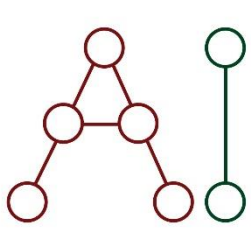

Intro to Machine Learning and A.I.

and Introduction to the ChE 197/297 Course

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Process Systems Engineering Laboratory
Department of Chemical Engineering
University of the Philippines Diliman

Outline

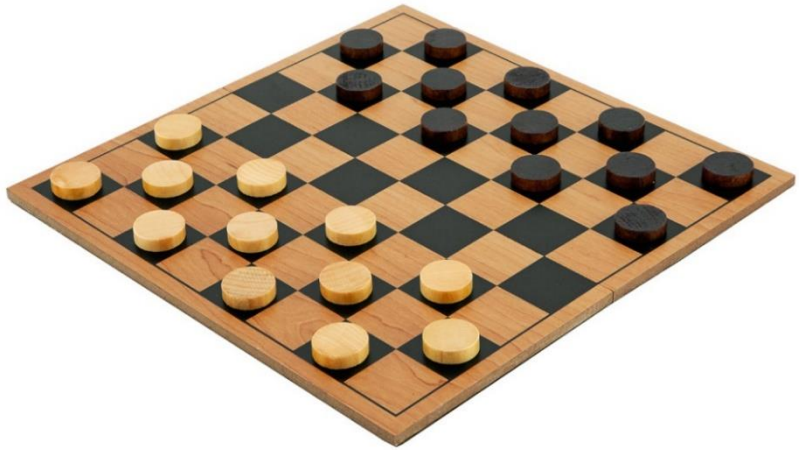
- What is Machine Learning?
  - Why only now?
  - Types of Learning Problems

- Intro to the Course
  - Course Delivery
  - Course Content
  - Course Requirements
  - Software

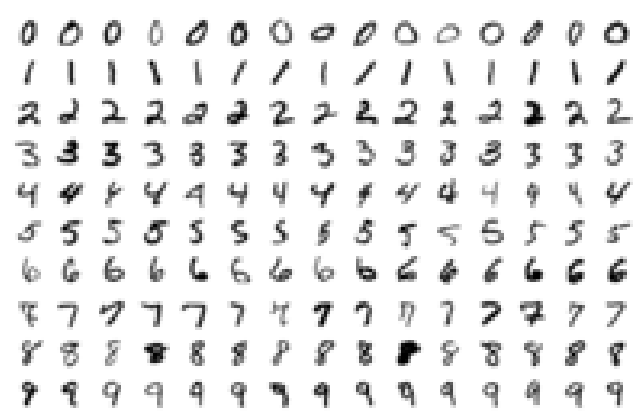
What is Machine Learning?

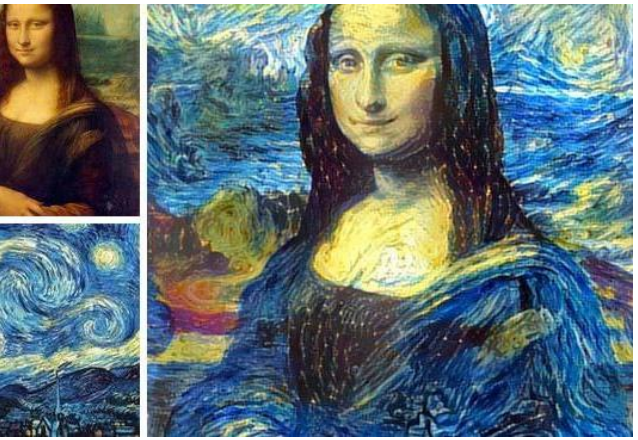
A field of study concerned with giving computers the *ability to learn* without being explicitly programmed.
(Arthur Samuel, 1959)

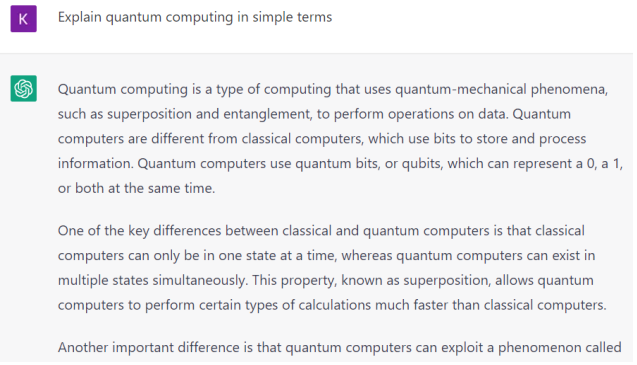
Arthur Samuel and the IBM 701 Computer



- Arthur Samuel was not a very good checkers player.
- But he was able to program a checkers bot that plays *better than a human*.
- The bot learned by playing millions of times against itself.
- In the process, it learns which moves lead to wins and which moves lead to losses.

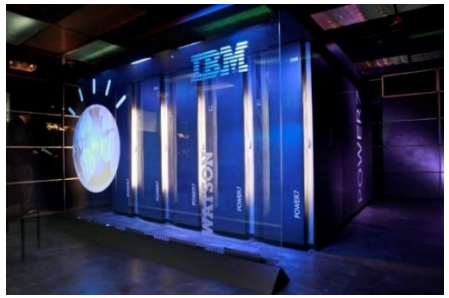






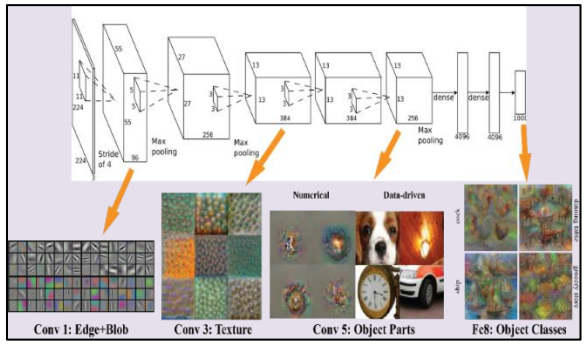
Typical ML Applications

- Filtering emails as spam / not spam
- Handwritten digits recognition
- Speech recognition, Natural Language Processing (NLP)
- Social media (Face recognition, News Feed Ranking, etc.)
- Image / Object Recognition, Image Segmentation
- Recommender systems (movies, products, videos, webpages, bookings)
- Finance (Stock market prediction, customer behaviour, etc.)
- Transportation (Self-driving cars, travel demand modelling)
- Healthcare (Early diagnostics, hospital demand forecasting)
- Bioinformatics (Protein folding and structure prediction, Gene function prediction, Biomedical image analysis)
- Chemometrics (GC-MS data analysis, drug discovery, compound classification, chemical property prediction)



IBM Watson

Jeopardy, **2011**

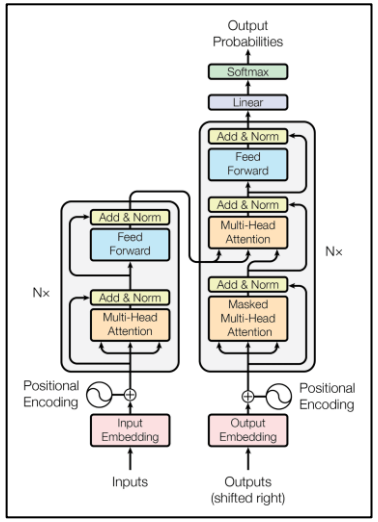


AlexNet

ImageNet Visual Recognition Challenge, **2012**

AlphaGo

Game of Go, **2016**



Transformers

2017

DALL-E

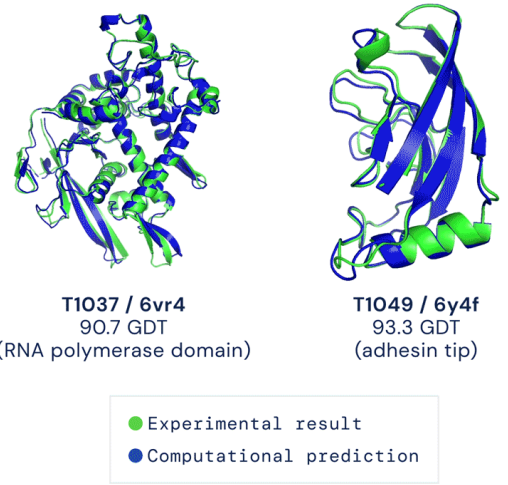
2021, 2022

IBM Deep Blue

Chess, **1997**

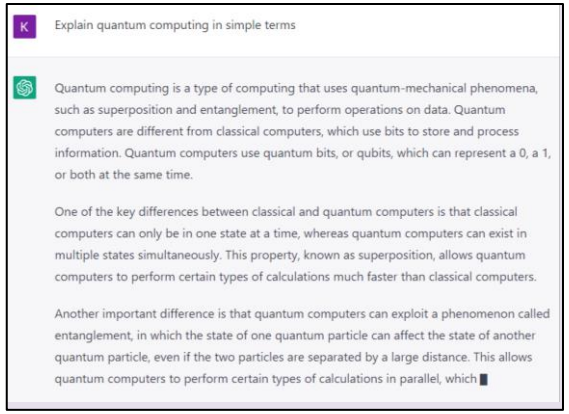
AlphaStar

StarCraft II, **2019**



AlphaFold

Protein Structure Prediction, **2016**, **2018**



ChatGPT

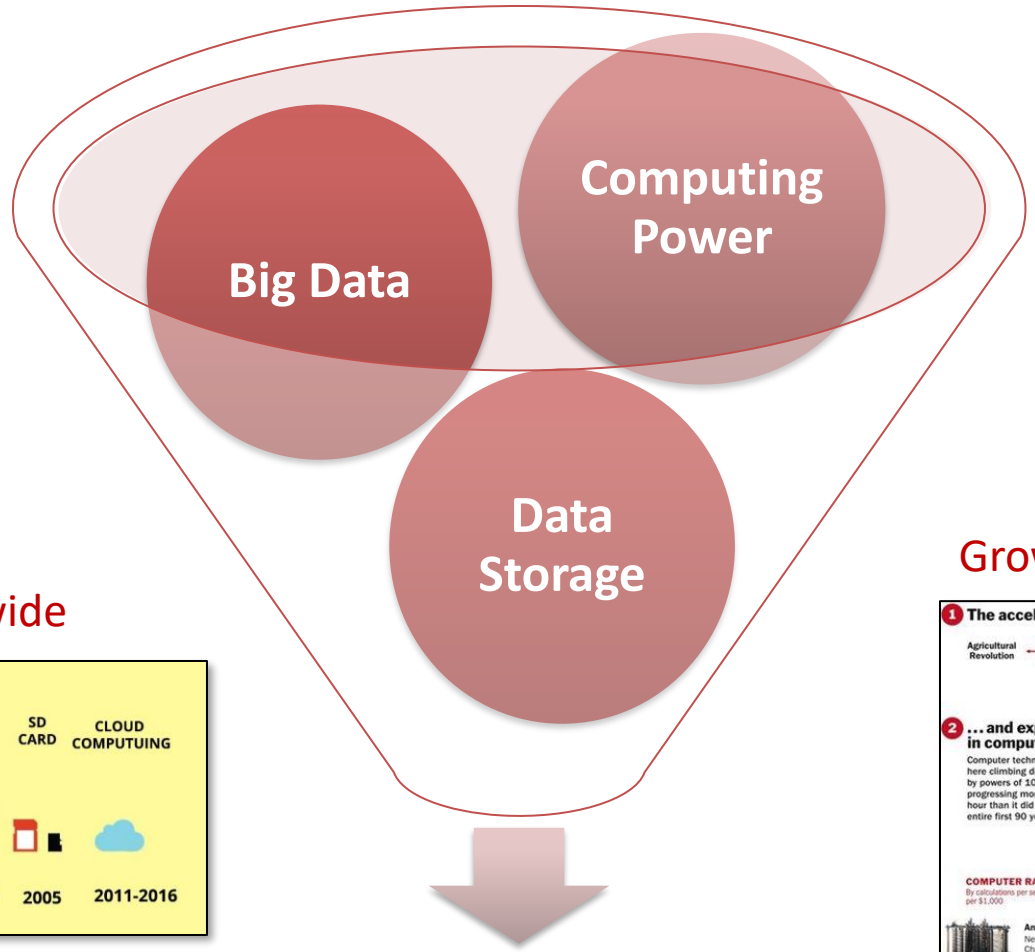
2022

Machine Learning,

Data Science,

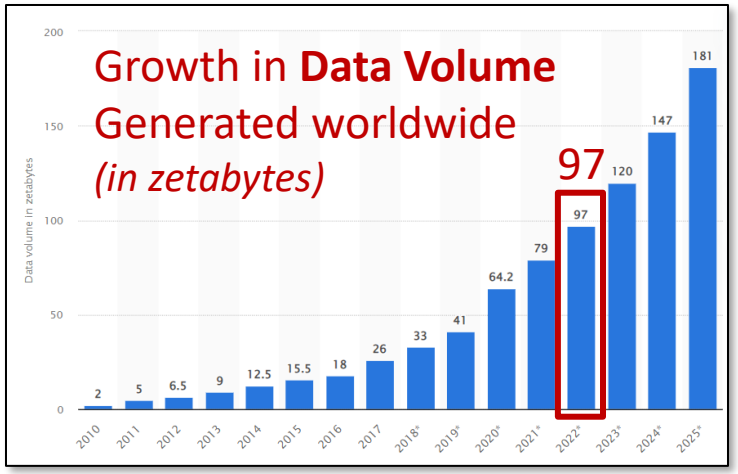
Data Analytics,

…why only now?



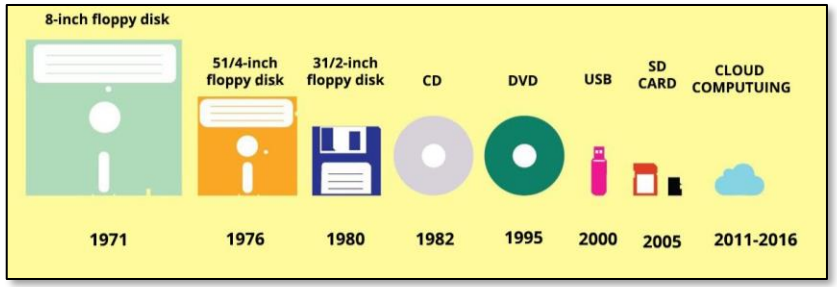
Machine Learning +

Practical Applications

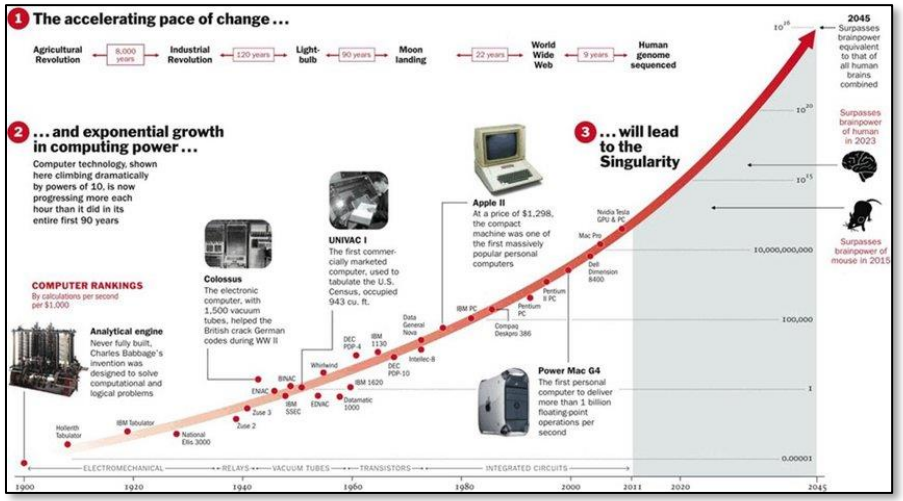


2022

Growth in **Data Storage** worldwide



Growth in **Computing Power** worldwide



Machine Learning,

Data Science,

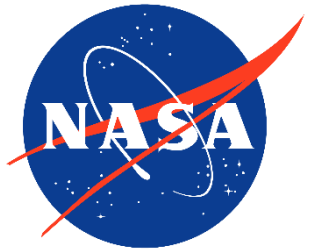
Data Analytics,

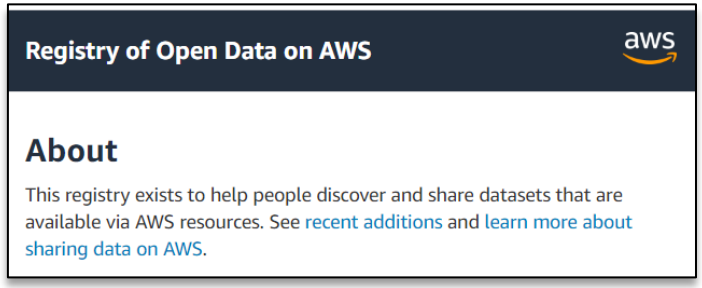
…why only now?

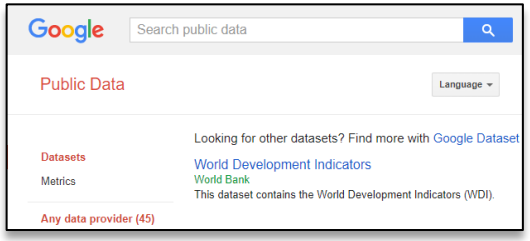
We are currently DROWNING[1] in data!

- There are about 1 trillion web pages.
- 1 hr of video is uploaded to Youtube every second.
- Human genomes have a length of 3.8×10^9 base pairs.
- Walmart handles more than 1 million transactions per hour.
- Etc…

Popular websites where we can get publicly available data:







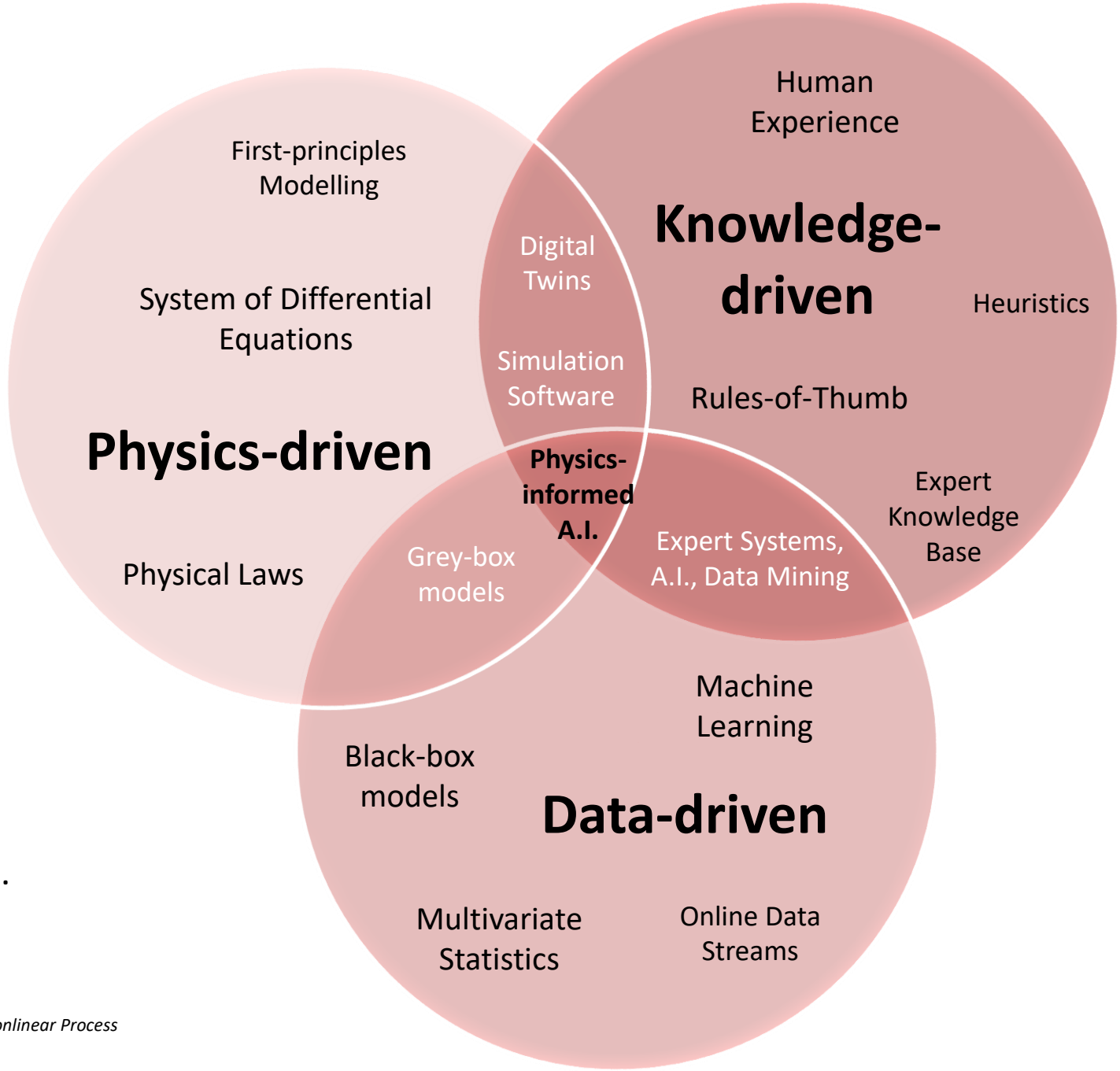
[1] Venkatasubramanian (2009). DROWNING IN DATA: Informatics and Modeling Challenges in a Data-Rich Networked World. *AIChE Journal.*
[2] Murphy (2012). Machine Learning: A Probabilistic Perspective. *MIT Press.*

Why use Machine Learning in your Engineering?

Three approaches to engineering problems:

1. Physics-driven Methods
2. Knowledge-driven Methods
3. Data-driven Methods

Machine learning is a **data-driven approach**.

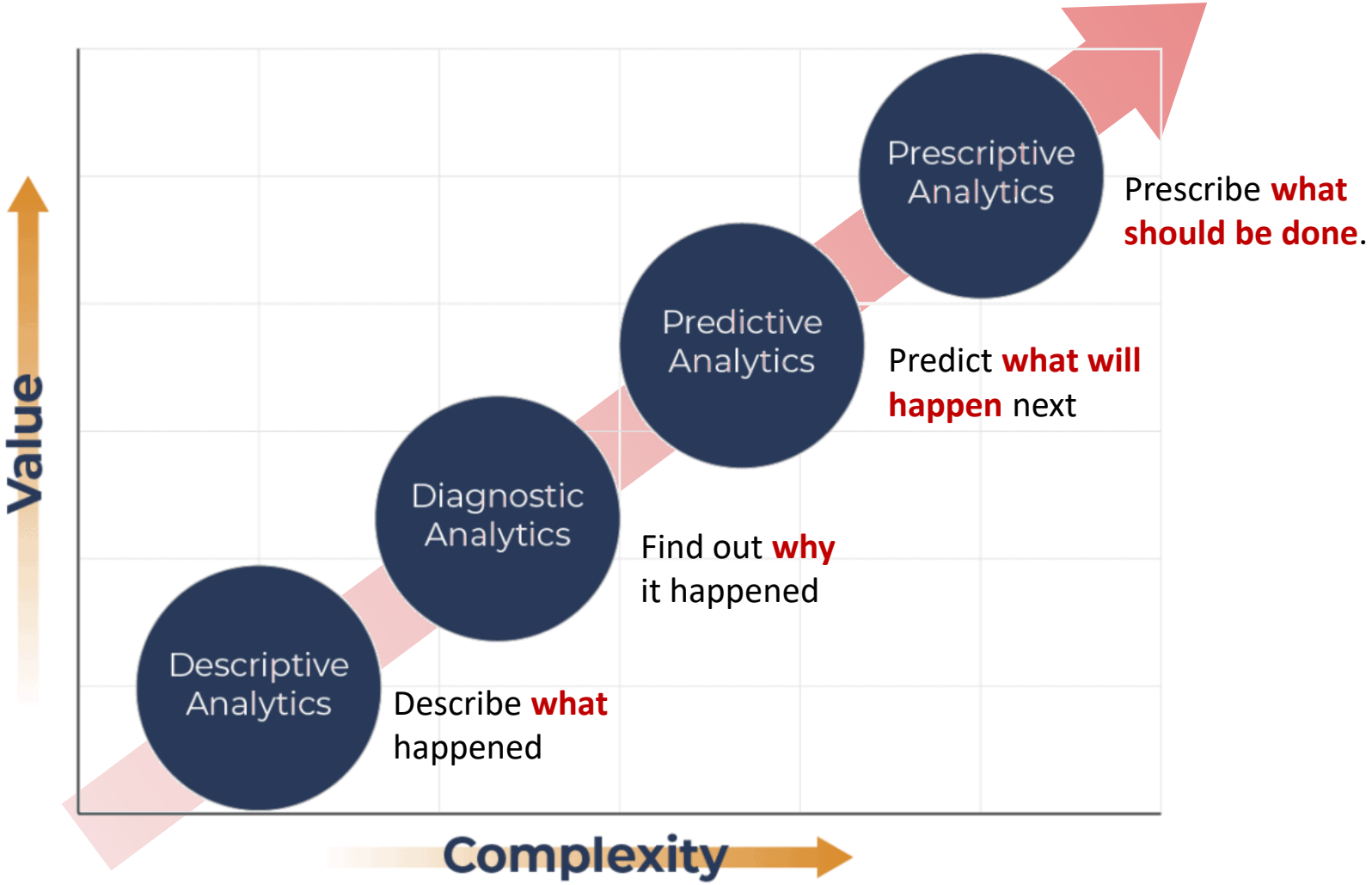


Reference: Pilario et al. (2020), *A Review of Kernel Methods for Feature Extraction in Nonlinear Process Monitoring.* MDPI: Processes, https://doi.org/10.3390/pr8010024

How to turn data into decisions?

Source: https://iterationinsights.com/article/where-to-start-with-the-4-types-of-analytics/

- Applying machine learning to your data is not enough.
- Don’t just let your data speak, let it change the way you do things. **The goal is prescriptive analytics!**
- Getting through each stage of analytics requires more and more effort, but also **more returns**.



Outline

- What is Machine Learning?
  - Why only now?
  - **Types of Learning Problems**

- Intro to the Course (AI 221)
  - Course Delivery
  - Course Content
  - Course Requirements
  - Software

Types of Learning Problems

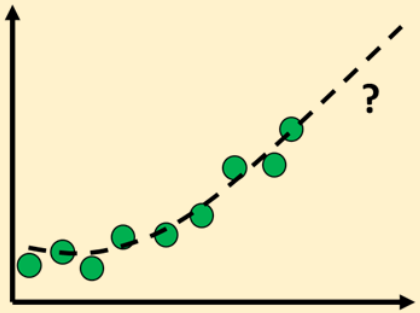
Supervised Learning

Learn a mapping or a function:

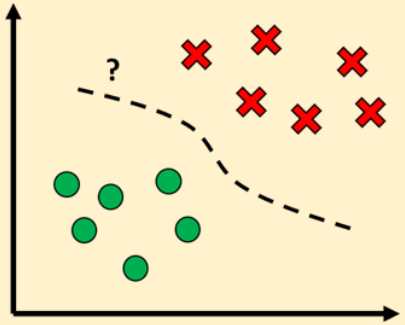
$$y = f(x)$$

from inputs (x) to outputs (y), *given a labelled set of input-output examples* (or).

Regression



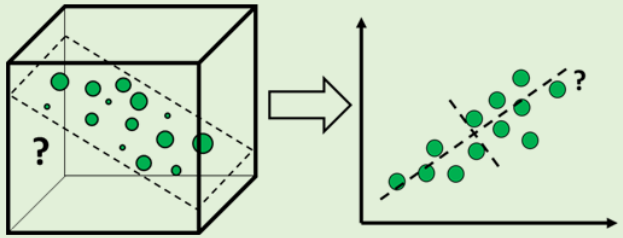
Classification



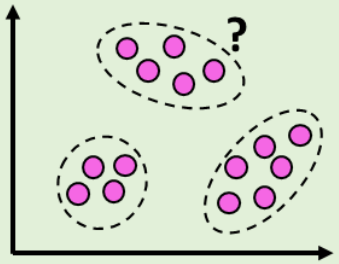
Unsupervised Learning

Discover *patterns or structure* from a data set ( ) without any label information.

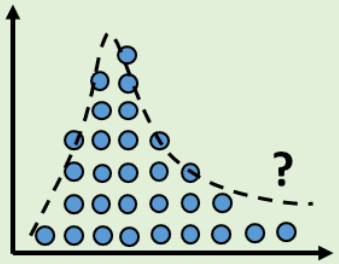
Dimensionality Reduction



Clustering



Density Estimation



Types of Learning Problems

A simple example…

Supervised Learning

These are images of dogs.

These are images of cars.

Now, what is this an image of?

Unsupervised Learning

Here are some images…

Is there an image that does not belong?

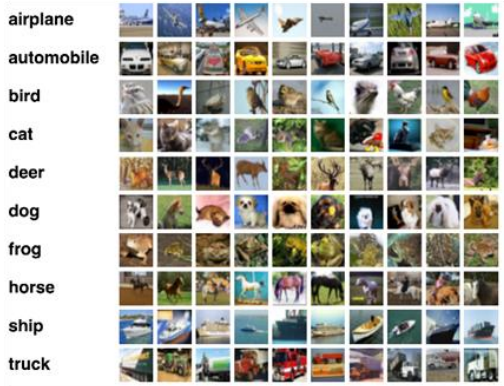
Are there images with similar patterns?

Types of Learning Problems

Semi-Supervised Learning

Goal: Make a computer learn from both labelled and unlabelled data.

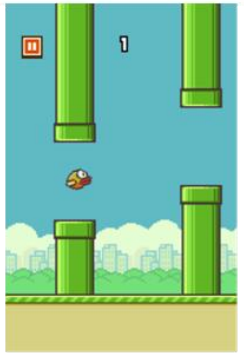
Labelled Data

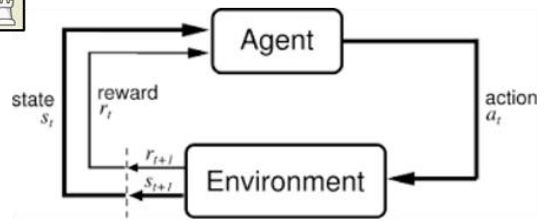


Unlabelled Data

Reinforcement Learning

Goal: Make a computer learn by letting it interact with the environment.





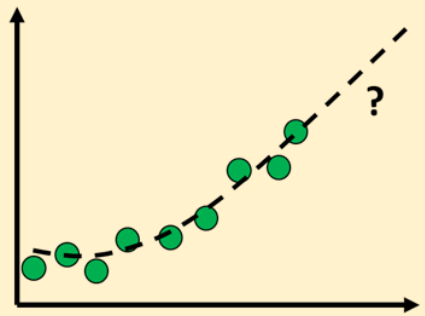
Supervised Learning

Learn a mapping or a function:

$$y = f(x)$$

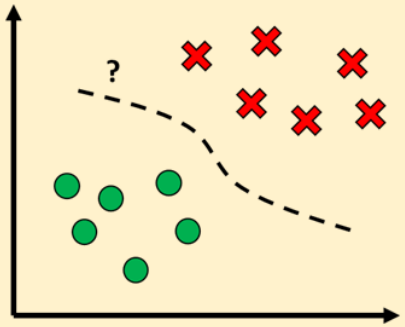
from inputs (x) to outputs (y), *given a labelled set of input-output examples* (● or ✖).

Regression



- **Given:** Training Data $\{\boldsymbol{x}_i, y_i\}_{i=1,2\ldots,N}$
- Target y_i is a **continuous** variable.
- Examples:
  - Forecasting future stock price
  - Forecasting energy resources
  - Prediction of key performance indicators
  - Predicting the properties of molecules based on their structure
  - Predicting the environmental impact of pollutants

Classification

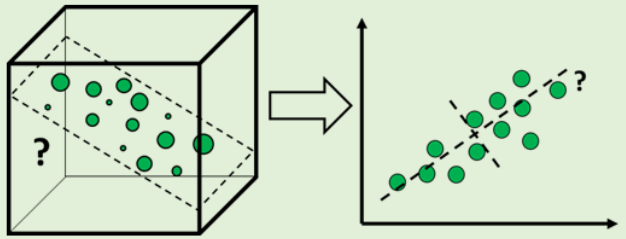


- **Given:** Training Data $\{\boldsymbol{x}_i, y_i\}_{i=1,2\ldots,N}$
- Target y_i is a **categorical** variable.
- Examples:
  - Classifying objects in images
  - Classifying chest X-ray images into COVID positive/negative
  - Handwritten digits recognition
  - Filter e-mails into spam/not spam
  - Classify critical equipment as to healthy or faulty
  - Activity recognition from wearable devices

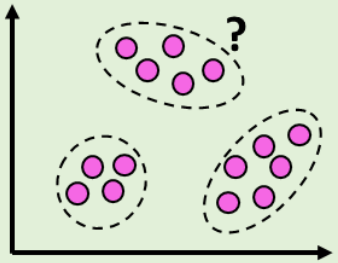
Unsupervised Learning

Discover *patterns or structure* from a data set (●) without any label information.

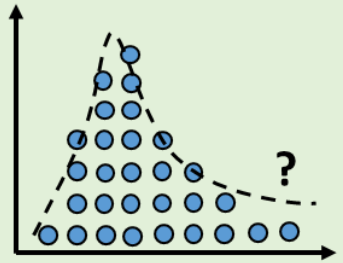
Dimensionality Reduction



Clustering



Density Estimation



Dimensionality Reduction

- **Given:** Data $\{x_i\}_{i=1,2\ldots,N}$
- **Reduce features** but retain the most important information from the original data.
- Examples:
  - Feature Engineering
  - Image compression
  - Filtering noise from signals
  - Source separation in audio
  - Data visualization

Clustering

- **Given:** Data $\{x_i\}_{i=1,2\ldots,N}$
- **Group** similar data points together.
- Examples:
  - Customer segmentation
  - Recommendation systems
  - Identifying fake news
  - Clustering documents, tweets, posts

Density Estimation

- **Given:** Data $\{x_i\}_{i=1,2\ldots,N}$
- **Estimate** the distribution of the data.
- Examples:
  - Anomaly Detection
  - Novelty Detection
  - Generative Models
  - Finding distribution modes
  - Spatio-temporal analytics

Can you identify the type of learning problem?

Regression, Classification, Dimensionality Reduction, Clustering, Density Estimation

Example 1

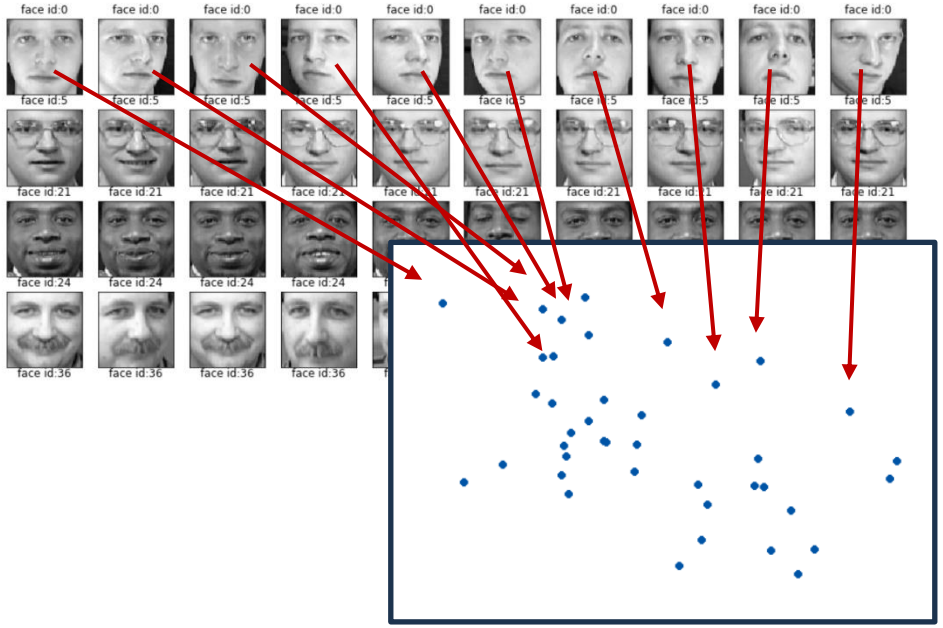
Given the weight of the car, its model year, and horsepower, predict its mileage in miles per gallon (mpg).

car_weight	model_year	horsepower	mileage
1522 kg	2020	150	18 mpg
1930 kg	2017	185	16 mpg
1321 kg	2018	200	21 mpg
2128 kg	2019	168	?
2498 kg	2018	170	15 mpg
1882 kg	2021	155	17 mpg
1956 kg	2019	190	?
1672 kg	2017	182	18 mpg

Answer: Regression

Example 2

Given images of faces with varying poses and expressions, *map* each image onto a 2D point so that similar-looking images are closer together on the map.



Answer: Dimensionality Reduction

Can you identify the type of learning problem?

Regression, Classification, Dimensionality Reduction, Clustering, Density Estimation

Example 3

Given a tweet, predict whether the sentiment is positive, negative, or neutral.

Tweet	Sentiment
I'm in pain…	Negative
Manifesting a promotion this year!	Positive
It's 2AM. Who's awake?	Neutral
Heavy traffic at EDSA	Negative
Family dinner… So full!	Positive
Spoiler alert: RIP Tony Stark	?
Tesla sucks!	?
It's a boy!	Positive

Answer: **Classification**

Example 4

Given student grades in 5 subjects: Math, Chemistry, Physics, English, and Reading, group the students with similar competencies.

Student	Math	Chemistry	Physics	English	Reading
1	81	85	88	94	92
2	95	80	94	93	85
3	92	94	89	81	80
4	94	83	90	91	84
5	88	84	90	97	95
6	90	93	88	85	82
7	92	94	91	87	81
8	87	82	85	93	94

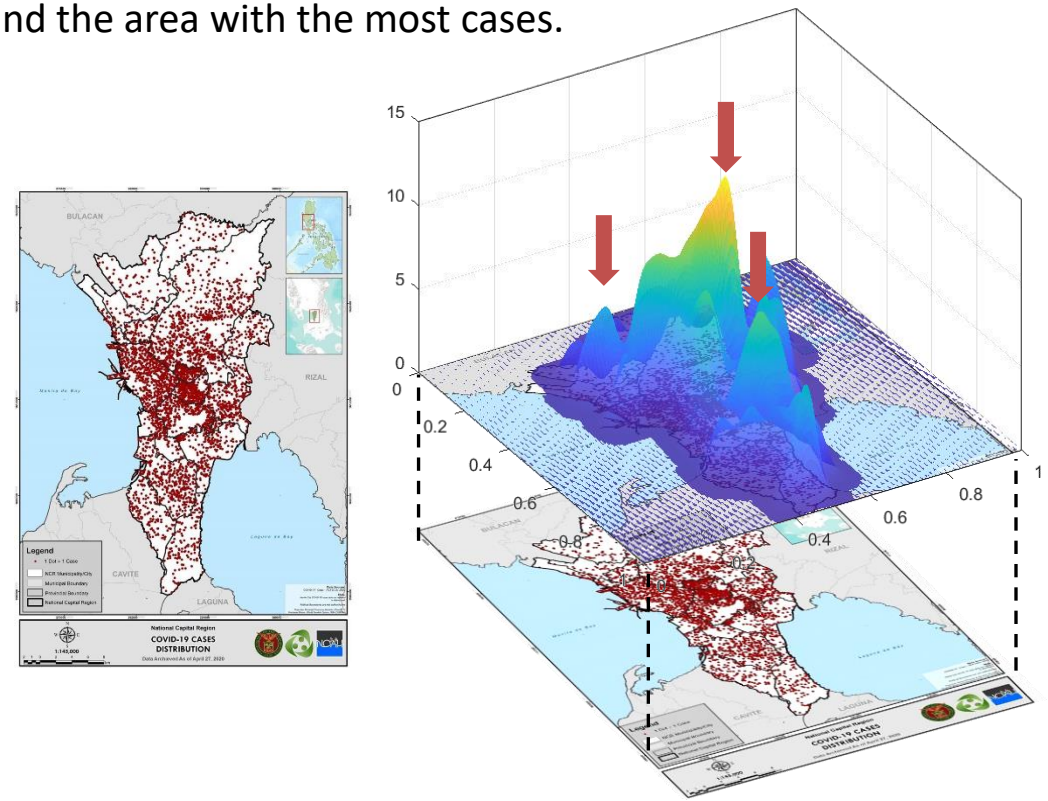
Answer: **Clustering**

Can you identify the type of learning problem?

Regression, Classification, Dimensionality Reduction, Clustering, Density Estimation

Example 5

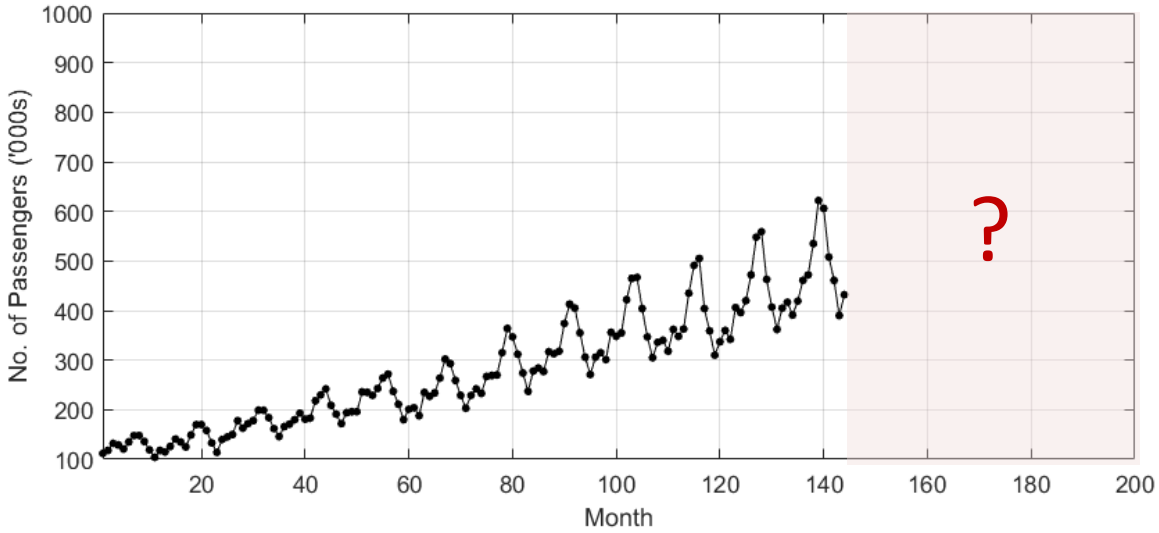
Given the spatial occurrence of Covid cases in Metro Manila, find the area with the most cases.



Answer: Density Estimation

Example 6

Given the number of airline passengers in the previous months, predict the number of passengers for the next few months.



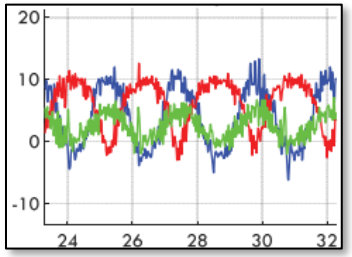
Answer: Regression

Can you identify the type of learning problem?

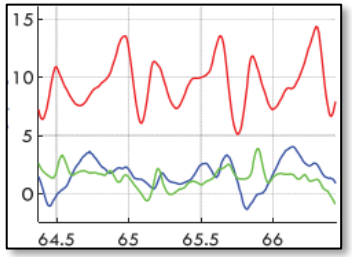
Regression, Classification, Dimensionality Reduction, Clustering, Density Estimation

Example 7

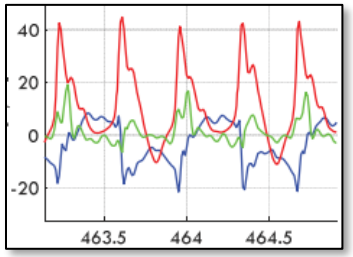
Given smartphone *accelerometer data* from a human doing exercise, predict the kind of exercise being done.



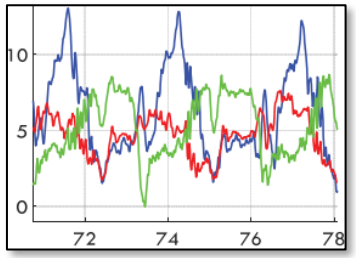
Push-up



Walking



Running



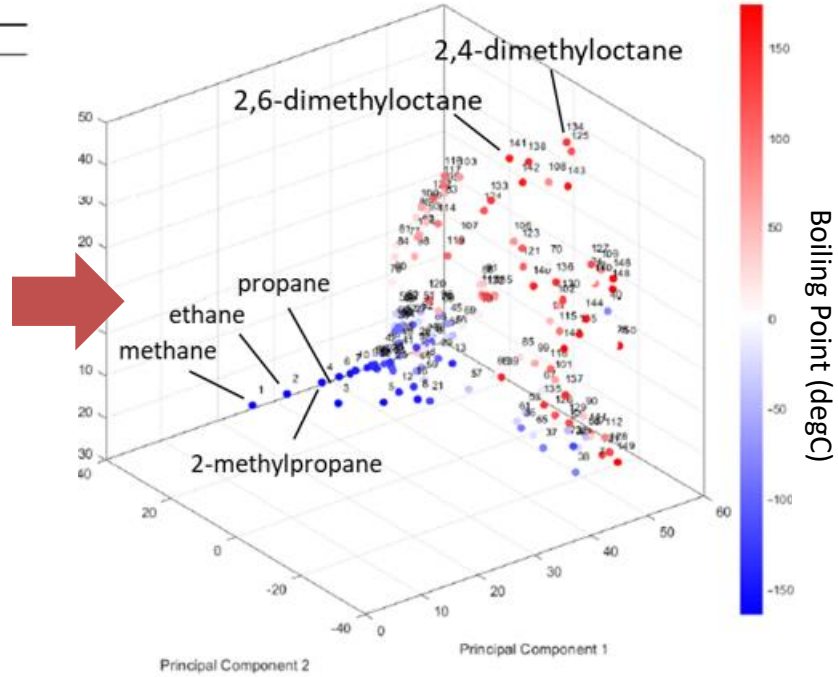
Squats

Answer: **Classification**

Example 8

Given the structural properties of alkane molecules, *map* them onto 3D space based on their similarities, then *predict* their boiling points.

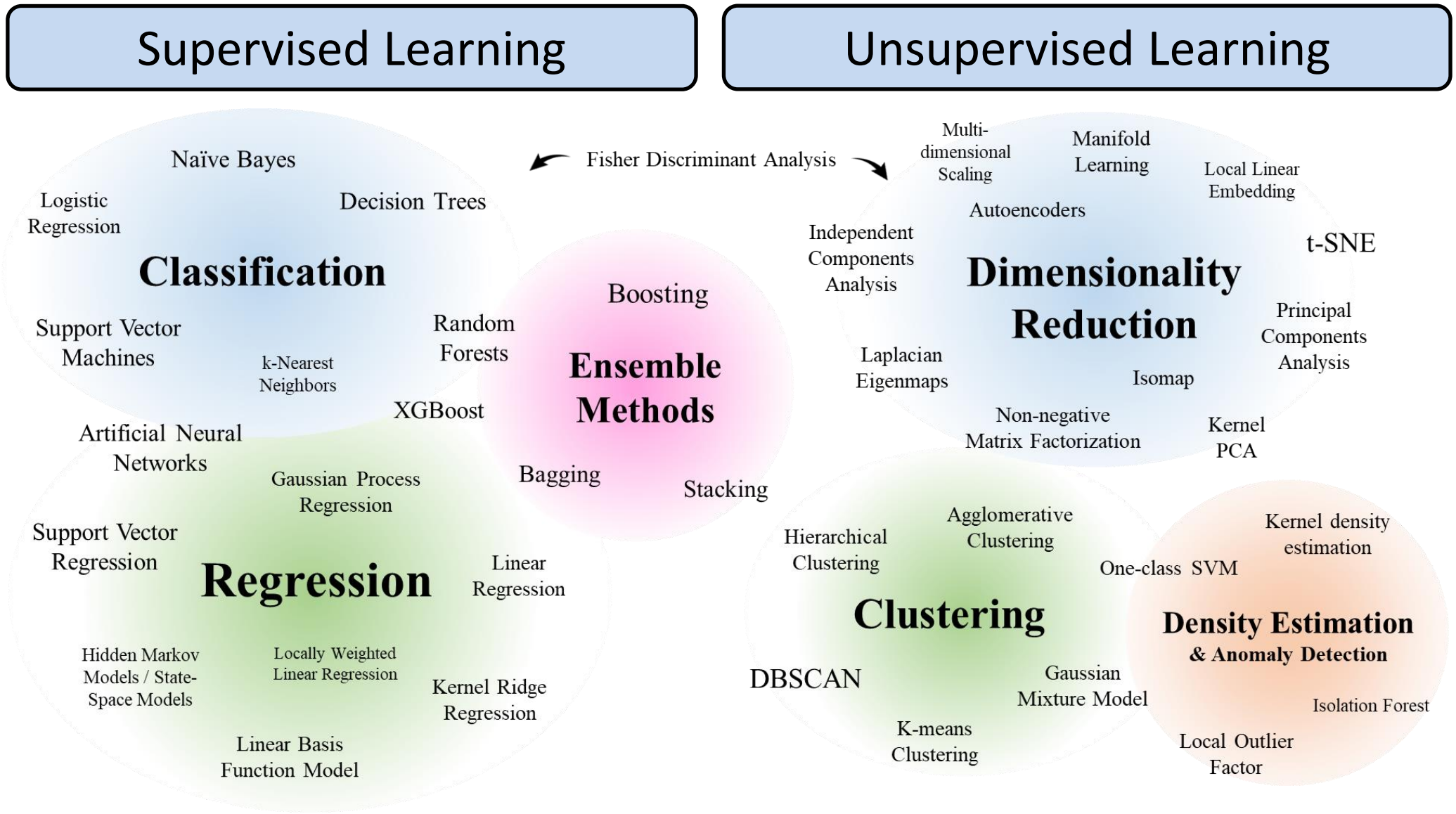
No.	BP	Alkane
1	-164	methane
2	-88.6	ethane
3	-42.1	propane
4	-11.7	2-methylpropane
5	-0.5	butane
6	9.5	2,2-dimethylpropane
7	27.8	2-methylbutane
8	36.1	pentane
9	49.7	2,2-dimethylbutane
10	58	2,3-dimethylbutane
11	60.3	2-methylpentane
12	63.3	3-methylpentane
13	69	hexane
14	80.9	2,2,3-trimethylbutane
15	79.2	2,2-dimethylpentane
16	86.1	3,3-dimethylpentane
17	89.8	2,3-dimethylpentane
18	80.5	2,4-dimethylpentane
19	90	2-methylhexane
20	92	3-methylhexane



Answer: **Dimensionality Reduction + Regression**

Source: https://ieeexplore.ieee.org/document/8472444

Machine Learning Methods



Reference: Pilario et al. (2020), *A Review of Kernel Methods for Feature Extraction in Nonlinear Process Monitoring.* MDPI: Processes, https://doi.org/10.3390/pr8010024

Outline

- What is Machine Learning?
  - Why only now?
  - Types of Learning Problems

- **Intro to the Course**
  - Course Delivery
  - Course Content
  - Course Requirements
  - Software

Introduction to the Course

COURSE NUMBER: ChE 197/297

COURSE TITLE: Introduction to AI/ML for Chemical Engineers

COURSE DESCRIPTION: Mathematical details, code implementations, and chemical engineering applications of basic machine learning and artificial intelligence methods.

COURSE CREDIT: 3 units

3.0 hours/week

COURSE LMS*: **UVLE Course Page: Intro to AI/ML for ChemE**

COURSE OUTCOMES:

After completing this course, the students should be able to:

1. Identify problem types in chemical engineering solvable using machine learning and artificial intelligence techniques.
2. Solve predictive problems in chemical engineering using machine learning.
3. Analyze chemical engineering data sets in both unsupervised and supervised learning settings.
4. **[ChE 297]** Assess the effectiveness of current research works that apply machine learning in chemical engineering problems.

*LMS = Learning Management System

Course Delivery

- **Meeting:** Every Tuesday, face-to-face, Room A301, Chemical Engineering Building.

Sunday	Monday	Tuesday	**Wednesday**	Thursday	**Friday**	Saturday
			1-2:30 PM		1-2:30PM	

- **Course Requirements:**

Requirement	ChE 197	ChE 297	Mode

• Final Project
  • Oral Presentation (40%)
  • Written Report (60%)
	50%	**40%**	Group (197)
			Indiv. (297)

• Machine Problems	**50%**	**40%**	Indiv., Async.
• Journal Critique		**20%**	Indiv. Async.

- **Grading System:**

[92,100]	[88,92)	[84,88)	[80,84)	[76,80)	[72,76)	[68,72)	[64,68)	[60,64)	[0,60)
1.00	**1.25**	**1.50**	**1.75**	**2.00**	**2.25**	**2.50**	**2.75**	**3.00**	**5.00**

Course Content

Feb 7	Week 1.	Introduction to Machine Learning
Feb 14	Week 2.	Linear Regression and Logistic Regression
Feb 21	Week 3.	Kernel Methods
Feb 28	Week 4.	Neural Networks
Mar 6	Week 5.	Trees and Ensemble Learning
Mar 13	Week 6.	Time Series Models
Mar 18	Week 7.	**MACHINE PROBLEM 1**
	----------	Reading Break + Lenten Break ----------
		(Week 8) (Week 9)
Apr 10	Week 10.	Dimensionality Reduction
Apr 17	Week 11.	Clustering
Apr 24	Week 12.	Density Estimation and Anomaly Detection
May 3	Week 13.	Hyper-parameter Tuning and Explainable AI
May 6	Week 14.	**MACHINE PROBLEM 2**
May 15	Week 15.	**Free Week**
May 22, 24	Week 16.	***Final Project Presentation***

Course Requirements

Final Project (50%, 40%)

- A team should have at most 3 members only (197).
- For ChE 297, this should be done individually.

- Aims:
  - Find a problem + data set that requires an ML solution.
  - Solve the problem using the ML methods discussed in class.
  - Present your results to the class.

- NO two teams should have the same problem.

- Grading and deadlines:
  - Oral Presentation (40%) – May 22 & 24, 2024
  - Written Report (60%) – May 31, 2024

Machine Problems (50%, 40%)

- Mode: Individual, take-home
- To be treated as a Long Exam.
- Submission deadline is **1 week** after release.

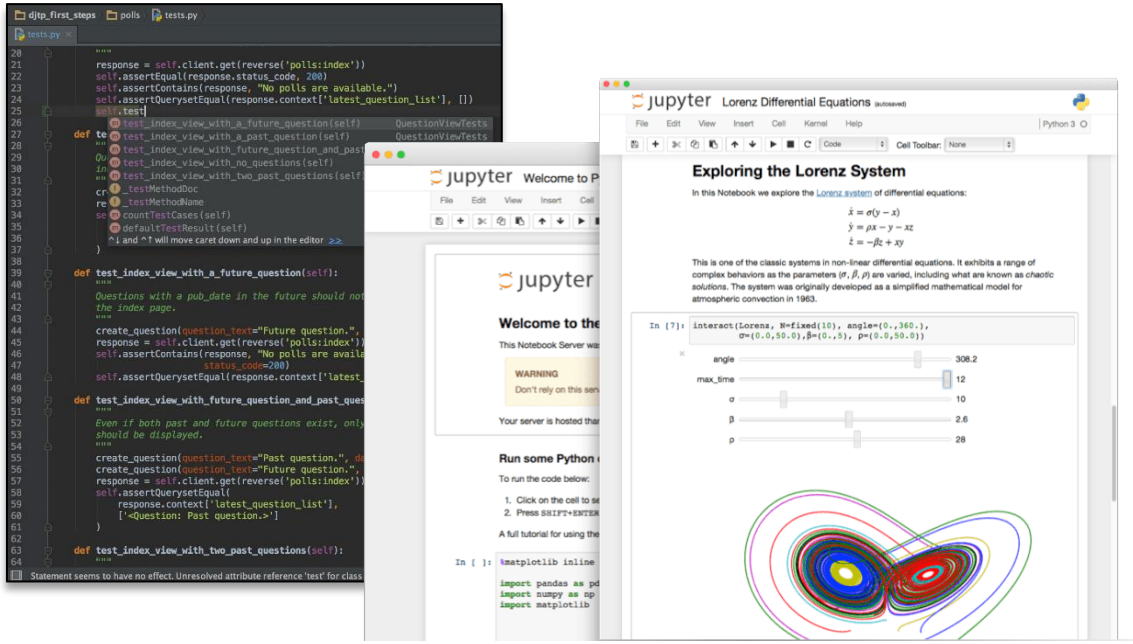
Journal Critique (0%, 20%)

- Mode: Individual, take-home
- Find a paper from a reputable journal.
  - Should at least have an impact factor.
  - Should be published in the last 5 years.
  - Review papers are NOT allowed.

- Send me the paper for approval first, then I will send guide questions for you to answer.

- Deadline for Paper approval: May 31, 2024
- Deadline for Critique submission: Jun 14, 2024

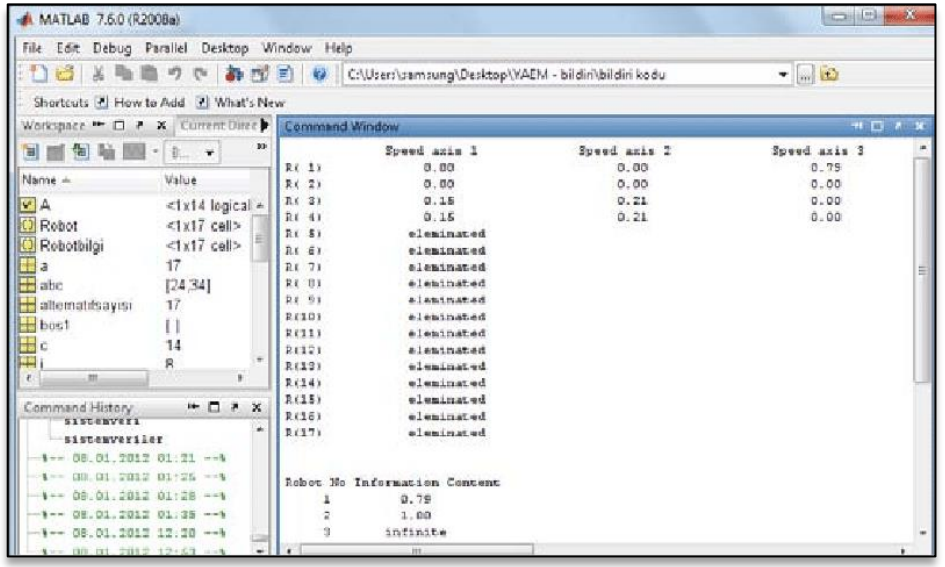
Required Software



- Anaconda >> Spyder
- Anaconda >> JupyterLab
- Google Colab
- Jupyter Notebook
- PyCharm
- JupyterLite
- Microsoft Excel (New)

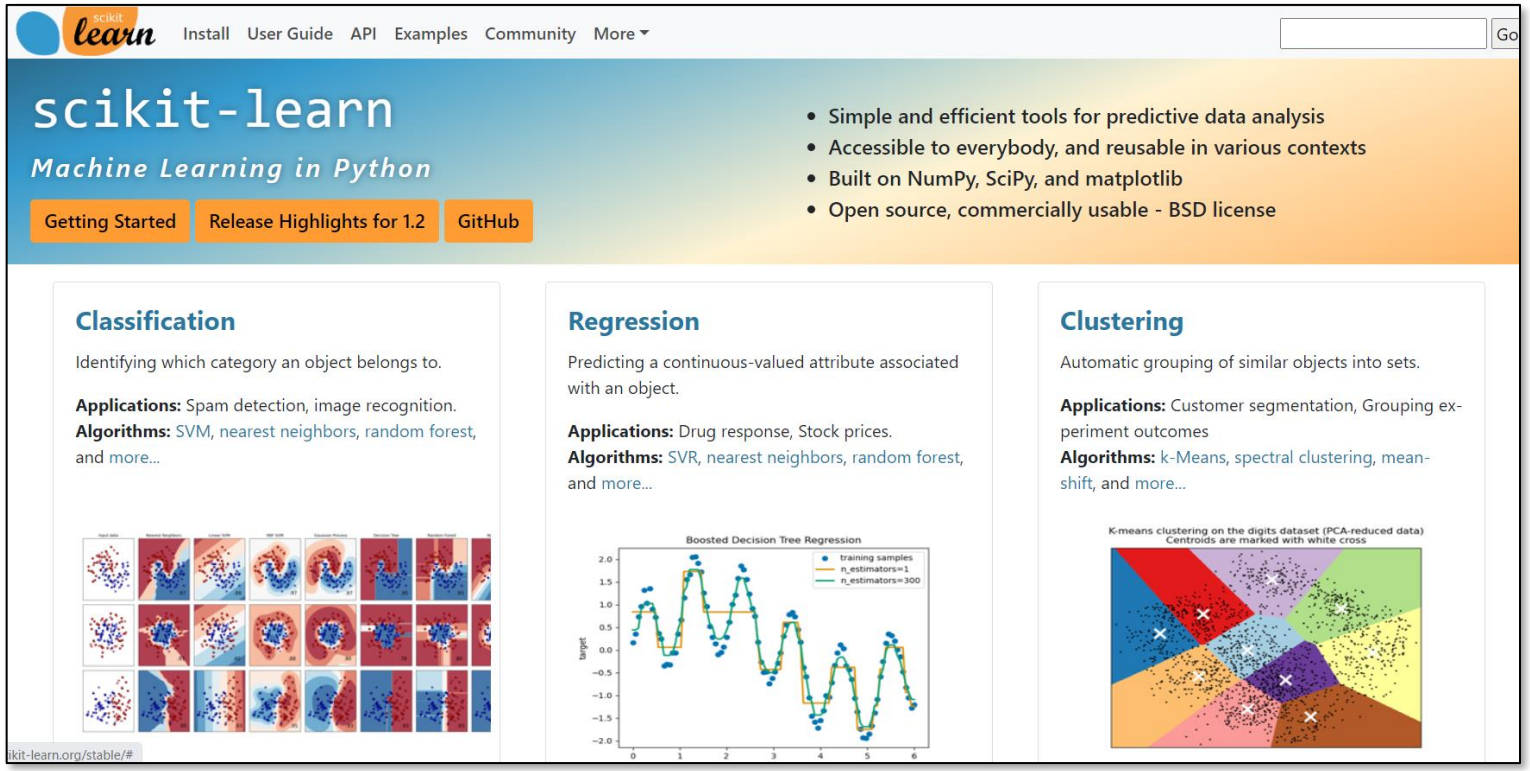
or

- You can download MATLAB by logging in to www.mathworks.com
  - Use your UP credentials!
- You can also use MATLAB online.



Required Software

- Python 3
  - https://www.python.org
- Numpy
  - http://www.numpy.org/
- Scikit-Learn
  - https://scikit-learn.org/
- Juptyer Lab
  - https://jupyter.org/try-jupyter/lab/
  - https://nbviewer.org/
- MS Excel



References

- Bishop (2006). *Pattern Recognition and Machine Learning.* Springer.
- Murphy, Kevin (2012). *Machine Learning: A Probabilistic Perspective.* MIT Press.
- Hastie et al. (2008). *The Elements of Statistical Learning.* 2nd Ed. Springer.
- Cristianini & Shawe-Taylor (2000). *An Introduction to Support Vector Machines and other kernel-based learning methods.* Cambridge University Press.
- Marsland, Stephen (2014). *Machine Learning: An Algorithmic Perspective*. Chapman and Hall. 2nd Ed.
- Rasmussen and Williams (2006). *Gaussian Processes for Machine Learning.* MIT Press. https://gaussianprocess.org/gpml/
- Geron, Aurelien (2019). *Hands-on Machine Learning with Scikit-Learn, Keras & TensorFlow*. O'Reilly Media.
- Journals and Conference Proceedings
- Python API, Sci-kit learn API: https://scikit-learn.org/stable/modules/classes.html
- Online Courses, Youtube Videos, etc.

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