear Regression procedure:

- We initialize a and b with some initial values (could be zero, random values, or something else).
- For a given number of iterations, we will apply the two update rules defined earlier.
- (Optionally, we might decide to stop iterating, if we realize that the values of a and b are no longer changing.
  This is called **early stopping**, and is typically implemented by tracking the changes on each iteration.
  We would then decide to break the GD loop if the changes on a and b are less than a threshold δ.)

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradient descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # COmpute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Initialize a and b as you please.

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradient descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # COmpute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Number of samples in dataset.

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradient descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # COmpute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Two possible stopping conditions, change < delta or counter > max_count.

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradient descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # COmpute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Update using our GD update rules from earlier.

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradient descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # Compute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Compute change on this iteration (to decide on early stopping if changes become insignificant).

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradident descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # COmpute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Calculate new MSE value using the new parameters of a and b. We also keep track of these losses by adding them to a list, used for display later.

```python
def gradient_descent_linreg(a_0, b_0, x, y, alpha = 1e-5, delta = 1e-5, max_count = 1000):
    # Define the initial values of a and b as a_0 and b_0
    a, b = a_0, b_0
    # Define N as the number of elements in the dataset
    N = len(x)
    # Keep track of how much a and b changed on each iteration
    change = float("Inf")
    # Counter as safety to prevent infinite looping
    counter = 0
    # List of losses, to be used for display later
    losses = []
    while change > delta:
        # Helper to visualize iterations of while loop
        print("-----")
        # Use gradident descent update rules for a and b
        D_a = -2/N*(sum([x_i*(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        D_b = -2/N*(sum([(y_i - (a*x_i + b)) for x_i, y_i in zip(x, y)]))
        a = a - alpha*D_a
        b = b - alpha*D_b
        print("Gradients: ", D_a, D_b)
        print("New values for (a, b): ", a, b)
        # Compute change
        change = max(abs(alpha*D_a), abs(alpha*D_b))
        print("Change: ", change)
        # COmpute and display current loss
        loss = loss_mse(a, b, x, y)
        losses.append(float(loss))
        print("Loss: ", loss)
        # Counter update, will break if iterations number exceeds max_count,
        # to prevent gradient descent from going indefinitely.
        # (Just a safety measure, for good practice, we would definitely prefer to see
        # the while loop break "naturally", because change eventually fell under the threshold stop.)
        counter += 1
        if(counter > max_count):
            print("Maximal number of iterations reached.")
            break
    return a, b, losses
```

Return trained parameters and losses evolution on each iteration.

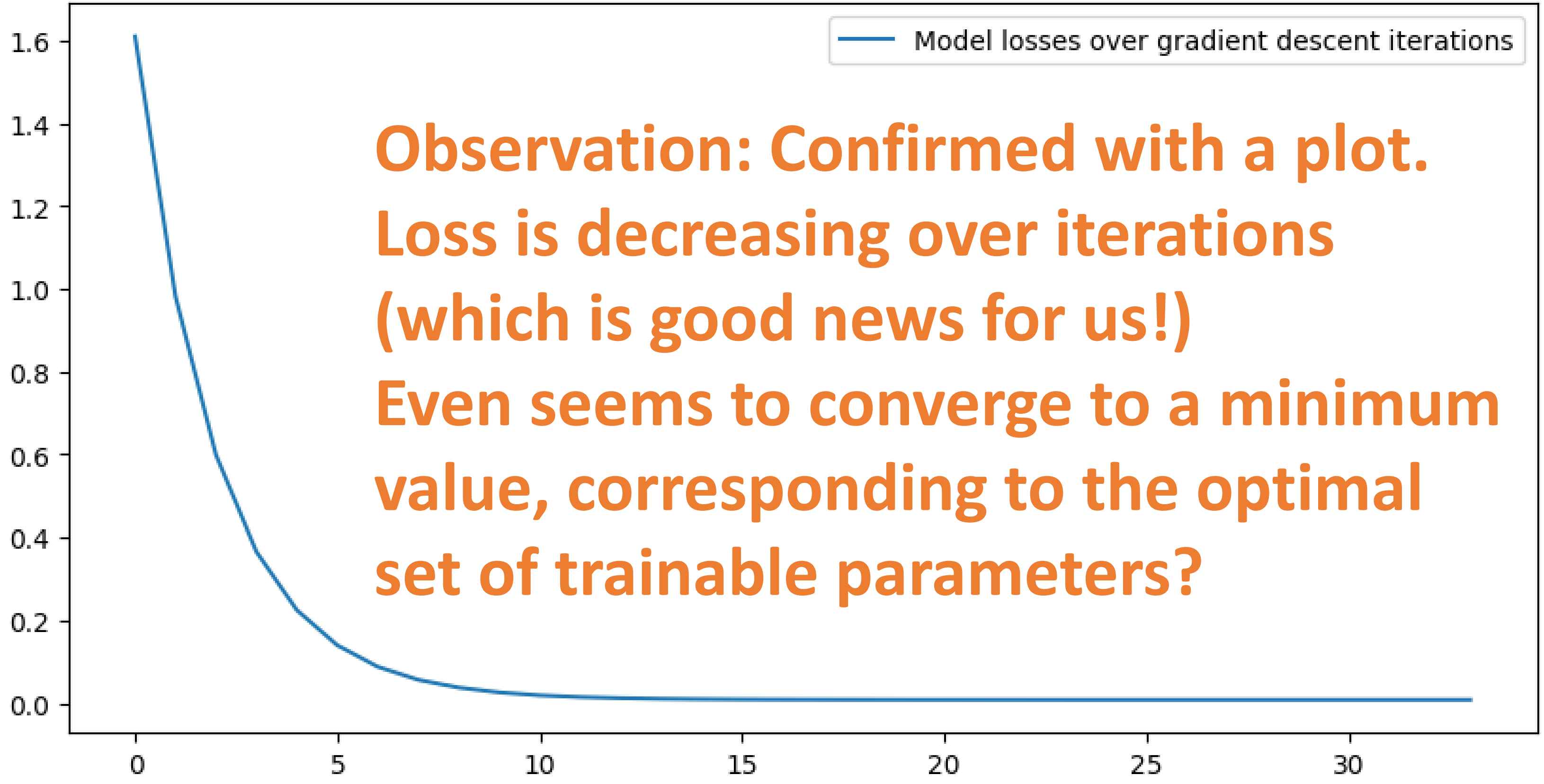
```
a_gd, b_gd, losses = gradient_descent_linreg(a_0 = 0, b_0 = 0, x = inputs, y = outputs, alpha = 1e-5, delta = 1e-6)
```

```
-----
Gradients:  -342.3996226384001 3.105429920000001
New values for (a, b):  0.003423996226384013 -3.105429920000001e-05
Change:  0.003423996226384013
Loss:  1.61e+00
-----
Gradients:  -266.62829357559235 2.4212214483389536
New values for (a, b):  0.006090279162139925 -5.526651368338955e-05
Change:  0.002666282935755923 6
Loss:  9.82e-01
-----
Gradients:  -207.62478780001163 1.8884249597020164
New values for (a, b):  0.008166527040140042 -7.415076328040972e-05
Change:  0.0020762478780001164
Loss:  5.99e-01
-----
Gradients:  -161.6784683033283 1.4735337252735503
New values for (a, b):  0.009783311723173324 -8.888610053314522e-05
Change:  0.0016167846830332 83
```

Observation: Loss is decreasing over iterations (which is good news for us!)

```python
# Display dataset
plt.figure(figsize = (10, 5))
plt.plot(losses, label = "Model losses over gradient descent iterations")

# Display
plt.legend(loc = 'best')
plt.show()
```



Observation: Confirmed with a plot.
Loss is decreasing over iterations (which is good news for us!)
Even seems to converge to a minimum value, corresponding to the optimal set of trainable parameters?

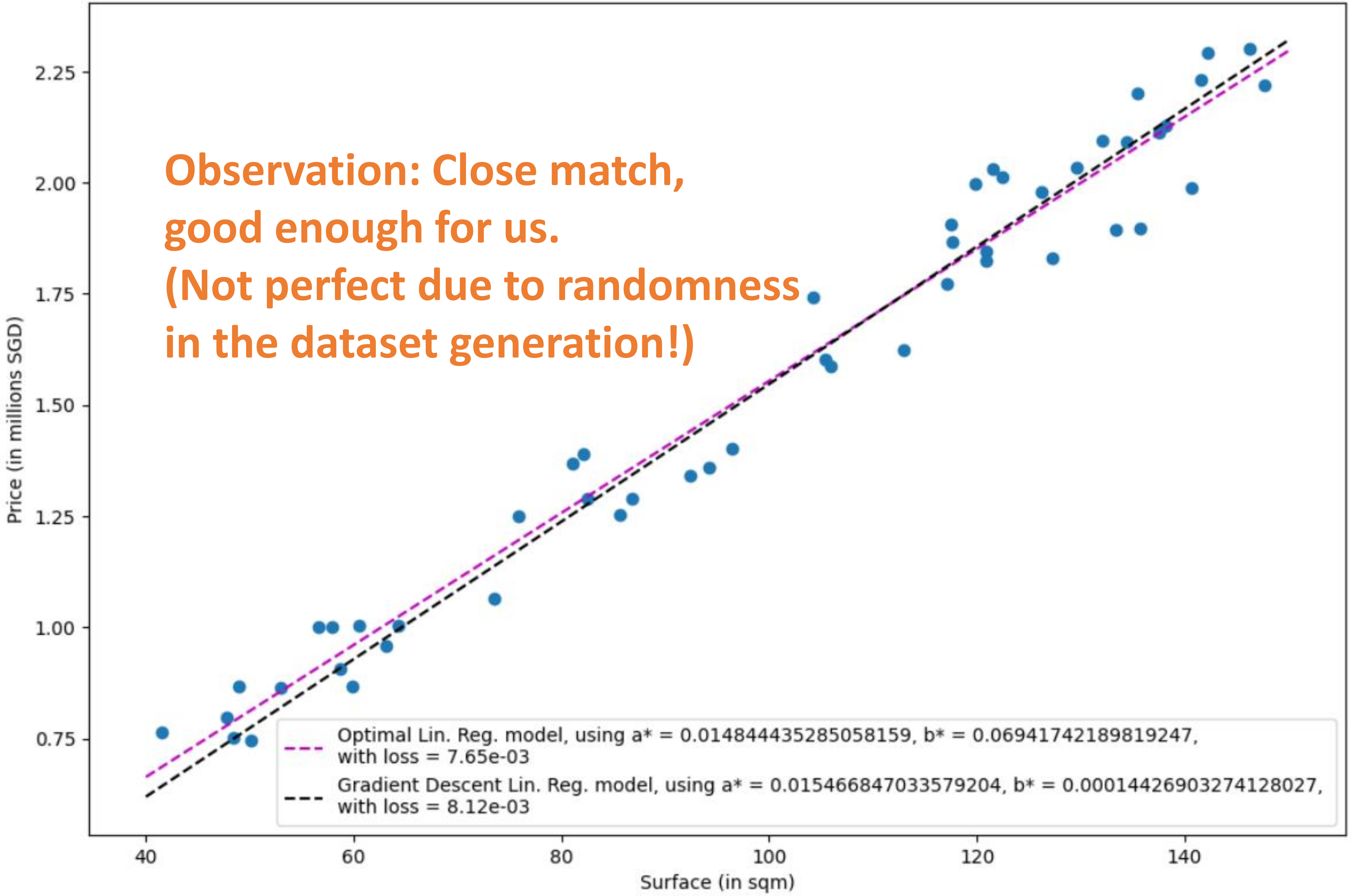
Checking for optimal parameters

We have generated the dataset ourselves, so we know the optimal values for a and b!

```python
print("Optimal a_star value: ", a_star)
print("Value for a_star, found by gradient descent: ", a_gd)
print("We used 14373/1000000 in the mock dataset generation, which is: ", 14373/1000000)
print("Optimal b_star value: ", b_star)
print("Value for b_star, found by gradient descent: ", b_gd)
print("The value we used in the mock dataset generation: ", 100000/1000000)
```

```
Optimal a_star value:  0.014844435285058159
Value for a_star, found by gradient descent:  0.015466847033579204
We used 14373/1000000 in the mock dataset generation, which is:  0.014373
Optimal b_star value:  0.06941742189819247
Value for b_star, found by gradient descent:  0.00014426903274128027
The value we used in the mock dataset generation:  0.1
```

Observation: Close match, good enough for us. (Not perfect due to randomness in the dataset generation!)



Using Sklearn for Linear regression

In practice, we never implement the linear regression model ourselves (but it is a good practice to try it at least once!)

- It is often better/faster to rely on the **sklearn** library and use the **LinearRegression** object!

```python
# Creating a sklearn Linear Regression model.
# It uses the same analytical formula from earlier, i.e. W^* = (X^T X)^{-1} X^T Y.
reg = LinearRegression().fit(sk_inputs, sk_outputs)
# The coefficients for a* and b* are found using coeff_ and intercept_ respectively.
a_sk = reg.coef_[0]
b_sk = reg.intercept_
print("Optimal a_star value: ", a_star)
print("Value for a_star, found by sklearn: ", a_sk)
print("Optimal b_star value: ", b_star)
print("Value for b_star, found by sklearn: ", b_sk)
```

```
Optimal a_star value:  0.014844435285058159
Value for a_star, found by sklearn:  0.014844435285058166
Optimal b_star value:  0.06941742189819247
Value for b_star, found by sklearn:  0.06941742189818956
```

Predicting using Sklearn Linear regression

After training, it is also good practice to check if the predictor makes sense, by **testing** it and asking it to predict the price of an apartment it has never seen before.

- Confirm the pertinence of predicted values manually, if possible.

```python
# We can later use this Linear Regression model, to predict the price of
# a new appartment with surface 105 sqm (price in millions SGD).
new_surf = 105
pred_price = reg.predict(np.array([[new_surf]]))[0]
print(pred_price)
```

```
1.628083126829297
```

```python
avg_price = 14373*new_surf + 100000
min_val = 0.9*avg_price
max_val = 1.1*avg_price
print("Min, max, avg prices: ", [min_val, max_val, avg_price])
```

```
Min, max, avg prices:  [1448248.5, 1770081.5000000002, 1609165]
```

More specifically

Specific topics in **linear algebra** to focus on:

- **Vectors, dot product, norms of vectors**
- **Matrices and their properties: determinant, rank, norm, trace, transpose**
- **Matrix multiplication and inversion**
- **Solving systems of linear equations**
- **Eigenvectors and eigenvalues**
- **Projections and orthonormality**
- (Symmetric matrices, positive semi-definite matrices)
- (Matrix decompositions, e.g. LU decomposition, SVD)

Restricted

More specifically

Specific topics in **calculus** to focus on:

- **Logarithmic and exponential functions**
- **Derivatives and partial derivatives, the chain rule of derivatives**
- (Integrals basics)
- **Multivariate calculus: functions of vectors and matrices and their gradients.**
- (Jacobian and Hessian)
- **Equations of lines and hyperplanes**
- **Solving optimization problems with Gradient Descent, Lagrange multipliers, and other methods.**

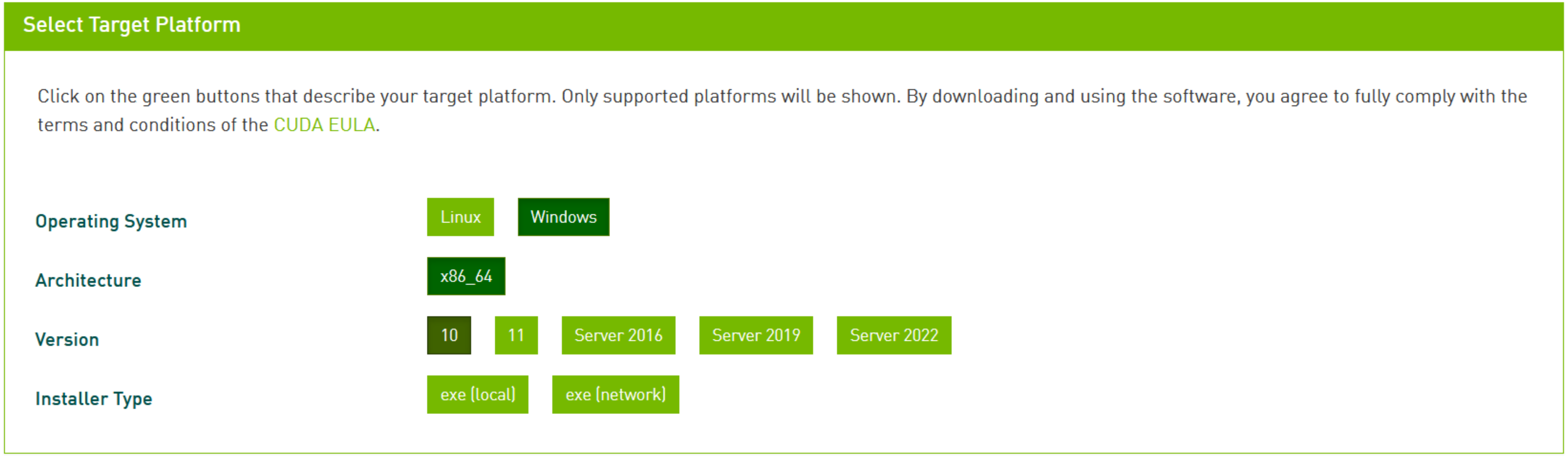
More specifically

Specific topics in **probabilities and statistics** to focus on:

- **Probability rules and axioms, random variables (both discrete and continuous)**
- **Standard distributions (Bernoulli, Binomial, Multinomial, Uniform and Gaussian)**
- **Expectation, variance, covariance and correlation**
- **Conditional probability, Bayes' theorem**
- (Law of total probability)
- (Joint and marginal probability distributions)
- **The central limit theorem**

Installing PyTorch and CUDA

- Check if your GPU is in the list of acceptable GPUs. https://developer.nvidia.com/cuda-gpus
- If so, install CUDA (check that you CUDA version number matchesthe one of your PyTorch install!) https://developer.nvidia.com/cuda-downloads



Installing PyTorch and CUDA

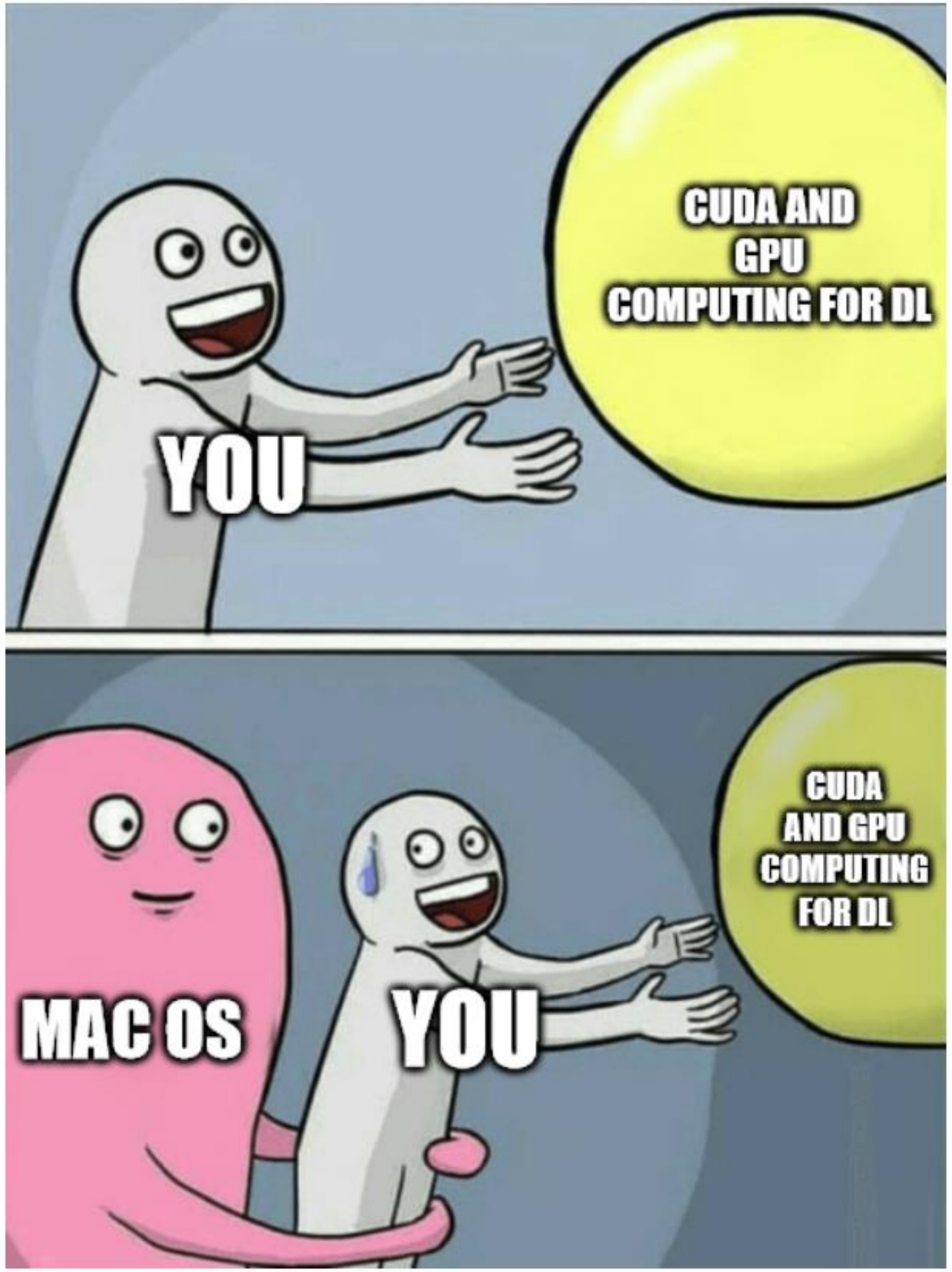
Question: How to use CUDA with MacOS?

Efforts are being made to make GPU computing compatible with AMD and MacOS GPUs, but still far from it (afaik).

Select Target Platform

Click on the green buttons that describe your target platform. Only supported platforms will be shown. By dowr terms and conditions of the CUDA EULA.

Operating System	Linux	Windows			
Architecture	x86_64				
Version	10	11	Server 2016	Server 2019	Server 2022
Installer Type	exe (local)	exe (network)			

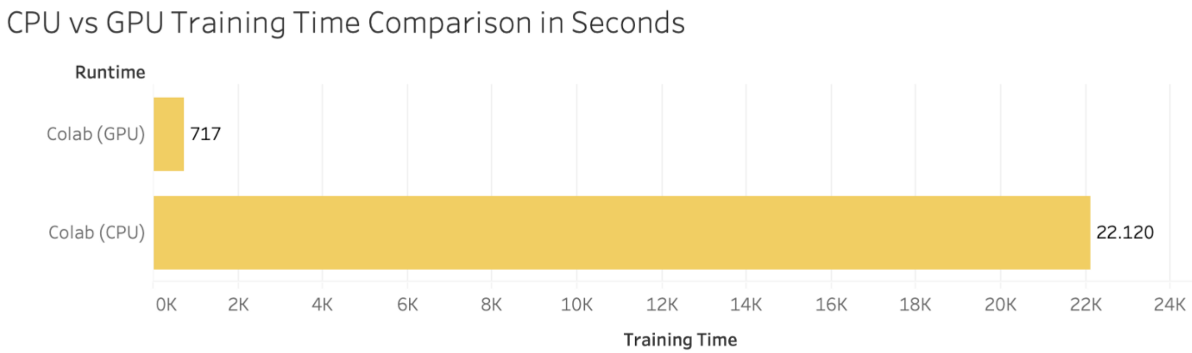


Installing PyTorch and CUDA

Your GPU not in the list of CUDA-enabled GPUs?

You bought a MacOS laptop?

- **Most notebooks can still run on CPU (but they might take significantly longer to run).**
- Also, always the option of using **Google Colab**, or create an education account on AWS.



Google Colaboratory

aws educate

Checking your PyTorch and CUDA install

- **Hello World for PyTorch:** to check you have PyTorch installed correctly. The code below should run and display a tensor.

```
import torch
x = torch.rand(5, 3)
print(x)
```

```
tensor([[0.3380, 0.3845, 0.3217],
        [0.8337, 0.9050, 0.2650],
        [0.2979, 0.7141, 0.9069],
        [0.1449, 0.1132, 0.1375],
        [0.4675, 0.3947, 0.1426]])
```

- **Hello World for CUDA:** to check you have correctly installed CUDA on top of PyTorch. The code below should print *True*, as the output of *torch.cuda.is_available()*

```
import torch
torch.cuda.is_available()
```

A quick word about PyTorch 2.0

PyTorch v2.0 is the current (latest version released in March 2023).

- Should be fully retro-compatible.
- Revising and testing notebooks (they were designed last year and tested on v1.13).
- Kindly let me know if you have any issues!
- Will let you know about new v2.0 features on W13.

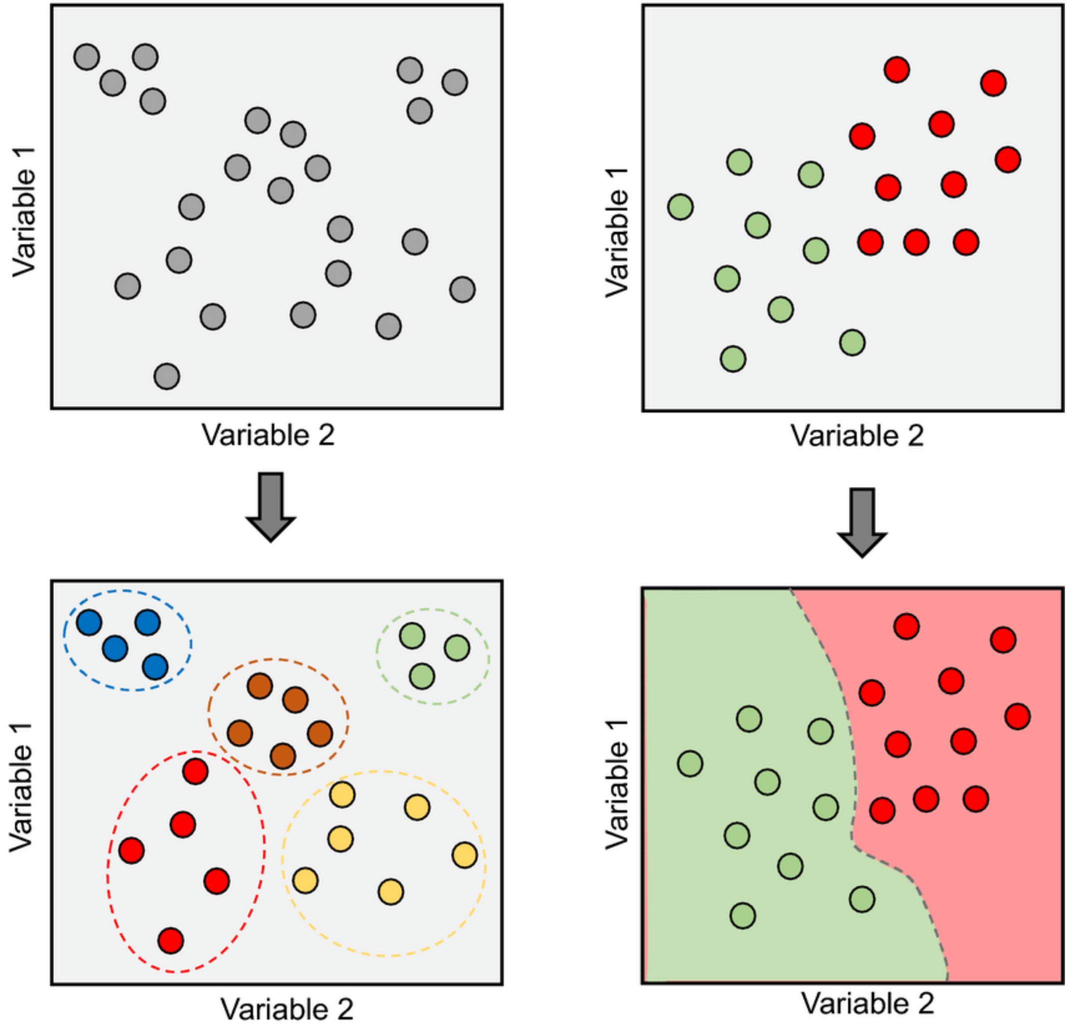
Supervised vs Unsupervised Learning

Definition (Supervised vs. Unsupervised Learning):

Supervised and **Unsupervised Learning** are the two techniques of ML.

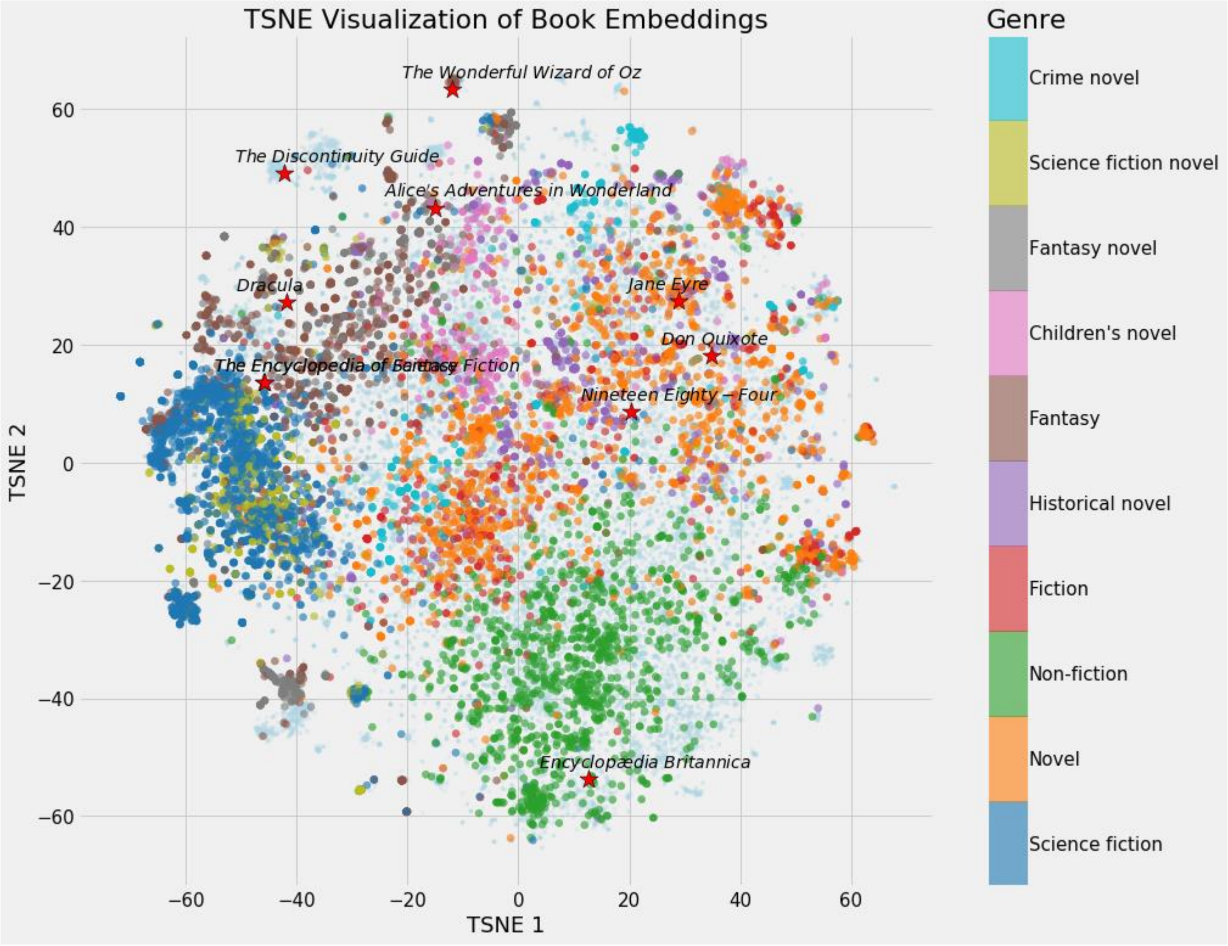
The main difference is **the need for labelled training data**:

- Supervised machine learning relies on labelled input and output data to learn and make predictions,
- while **unsupervised learning does not require labelled data.**



Unsupervised Learning Examples

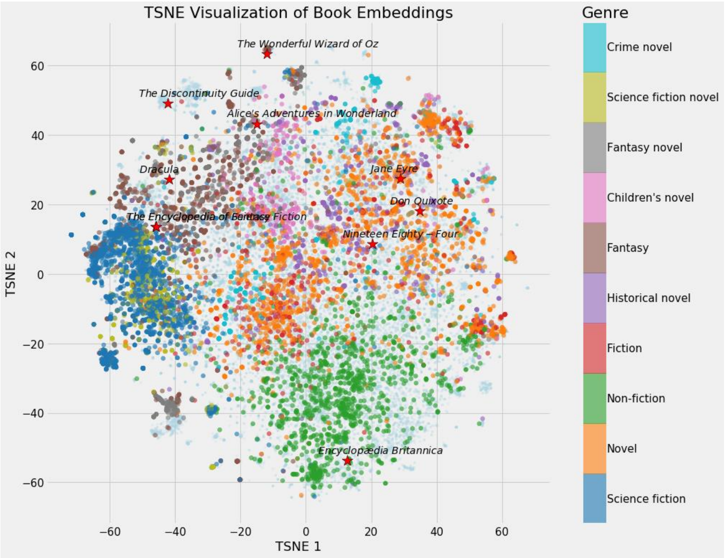
- Examples of **unsupervised learning:** clustering customers based on their behaviors, segmenting images, and identifying topics in a document.

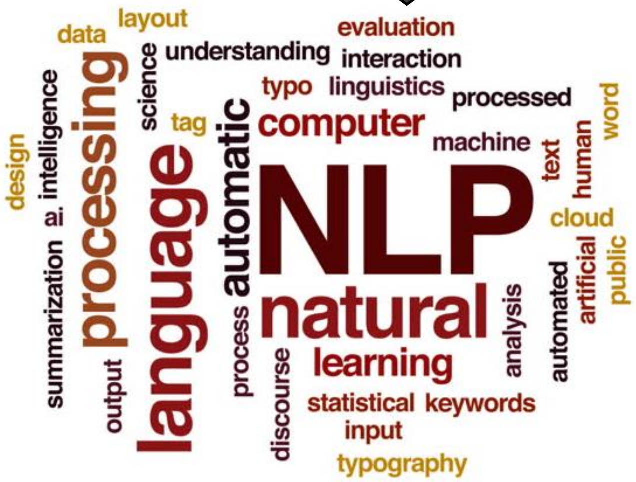


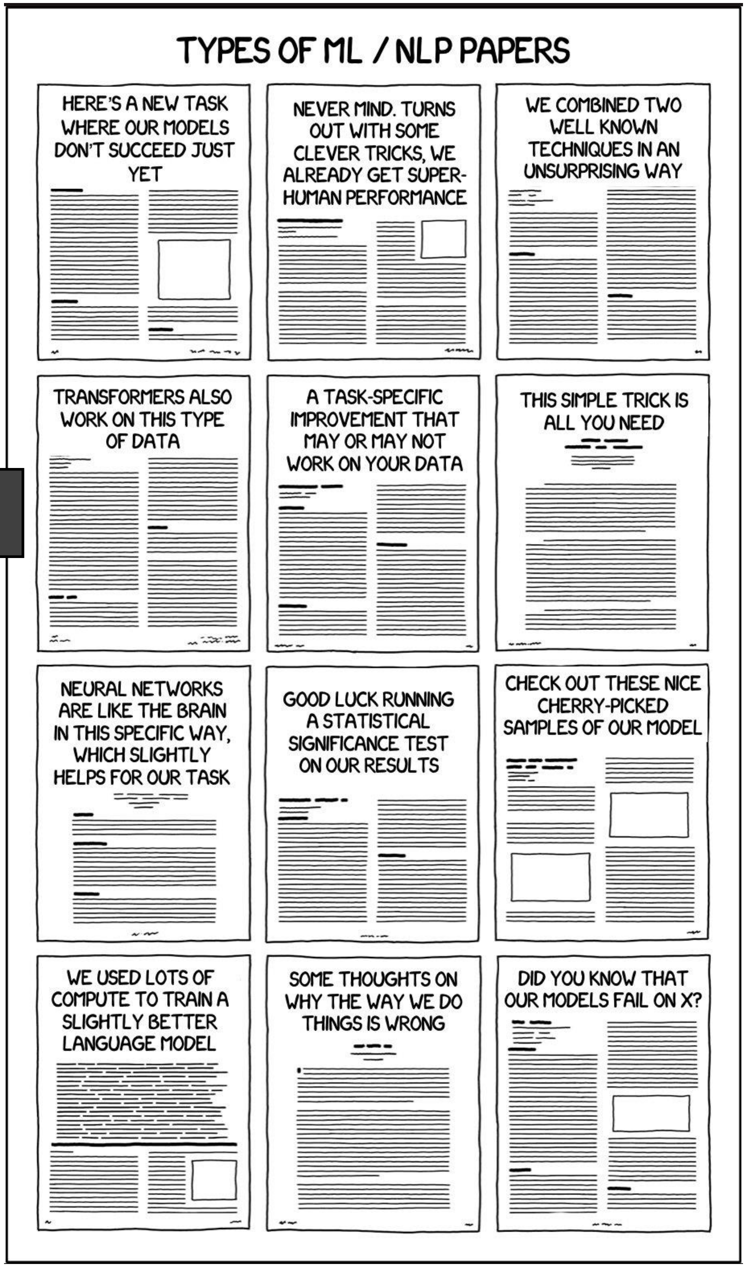
Unsupervised Learning Examples

- Examples of **unsupervised learning:** clustering customers based on their behaviors, segmenting images, and identifying topics in a document.

Identify topics that seem to appear in those papers and their prominence







Clustering vs. Association (Unsupervised)

Definition (Clustering vs. Association):

Unsupervised learning can be used for two types of problems: **Clustering** and **Association**.

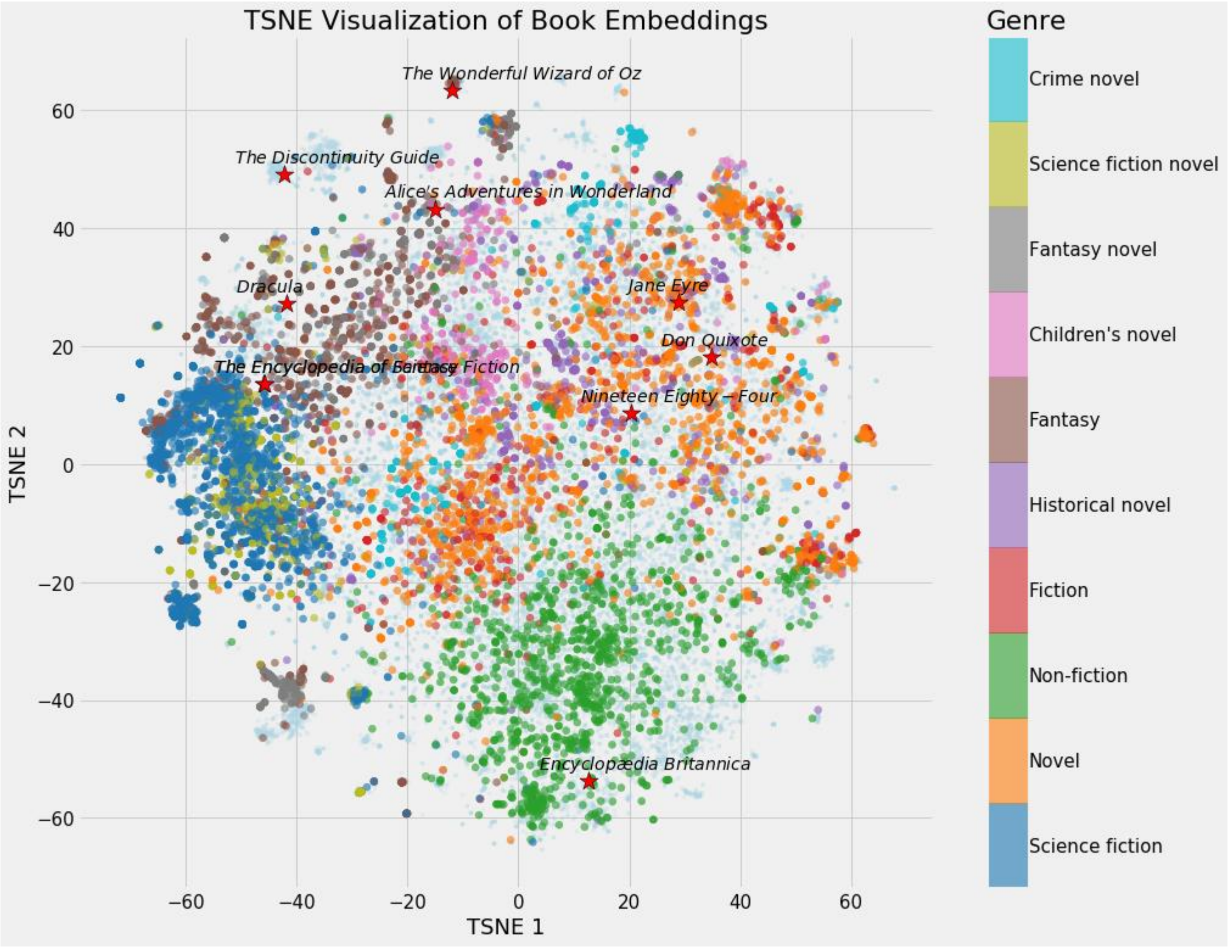
The main difference is that

- **clustering groups data based on similarity**,
- while **association looks for relationships between variables**.

Clustering vs. Association (Unsupervised)

Examples of clustering:

- Group customers into clusters based on the similarities in their purchasing behaviours, such as their spending habits or types of products they like.
- Group the catalogue of movies available on Netflix and identify what movies have in common, so you can later recommend a movie to a user based on what he/she has seen before.



Clustering vs. Association (Unsupervised)

Example of association:

- Finding the relationship between customer buying behaviors and customer satisfaction.
- Association can be used to understand how changes in customer behavior impacts customer satisfaction, such as if buying a certain product increases customer satisfaction (or the opposite).

Proof of the Normal Equation

Using the notations

$$X = \begin{pmatrix} 1 & x_1 \\ \dots & \dots \\ 1 & x_N \end{pmatrix},$$

$$Y = \begin{pmatrix} y_1 \\ \dots \\ y_N \end{pmatrix},$$

$$W^* = \begin{pmatrix} b^* \\ a^* \end{pmatrix}$$

We have, in matrix form

$$XW^* = \begin{pmatrix} a^* x_1 + b^* \\ \dots \\ a^* x_N + b^* \end{pmatrix}$$

And, then it follows that

$$XW^* - Y = \begin{pmatrix} a^* x_1 + b^* - y_1 \\ \dots \\ a^* x_N + b^* - y_N \end{pmatrix}$$

Proof of the Normal Equation

Our loss function, the MSE L, is therefore defined, in matrix format as:

$$L = \frac{1}{N}(XW^* - Y)^T(XW^* - Y)$$

This is equivalent to

$$L = \frac{1}{N}\left((XW^*)^T - Y^T\right)(XW^* - Y)$$

Proof of the Normal Equation

We then get

$$L = \frac{1}{N}\left({W^*}^T X^T - Y^T\right)(XW^* - Y)$$

Expanding

$$L = \frac{1}{N}({W^*}^T X^T X W^* - Y^T X W^* - \ {W^*}^T X^T Y + Y^T Y)$$

Proof of the Normal Equation

Recall that we are trying to find the solution to optimization problem

$$(a^*, b^*) = \arg\min_{a,b}[L(a, b, x, y)]$$

With

$$L = \frac{1}{N}({W^*}^T X^T X W^* - Y^T X W^* - {W^*}^T X^T Y + Y^T Y)$$

Recognizing that $Y^T X W^* = {W^*}^T X^T Y$, differentiating our function L with respect to W and equating it to zero gives:

$$\frac{\partial L}{\partial W} = \frac{1}{N}(2X^T X W - 2X^T Y) = 0$$

Proof of the Normal Equation

This is equivalent to

$$(X^T X W^* - X^T Y) = 0$$

Or,

$$X^T X W^* = X^T Y$$

Assuming $\boldsymbol{X^T X}$ is invertible (and that might not always be the case based on your dataset!), this finally gives:

$$\boldsymbol{W^* = (X^T X)^{-1} X^T Y}$$