Introduction to Machine Learning

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Outline

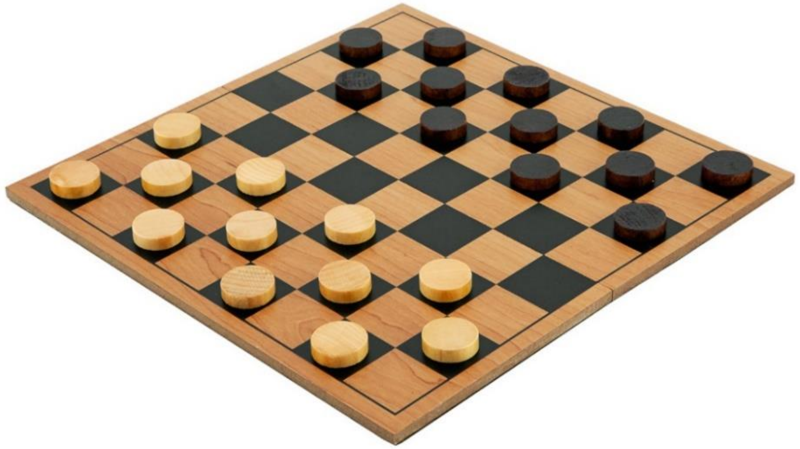
- What is Machine Learning?
  - Why only now?
  - Types of Learning Problems

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

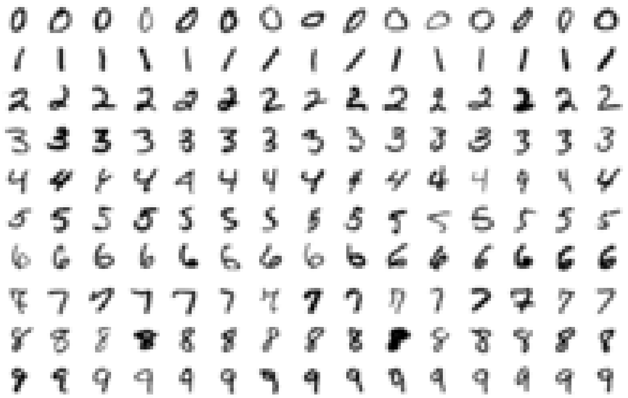
What is Machine Learning?

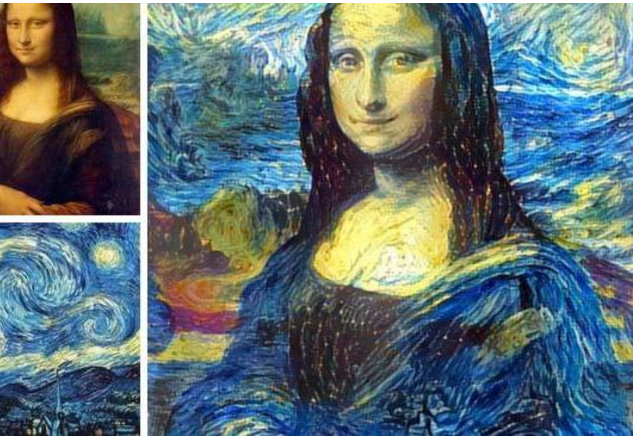
A field of study concerned with giving computers the *ability to learn* without being explicitly programmed.
(Arthur Samuel, 1959)

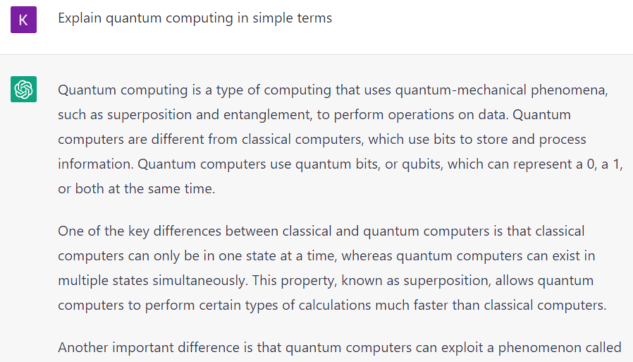
Arthur Samuel and the IBM 701 Computer



- 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.



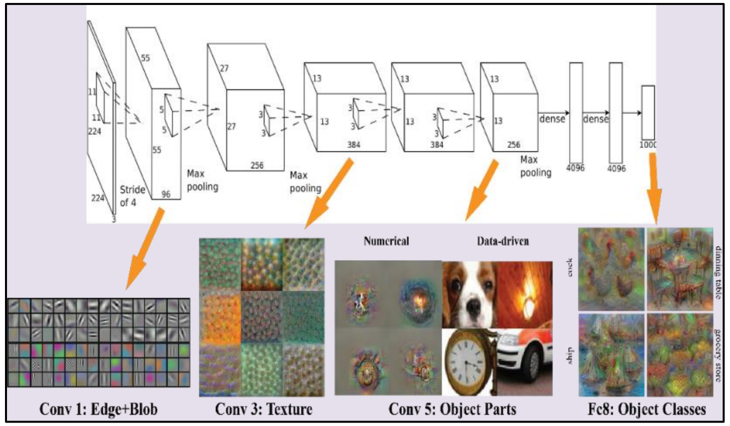




Typical ML Applications

- 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**



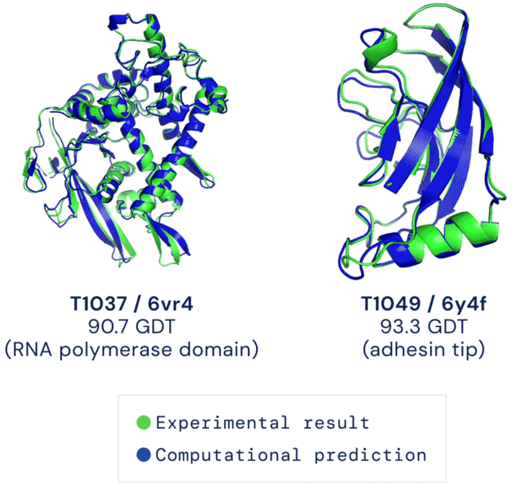
AlexNet
ImageNet Visual Recognition Challenge, **2012**

AlphaGo
Game of Go, **2016**

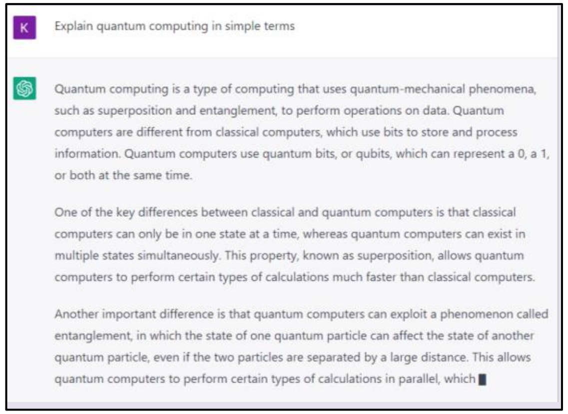
DALL-E
2021, 2022

IBM Deep Blue
Chess, **1997**

AlphaStar
StarCraft II, **2019**



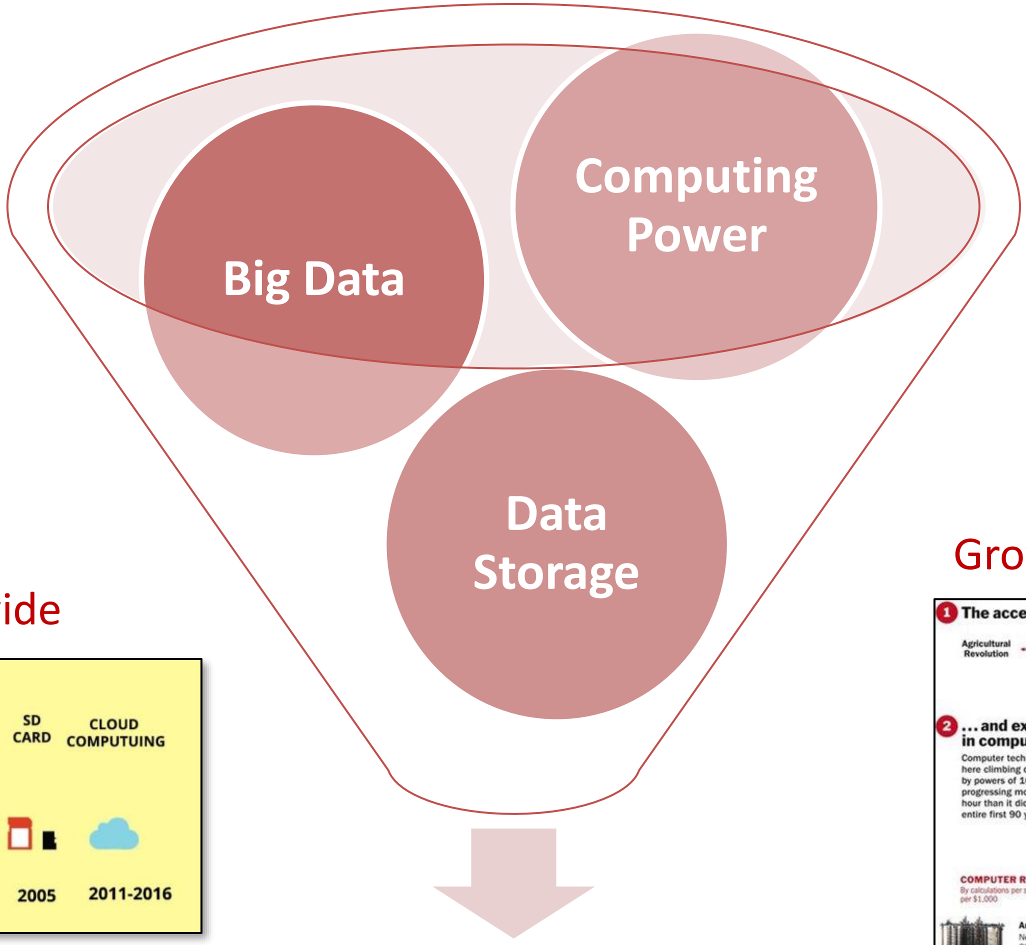
AlphaFold
Protein Structure Prediction,
2016, **2018**



ChatGPT
2022

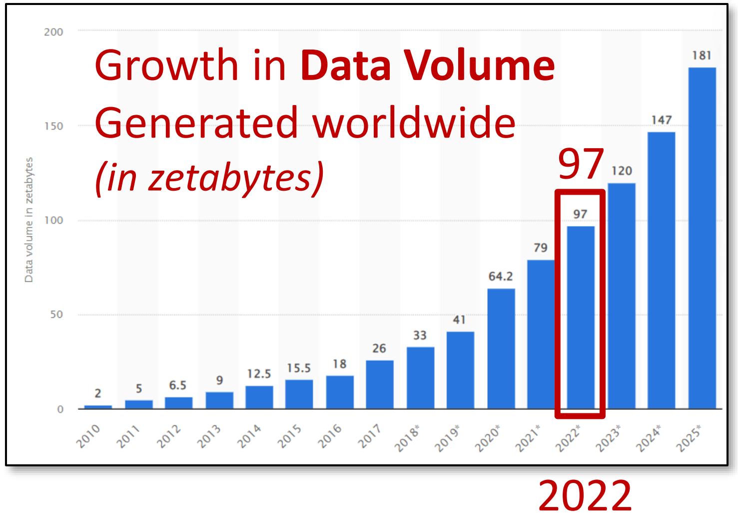
Machine Learning,
Data Science,
Data Analytics,

…why only now?

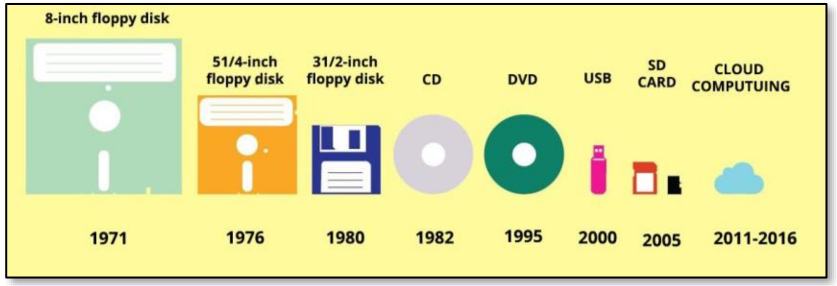


Machine Learning +

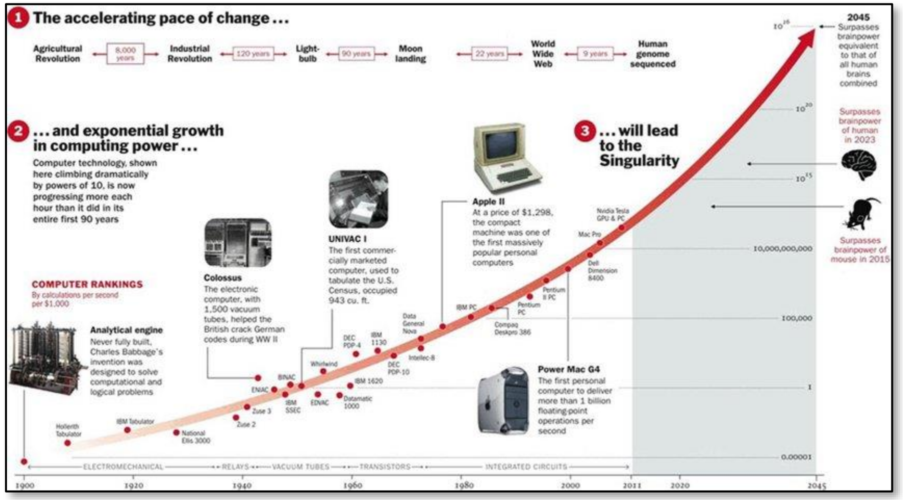
Practical Applications



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!

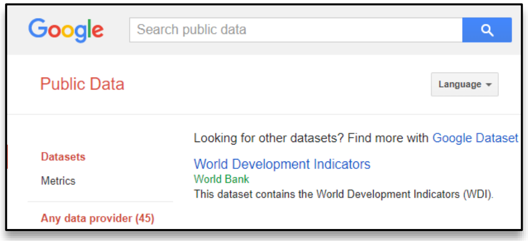
- There are about 1 trillion web pages.
- 1 hr of video is uploaded to Youtube every second.
- Human genomes have a length of 3.8×10^9 base pairs.
- Walmart handles more than 1 million transactions per hour.
- Etc…

Popular websites where we can get publicly available data:

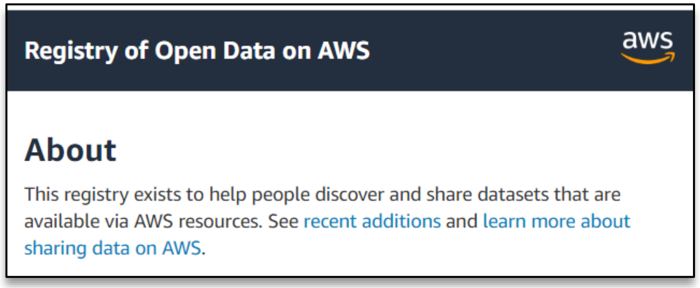
UCI Machine Learning Repository
Center for Machine Learning and Intelligent Systems

kaggle

OpenML
A worldwide machine learning lab



NASA



THE WORLD BANK
IBRD • IDA
Data

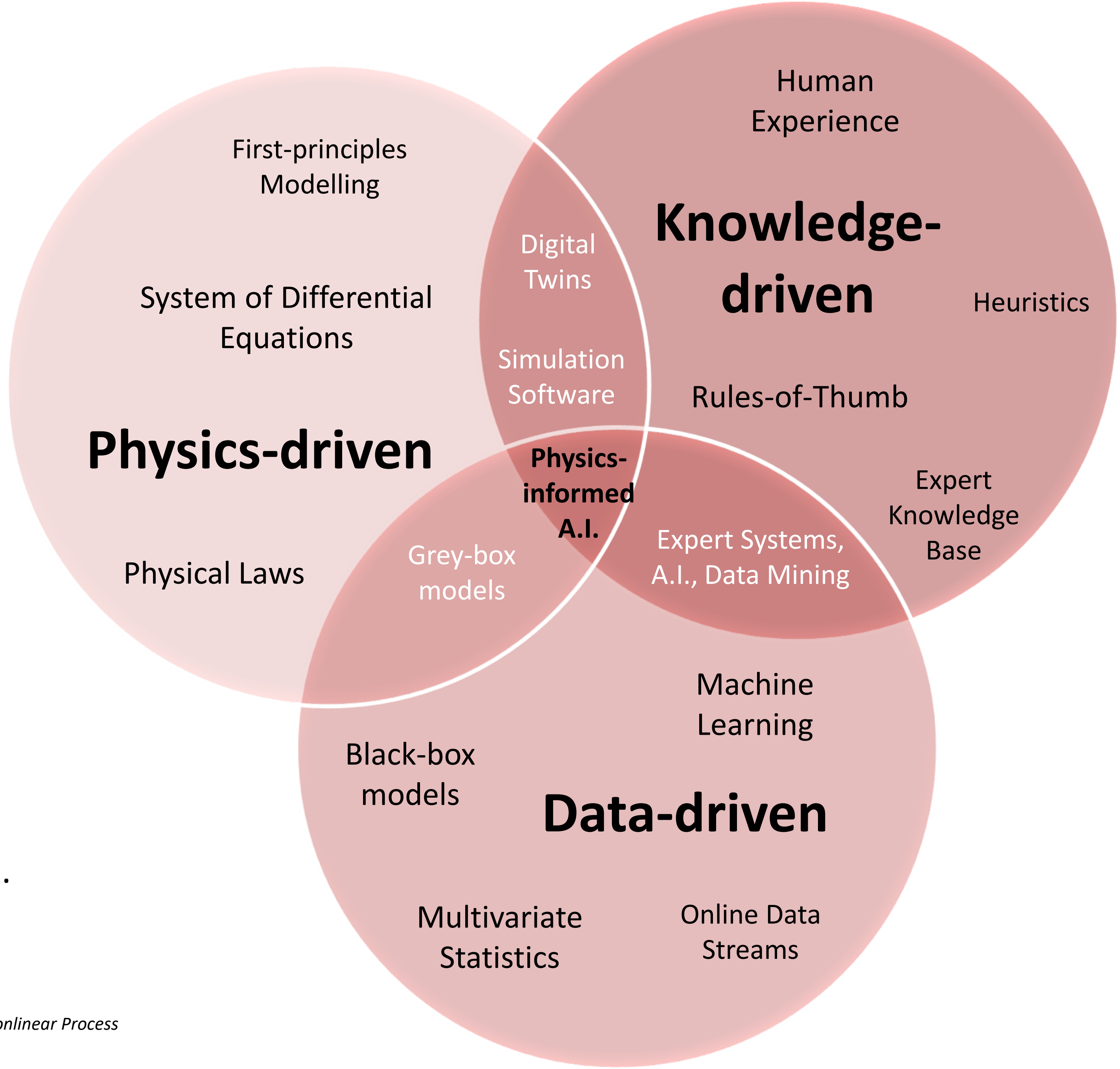
[1] Venkatasubramanian (2009). DROWNING IN DATA: Informatics and Modeling Challenges in a Data-Rich Networked World. *AIChE Journal.*
[2] Murphy (2012). Machine Learning: A Probabilistic Perspective. *MIT Press.*

Why use Machine Learning in your Industry?

Three approaches to engineering problems:

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

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

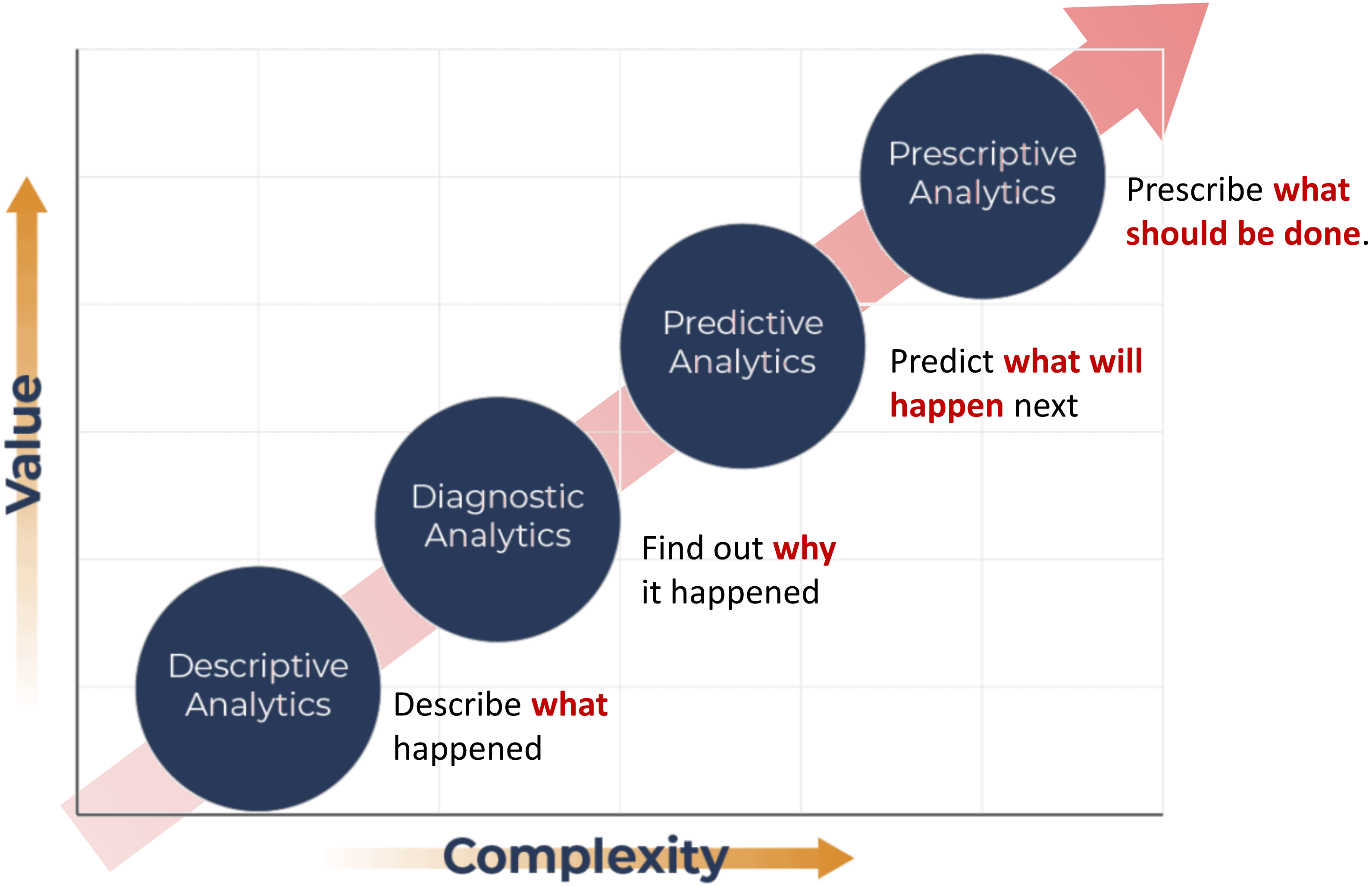


Reference: Pilario et al. (2020), *A Review of Kernel Methods for Feature Extraction in Nonlinear Process Monitoring.* MDPI: Processes, https://doi.org/10.3390/pr8010024

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.
- Ask yourself the purpose for using ML and AI.
- 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.



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  - **Types of Learning Problems**

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

Types of Learning Problems

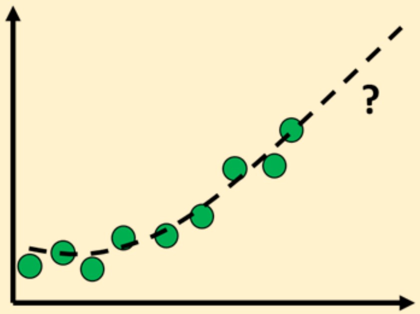
Supervised Learning

Learn a mapping or a function:

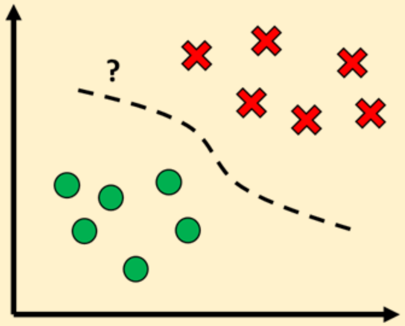
$$y = f(x)$$

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

Regression



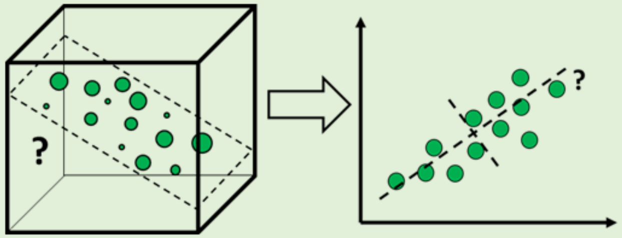
Classification



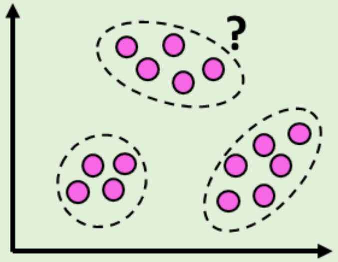
Unsupervised Learning

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

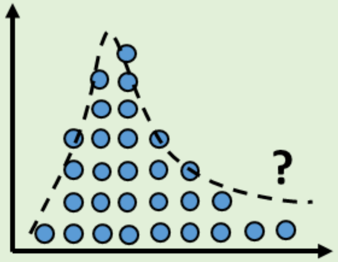
Dimensionality Reduction



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?

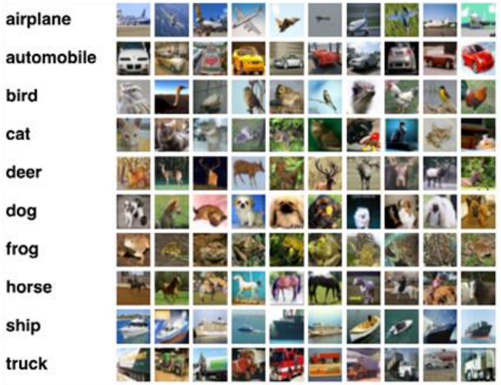
Are there images with similar patterns?

Types of Learning Problems

Semi-Supervised Learning

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

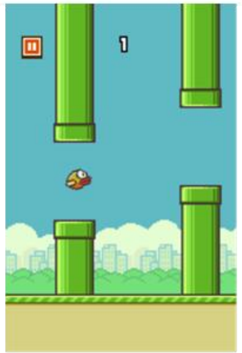
Labelled Data

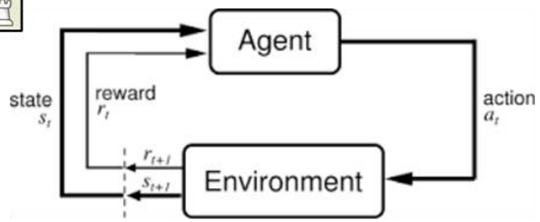


Unlabelled Data

Reinforcement Learning

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





Supervised Learning

Learn a mapping or a function:

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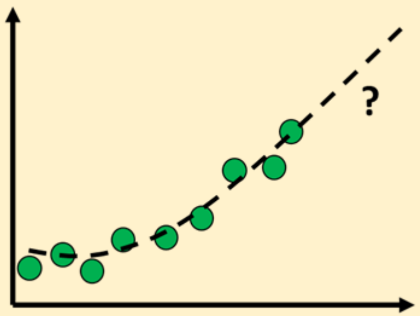
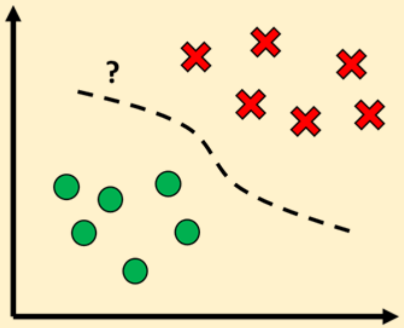
Regression



- **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

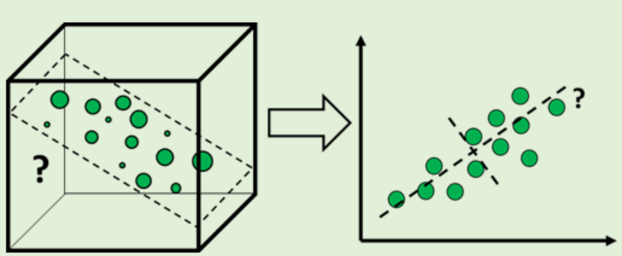


- **Given:** Training Data $\{\boldsymbol{x}_i, y_i\}_{i=1,2\ldots,N}$
- Target y_i is a **categorical** variable.
- Examples:
    - Classifying objects in images
    - Classifying chest X-ray images into COVID positive/negative
    - Handwritten digits recognition
    - Filter e-mails into spam/not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

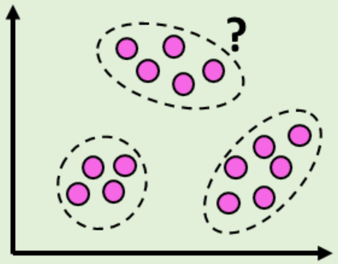
Unsupervised Learning

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

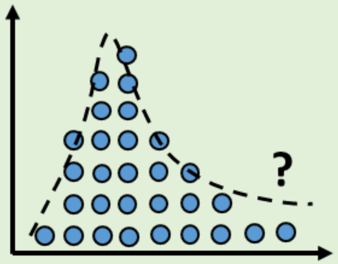
Dimensionality Reduction



Clustering



Density Estimation



Dimensionality Reduction

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

Clustering

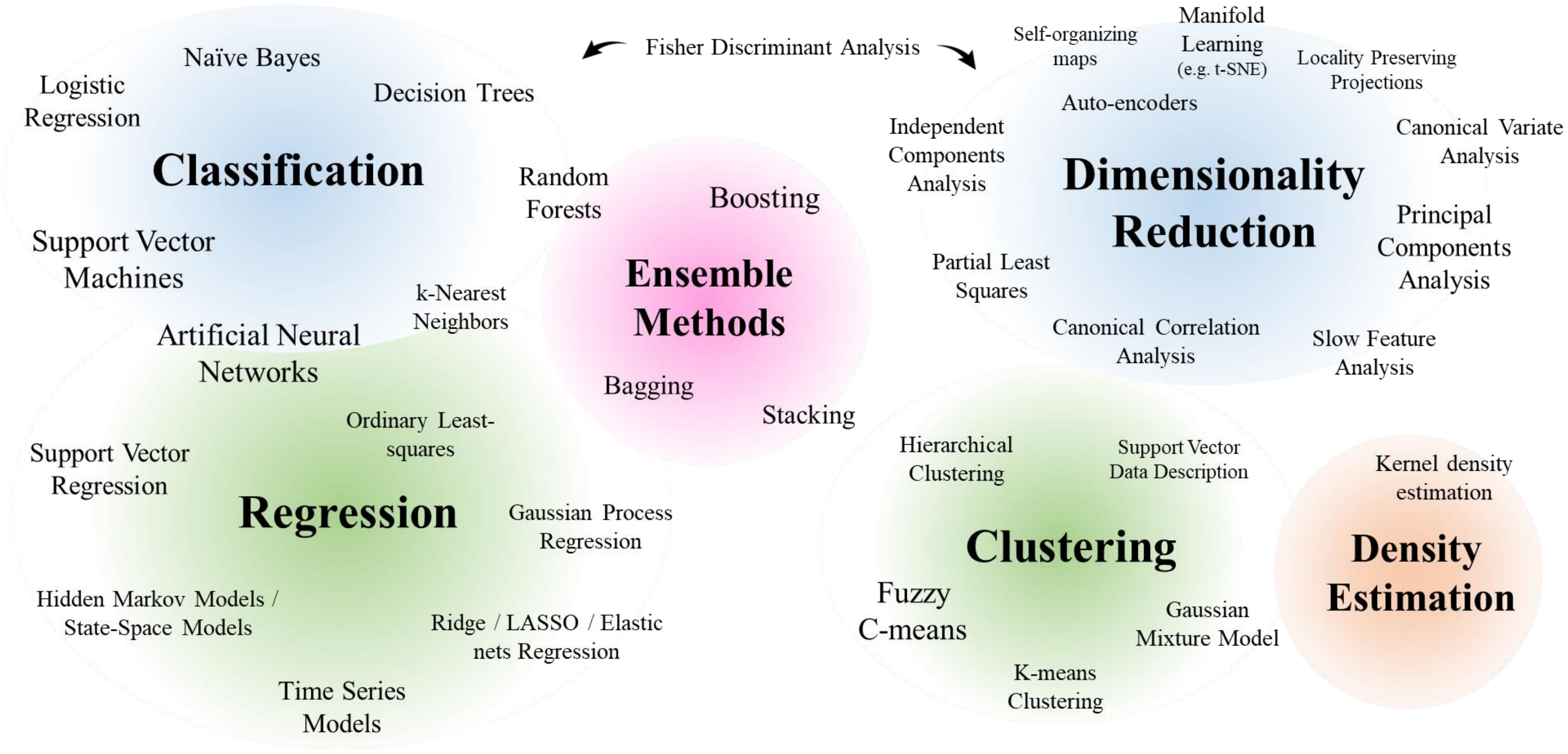
- **Given:** Data $\{\boldsymbol{x}_i\}_{i=1,2\dots,N}$
- **Group** similar data points together.
- <u>Examples:</u>
  - Customer segmentation
  - Recommendation systems
  - Identifying fake news
  - Clustering documents, tweets, posts

Density Estimation

- **Given:** Data $\{\boldsymbol{x}_i\}_{i=1,2\dots,N}$
- **Estimate** the distribution of your data.
- <u>Examples:</u>
  - Anomaly Detection
  - Novelty Detection
  - Generative Models
  - Finding distribution modes
  - Spatio-temporal analytics

Machine Learning Methods

Supervised Learning | Unsupervised Learning



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Outline

- What is Machine Learning?
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  - Types of Learning Problems

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

Introduction to the Course

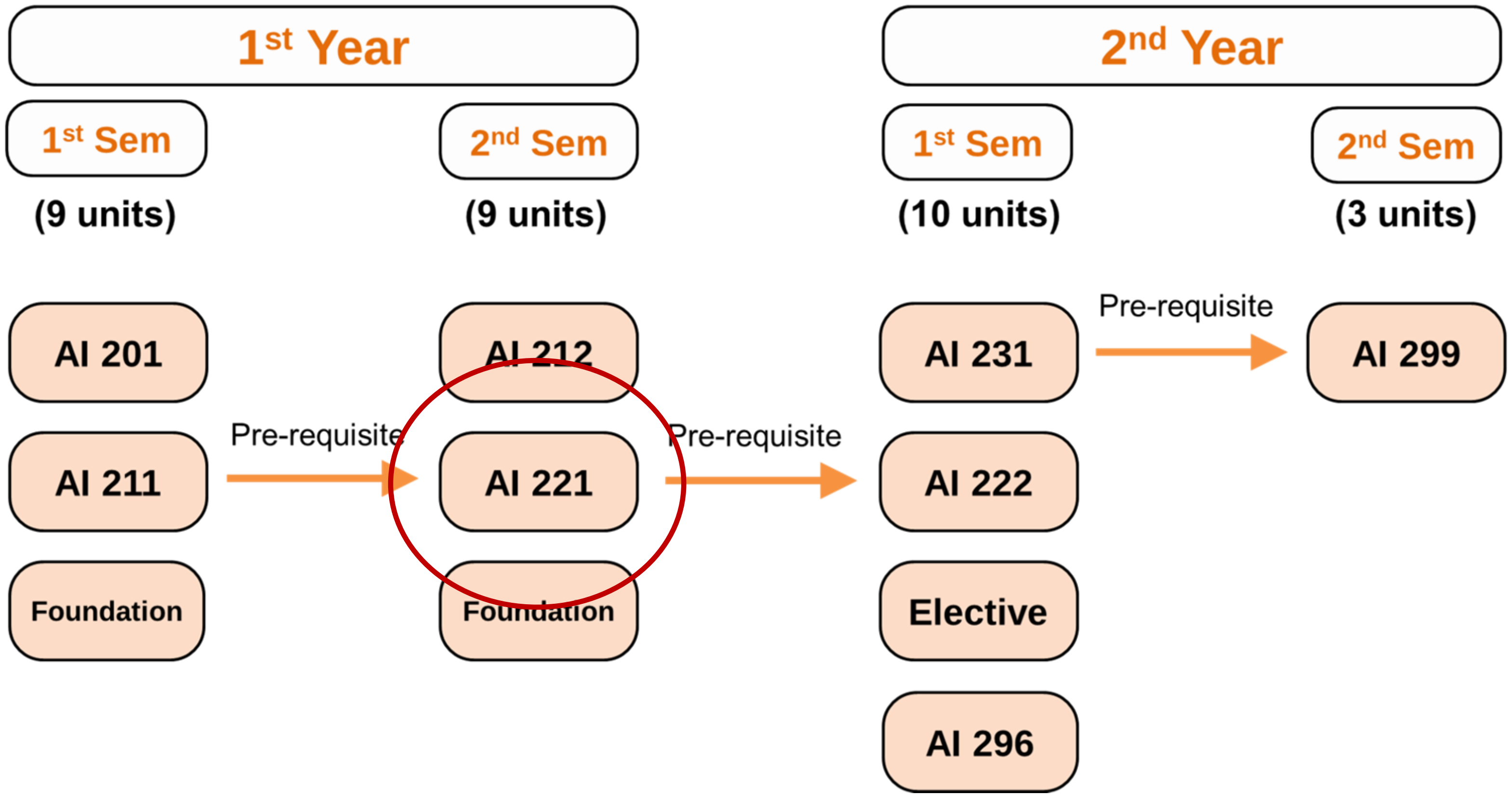
COURSE NUMBER:	AI 221
COURSE TITLE:	Classical Machine Learning
COURSE DESCRIPTION:	Linear Models. Kernel Methods. Neural Networks. Trees. Clustering. Dimensionality Reduction. Feature Engineering. Density Estimation. Ensemble Learning. Gaussian Processes. Bayesian Methods. Hyperparameter Search. AutoML. Explainability.
COURSE CREDIT:	3 units
	3.0 hours/week
COURSE LMS*:	**UVLE Course Page: AI 221 [SQRU]**
Github:	https://github.com/kspilario/AI221

*LMS = Learning Management System

Introduction to the Course

MEngg in Artificial Intelligence

Total Units: 31 Units

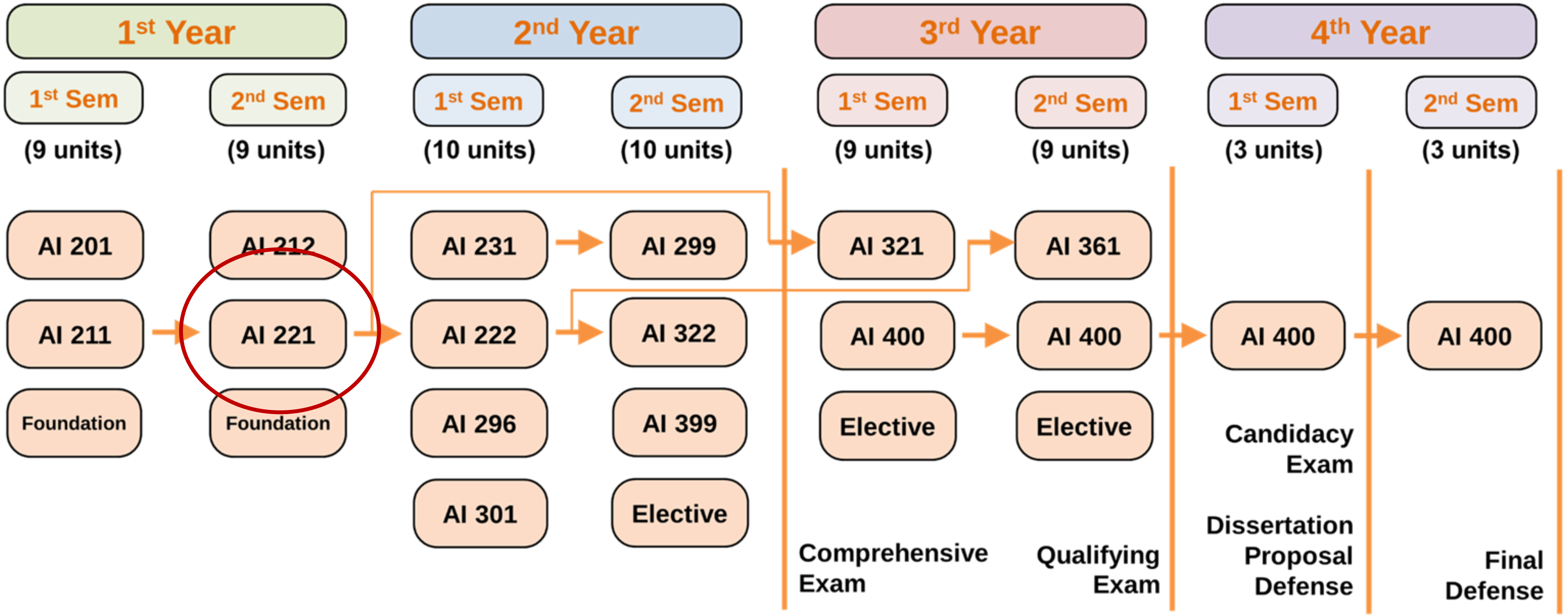


Introduction to the Course

PhD in Artificial Intelligence

Option A

Total Units: 62 Units
Requirement: 2 Publications



AI 221 Course Delivery

- **Meeting:** Every Saturday online via Zoom, except for the *Team Project Presentation.*

Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	**Saturday**

- **Course Requirements:**

Requirement	% of Final Grade	Mode

• Team Project
  • Oral Presentation (40%)
  • Written Report (60%)
	40%	"Teams" of 1 to 3 members only, Face-to-face

• Machine Exercises	**40%**	Individual, Asynchronous
• Journal Critique	**20%**	Individual, Asynchronous

- **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**

AI 221 Course Content

Feb 18	Week 1.	Introduction to Machine Learning
Mar 4	Week 2.	Linear and Logistic Regression
Mar 11	Week 3.	Support Vector Machines and Kernel Methods
Mar 18	Week 4.	Cross-validation and Hyper-parameter Optimization
Mar 25	Week 5.	Linear Dimensionality Reduction + Discriminant Analysis
Apr 1	Week 6.	Nonlinear Dimensionality Reduction
Apr 22	Week 7.	Clustering, Density Estimation, and Anomaly Detection
Apr 29	Week 8.	Trees, Weak Learners, and Ensemble Learning (Boosting, Bagging, Stacking)
May 6	Week 9.	Neural Networks for Classification, Regression, and Dim. Reduction
May 13	Week 10.	Neural Networks for Time Series
May 20	Week 11.	Gaussian Processes and Bayesian Optimization
May 27	Week 12.	AutoML and ML Explainability
Jun 3	Week 13.	***Team Project Presentation***

AI 221 Course Requirements

Team Project (40%)

- A team should have at most 3 members only.
- Aims:
  - Find a problem + data set that requires an ML solution.
  - Solve the problem using the ML methods discussed in class.
  - Present your results face-to-face.
- NO two teams should have the same problem.
- Grading:
  - Oral Presentation (40%)
  - Written Report (60%)

Machine Exercises (40%)

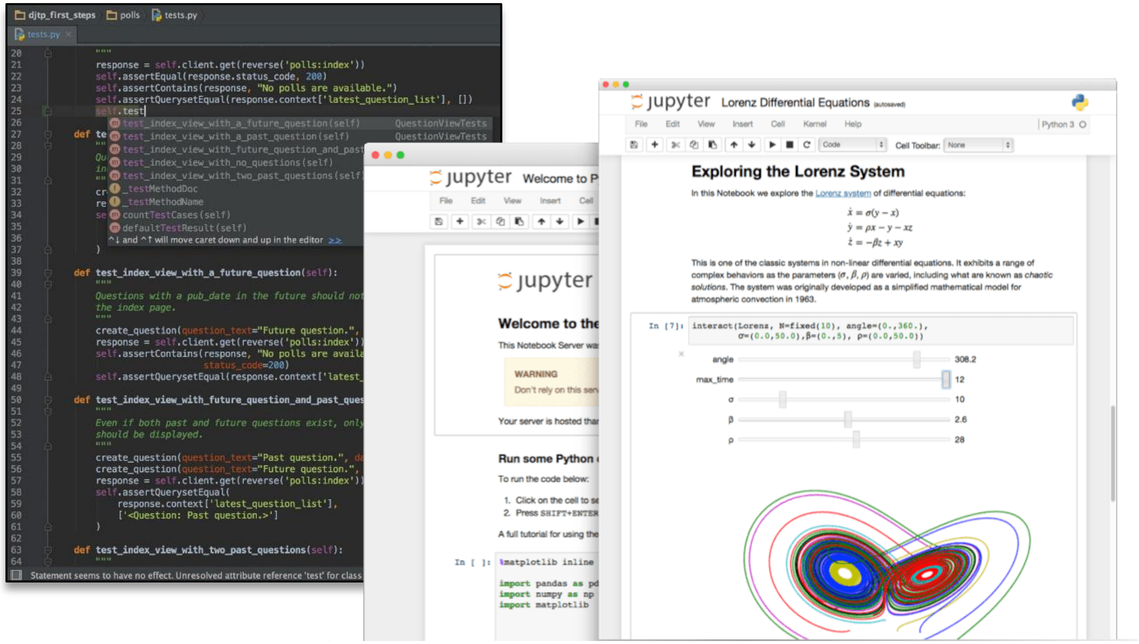
- Mode: Individual, asynchronous
- To be given every lecture week (Weeks 2-12).
- Submission deadline for all MEX is at the end of classes, June 8, 2023.

Journal Critique (20%)

- Mode: Individual, asynchronous
- Find a paper from a reputable journal / conference proceedings related to your field.
  - Should have an impact factor of 2 or higher.
  - Should be published in the last 3 years.
  - Send me the paper for approval first.
- Critique the paper. More guidelines to follow.

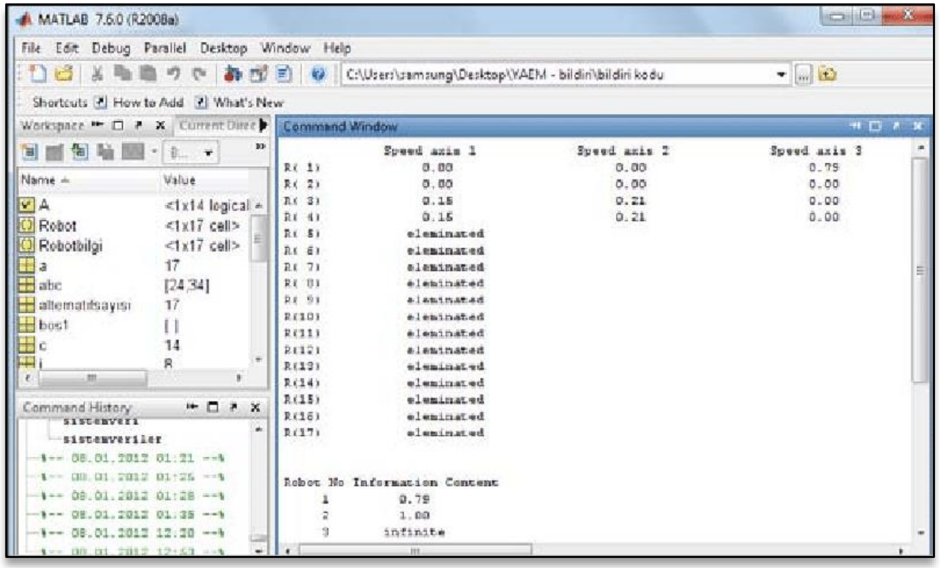
AI 221 Required Software

- Anaconda >> Spyder
- Google Colab
- Jupyter Notebook
- PyCharm

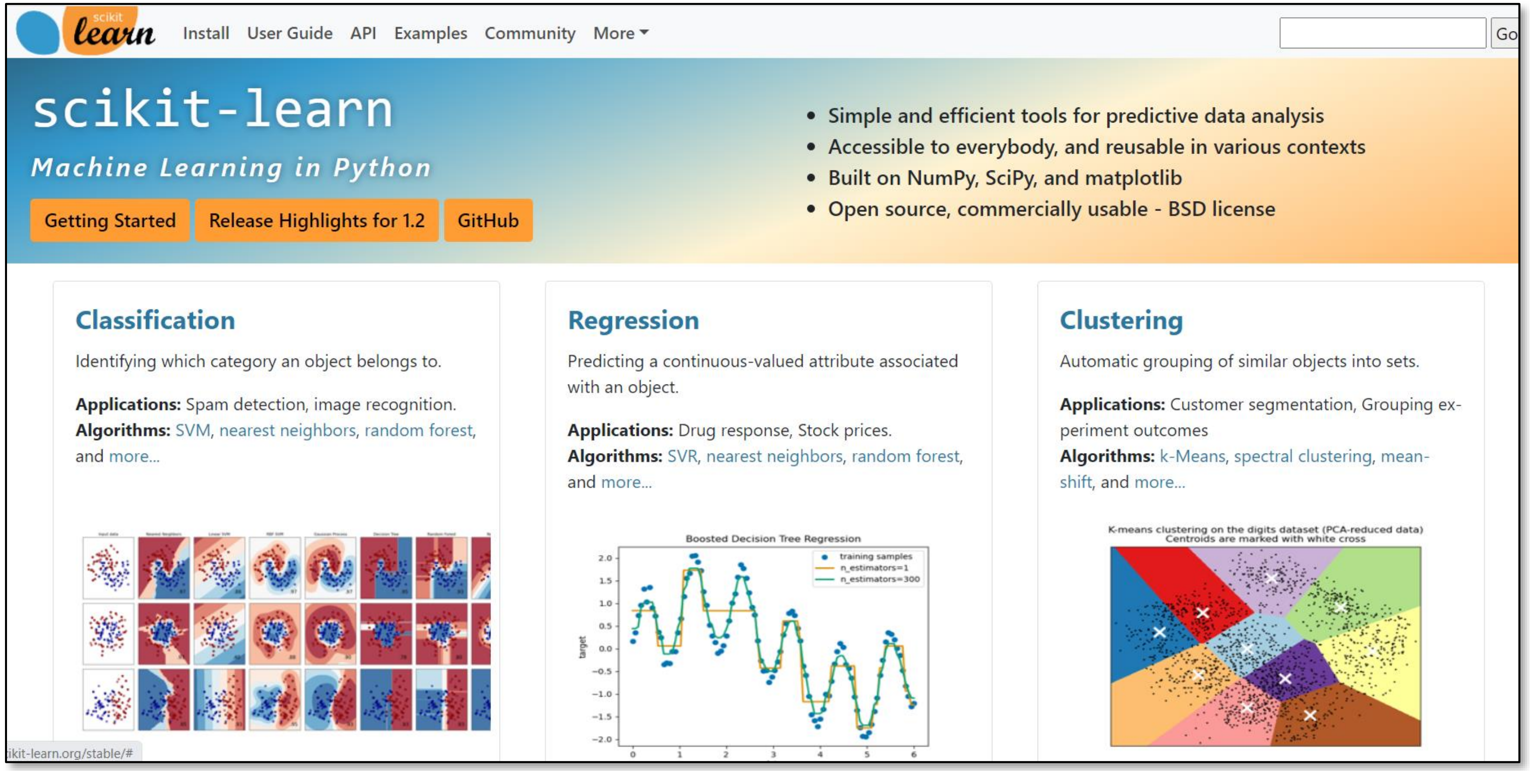


or

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



AI 221 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/

AI 221 Course Instructor

Current Position

Karl Ezra S. Pilario
Associate Professor
Department of Chemical Engineering
University of the Philippines, Diliman

- Process Dynamics & Control
- Programming in MATLAB, Python, Aspen HYSYS
- Numerical Methods in Engineering
- Plant Design and Research
- Machine Learning and Artificial Intelligence

University of the Philippines, Diliman

Research Lab

Head, Process Systems Engineering Laboratory (PSEL)
Department of Chemical Engineering
University of the Philippines - Diliman

Education

- **Bachelor's Degree:**
  Chemical Engineering, *SCL* (**2012**)
  University of the Philippines Diliman
- **Master's Degree:**
  Chemical Engineering (**2015**)
  University of the Philippines Diliman
- **PhD Degree:**
  PhD Energy and Power (**2020**)
  Cranfield University, United Kingdom

Research Interests

- Process Data Analytics
- Process Systems Engineering
- Industrial Process Monitoring and Predictive Maintenance
- Machine Learning for Energy, Water, and Environment
- Cheminformatics and Materials Informatics

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