



National Institute of
Diabetes and Digestive
and Kidney Diseases

Central Repository

NIDDK-CR Resources for Research

Data Science and Meet the Expert Webinar Series



February 27, 2025

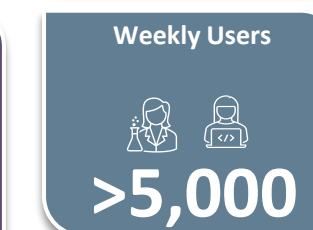
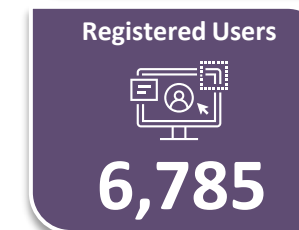
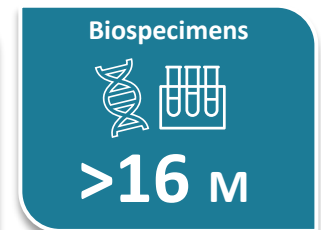
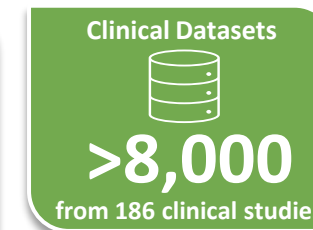
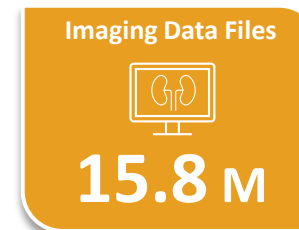
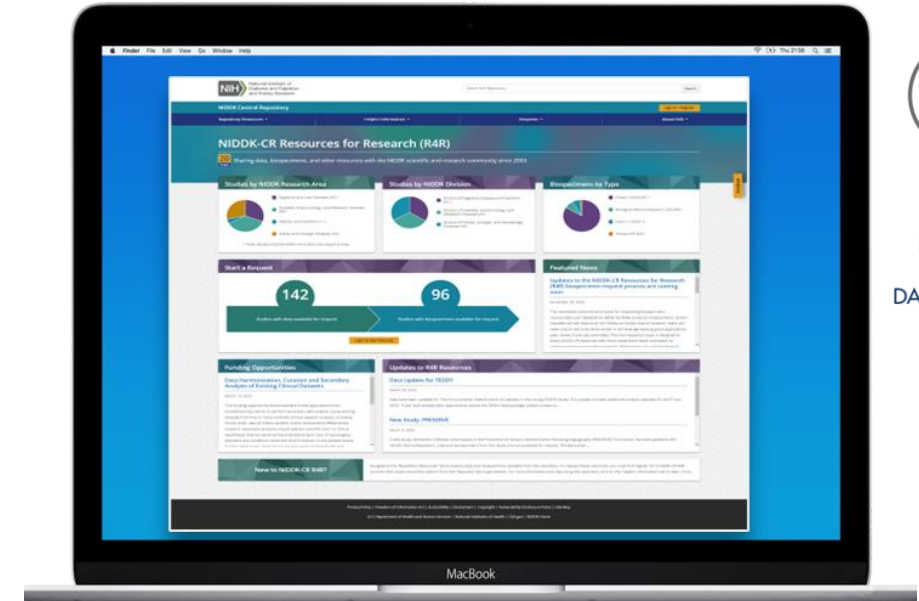


NIDDK Central Repository Overview

Mission

Established in 2003 to **facilitate the sharing of data, specimens, and other resources** generated from studies supported by NIDDK and within NIDDK's mission by making these **resources available for request to the broader scientific and research community.**

- Supports receipt and distribution of data and specimens in a manner that is ethical, equitable, and efficient
- Enables investigators not involved with the original work to test new hypotheses without the need to collect new resources
- Promotes FAIR (Findable, Accessible, Interoperable, and Reusable) and TRUST (Transparency, Responsibility, User focus, Sustainability, and Technology) principles



Recorded past tutorials, webinars, and other educational resources can be found on the NIDDK-CR website

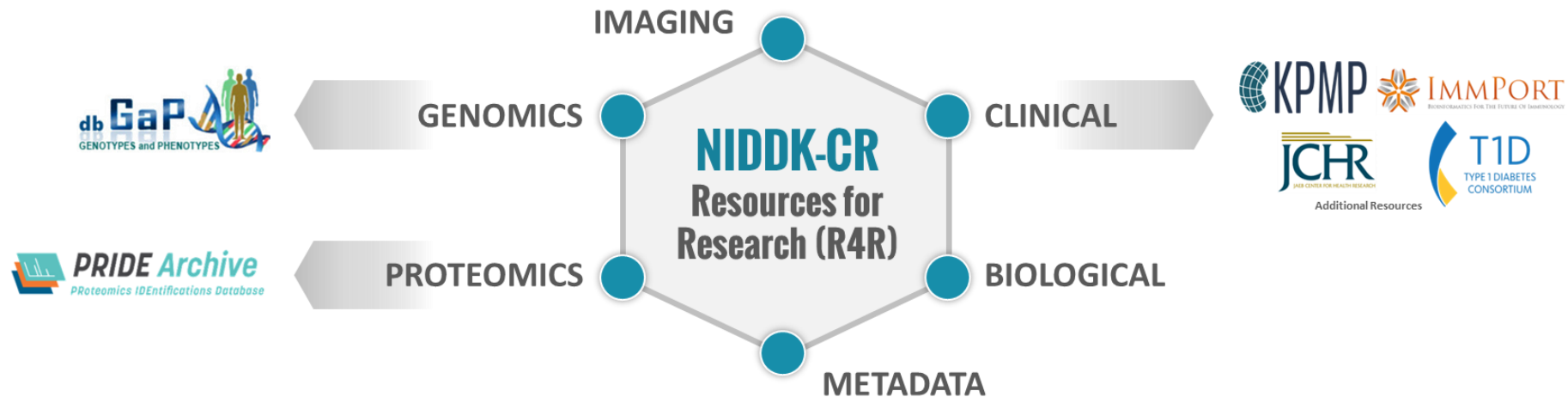


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NIDDK Data Sharing Ecosystem

The NIDDK-CR is a part of the broader NIDDK-funded biomedical data ecosystem and plays a key role in NIH's FAIRness and TRUSTworthiness goals. The NIDDK-CR houses a broad range of data types for secondary research and provides access to specimens and direct links to other repositories with additional resources such as genomics data.



FAIRsharing.org
standards, databases, policies

DataCite
FIND, ACCESS, AND REUSE DATA

re3data.org
REGISTRY OF RESEARCH DATA REPOSITORIES



Google Dataset Search /

Schema.org

NIH U.S. National Library of Medicine
ClinicalTrials.gov

Vivli
CENTER FOR GLOBAL CLINICAL RESEARCH DATA

PLANNING
PHASE

figshare

NIH
HEAL
INITIATIVE



Future Functionality: Analytics Workbench

Streamlining end-to-end data science lifecycle and discovery of data-driven biomedical insights.

Innovation and ease of use

A cloud-based analytics environment where researchers and data scientists can access a suite of integrated analytics tools and cloud computing resources to participate in data challenges and AI innovation.

Expected Benefits of Analytics Workbench:

Promote Collaboration

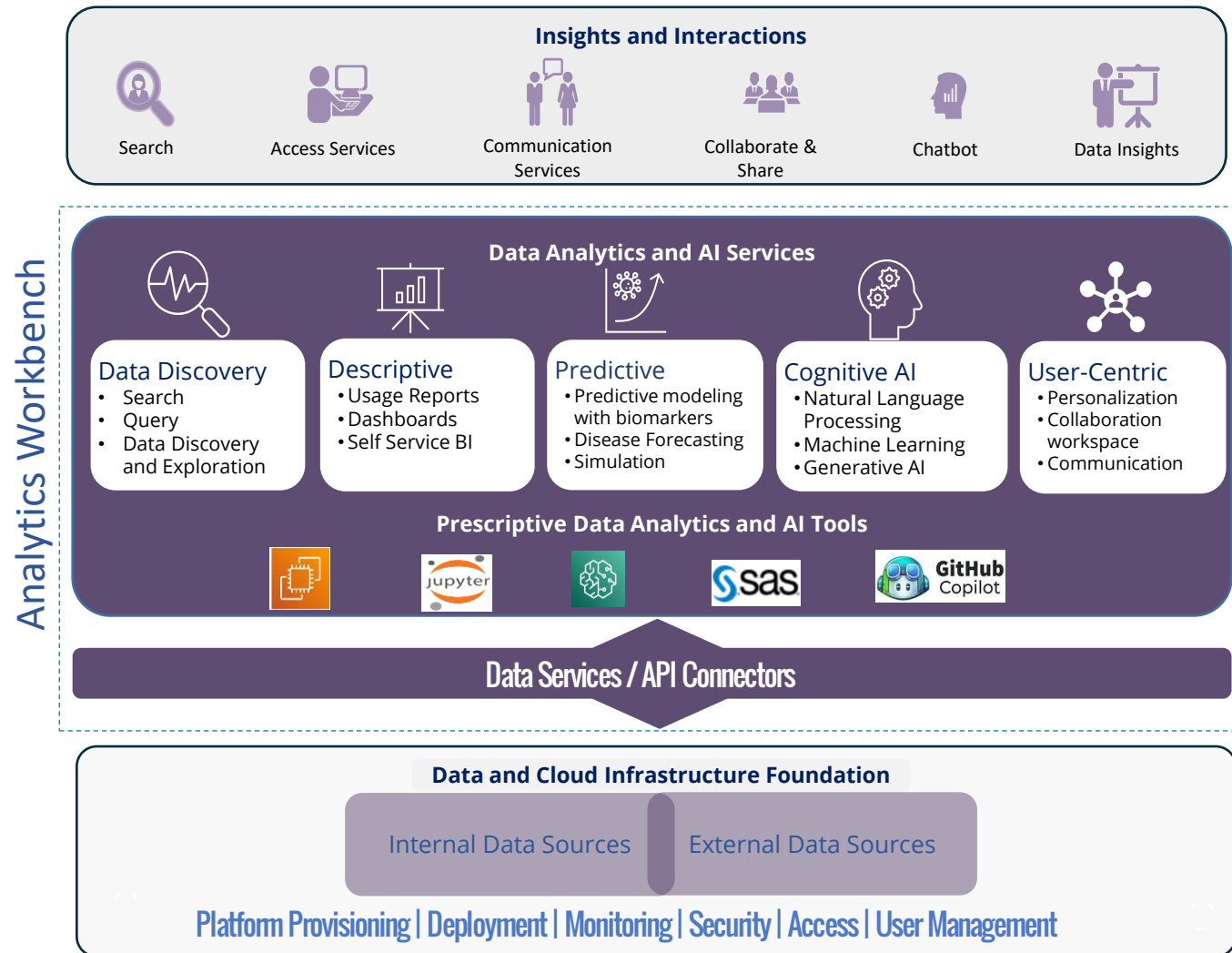
Support AI Innovation

Minimize Data Movement

Improve User Experience

Discover Data Insights

Advance NIDDK Research Mission





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Data Science Centric Challenge Series

Goals of NIDDK-CR Data-science centric challenge series

- Develop tools, approaches, models and/or methods to increase data interoperability and usability for artificial intelligence (AI) and machine learning (ML) applications
- Augment and enhance existing data for future secondary research, including data-driven discovery by AI/ML researchers
- Discover innovative approaches to enhance the utility of datasets for AI/ML applications



Visit our website for more information on our data-centric movement and to learn more about our past data-challenges



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Data Science and Meet the Expert Webinar Series

About the Series

- Aims to accelerate data science and AI-driven biomedical research by fostering collaboration between biomedical researchers and experts in the field
- Monthly webinar held on the **last Thursday of each month**

Upcoming Webinars

- Data science fundamentals
- Artificial Intelligence fundamentals
- FAIR data sharing
- Privacy protections for sharing human research participants' data
- Different privacy preserving techniques and implications for secondary researchers
- Challenges, opportunities, and considerations for secondary researchers using electronic health records and real-world data sources
- Impact and innovations realized



Learn more about the webinar series, register for future webinars, and access past webinar materials and recordings



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Meet the Experts



Arica Christensen is a Lead Associate Data Scientist at Booz Allen Hamilton, with a B.S. in Industrial and Systems Engineering from the University of San Diego. She specializes in natural language processing techniques and supervised machine learning. Arica has supported NAVWAR C4I PMW 130 on Project RAVEN applying predictive and proactive analytics for fleet readiness and cyber awareness. Currently Arica supports the Chief Digital Artificial Intelligence Office focusing on the development of dashboards and data pipelines measuring risk and resilience for all sailors at the individual and UIC level. Additionally, Arica leads the NAVWAR 4.0 Data Science Learning Program to create and facilitate trainings Navy wide on data science, machine learning, and artificial intelligence techniques.



Gordon Aiello is a Lead Scientist at Booz Allen Hamilton with a PhD in Applied Mathematical and Computational Sciences. He works full-time developing and delivering specialized data science, artificial intelligence, machine learning, and Python trainings for clients in the Navy and Intelligence Community. Prior to joining Booz Allen Hamilton, Dr. Aiello worked in the Office of Macroeconomic Affairs at the U.S. Department of State, using machine learning techniques to analyze developing and emerging market economies. Additionally, he has taught courses on data science and the R programming language for the Foundation for Advanced Education in the Sciences (FAES) at the NIH. He is passionate about working with others to expand their understanding of data science techniques and their applications.



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Data Science Fundamentals

NIDDK-CR Data Science

Meet the Experts Webinar Series

Feb 27th, 2025

Presented by: Booz Allen Hamilton





Training Guidance

- Avoid CUI/PII/PHI conversations
- Questions in Teams Chat are encouraged
- Due to size of class, stay on mute until end of class





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Instructor Introductions



Data Science Learning Program

If you're new to data science, start your learning journey with the **Foundations** courses. A more in-depth learning track starts with the **Data Science Fundamentals** course and continues to the **Data Science Labs**. Those interested in more specialized topics can explore courses in the **Select Topics** track.

Foundations for Data Citizens

- Data Citizen best practices
- Data governance
- Data-driven organization



Foundations of Data Analytics

- For NAVWAR supervisors
- Data Science Overview
- Machine Learning and Artificial Intelligence



Data Science Fundamentals

- Comprehensive intro to Data Science
- Python programming
- Statistics, Probability and Linear Algebra refresher
- Machine learning and Artificial Intelligence



10.5 hours (3 sessions)



Data Science Project Lab*

- Theory-to-practice
- Case study format
- Hands-on exercises
- Tabular data cleansing and processing techniques
- Full-cycle analytics process



12 hours (3 sessions)



Data Science NLP Lab*

- Theory-to-practice
- Case study format
- Hands-on exercises
- Natural Language Processing Techniques
- Large Language Models



12 hours (3 sessions)



INTRODUCTION

THEORY-TO-PRACTICE

*Completion of the Introduction to Python course is recommended for those without programming experience.

Introduction to Data Visualization

- Telling a story with your data
- How to create more impactful briefings
- Not product specific



3 hours



Python Fundamentals for Data Science

- Foundational Python syntax
- Develop essential analytic skills
- Machine Learning and Artificial Intelligence



7 hours (2 sessions)



Artificial Intelligence Fundamentals

- AI initiatives and foundational AI
- AI ecosystems and AI operations
- Responsible and Ethical AI
- Neural Networks



7 hours (2 sessions)

Data Science for Managers

Developed in partnership with NGA

- Management responsibilities in Data Science Projects
- Ethical considerations in Data Science
- Data Science and AI Opportunities

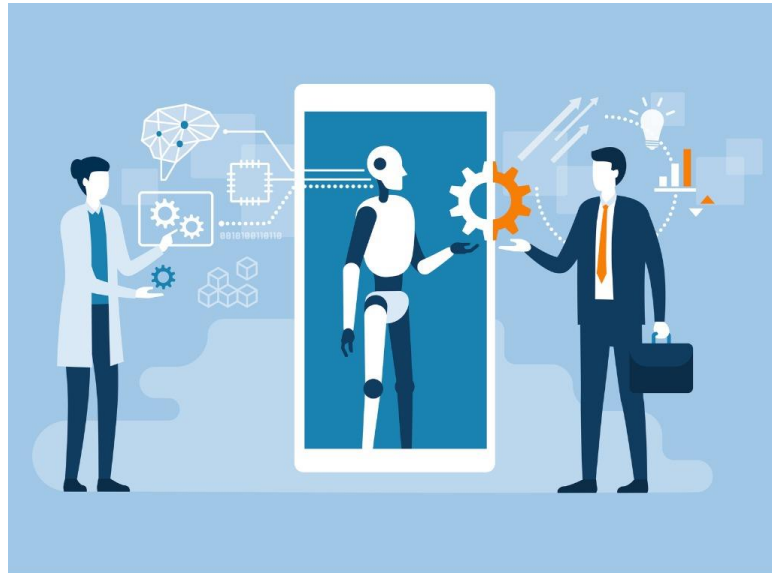


8 hours

SELECT TOPICS



Agenda



1. The Data Science Process
2. Supervised and Unsupervised Learning Techniques
3. Deep Learning
4. Specialized Data Science Topics
 1. Computer Vision
 2. Time Series
 3. Natural Language Processing



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The Data Science Process





Data Science Defined

The goal of data science is to extract meaningful insights from data.

Data – any kind of qualitative or quantitative set of values

- Common examples in data science today:

- Natural text: "I'm cold," "I'm not very cold"
- Categories: "yellow," "green," "red"
- Numbers: 1, 2.53, -4
- Images:



- Sometimes you have the data, sometimes you need to procure the data

Science – a systematic approach to building knowledge by testing hypotheses

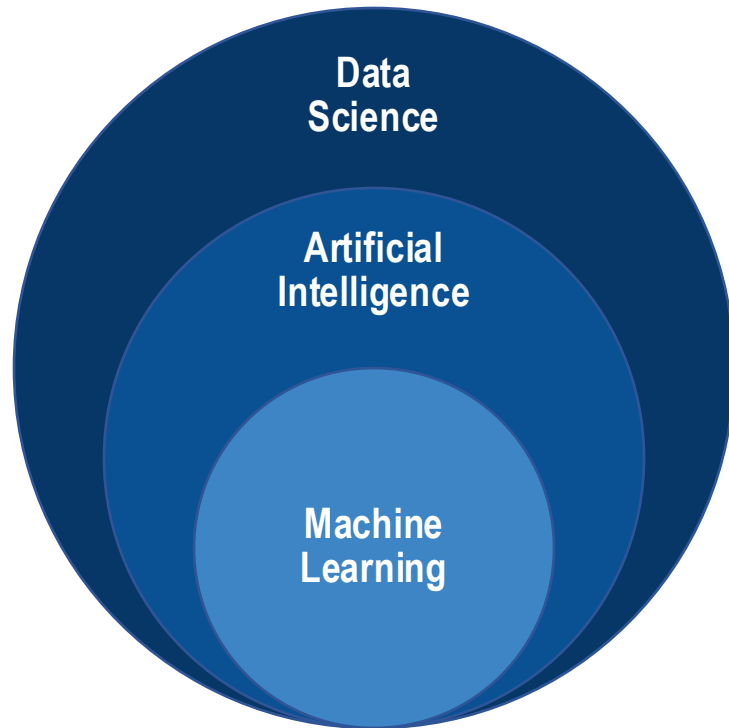
- Think Scientific Method:

Define a hypothesis → Collect the data → Analyze results → Draw conclusions

- Hypotheses must be testable, and experiments must be reproducible



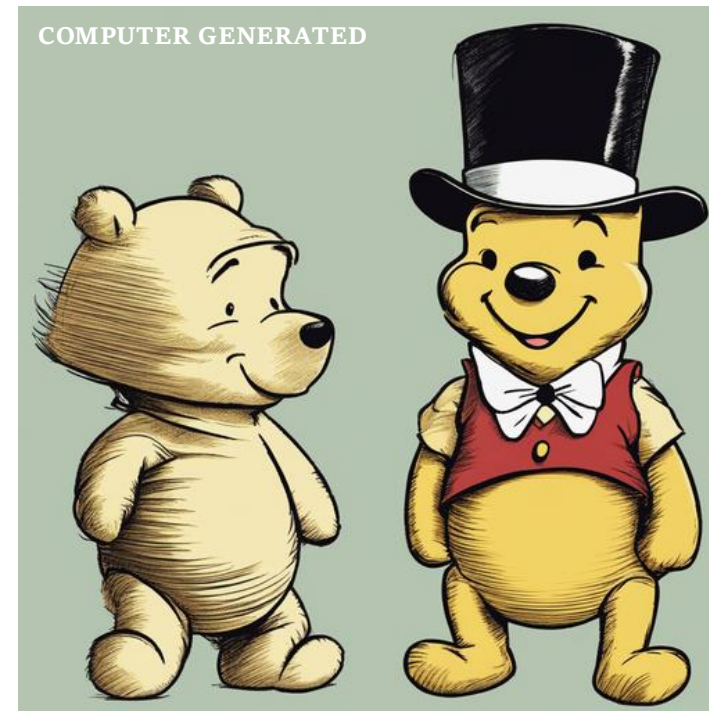
AI Is a Subset of Data Science



Artificial Intelligence (AI)

The theory and development of computer systems able to perform tasks normally requiring human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages

Machine Learning is an application of **Artificial Intelligence**, and Machine Learning is part of **Data Science** by applying algorithms and statistics to extract knowledge and insights from data



Statistics

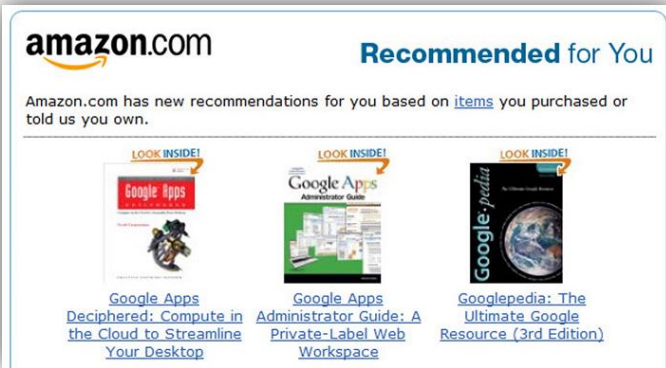
Data Science



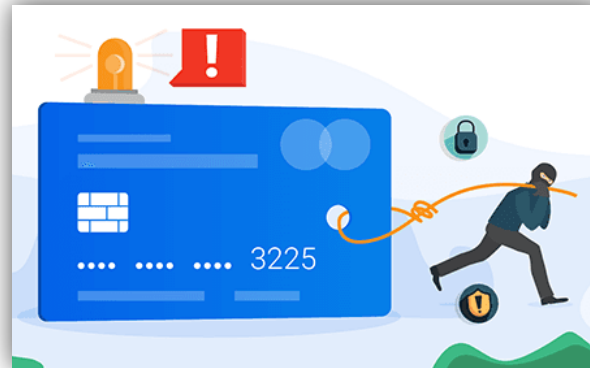
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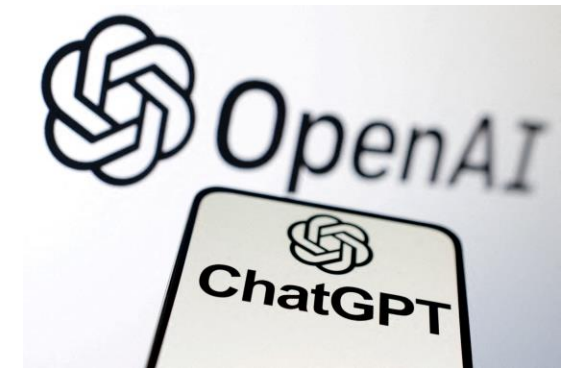
Data Science in the Commercial Space



Amazon: Recommendation Systems



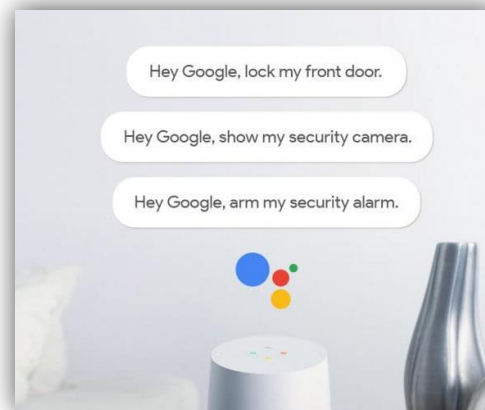
Credit Card Fraud Detection



ChatGPT



Snapchat: Computer Vision



Google Voice Recognition



UPS ORION (On-Road Integrated Optimization and Navigation)



Data Science in Healthcare

- **Predictive Analytics for Early Diagnosis** – Data science enables early detection of diseases by analyzing patient data, identifying risk factors, and improving treatment outcomes.
- **Personalized Medicine** – Machine learning models help tailor treatments based on a patient's genetic profile, lifestyle, and medical history, leading to more effective therapies.
- **Early Detection and Progression Monitoring of Kidney Disease** – Data science helps analyze lab results (e.g., creatinine levels, eGFR) to detect kidney disease in its early stages and predict progression, allowing for timely intervention.
- **Diabetes Prediction and Management** – Machine learning models can analyze patient data, including glucose levels and lifestyle factors, to predict diabetes risk, personalize treatment plans, and optimize insulin management.

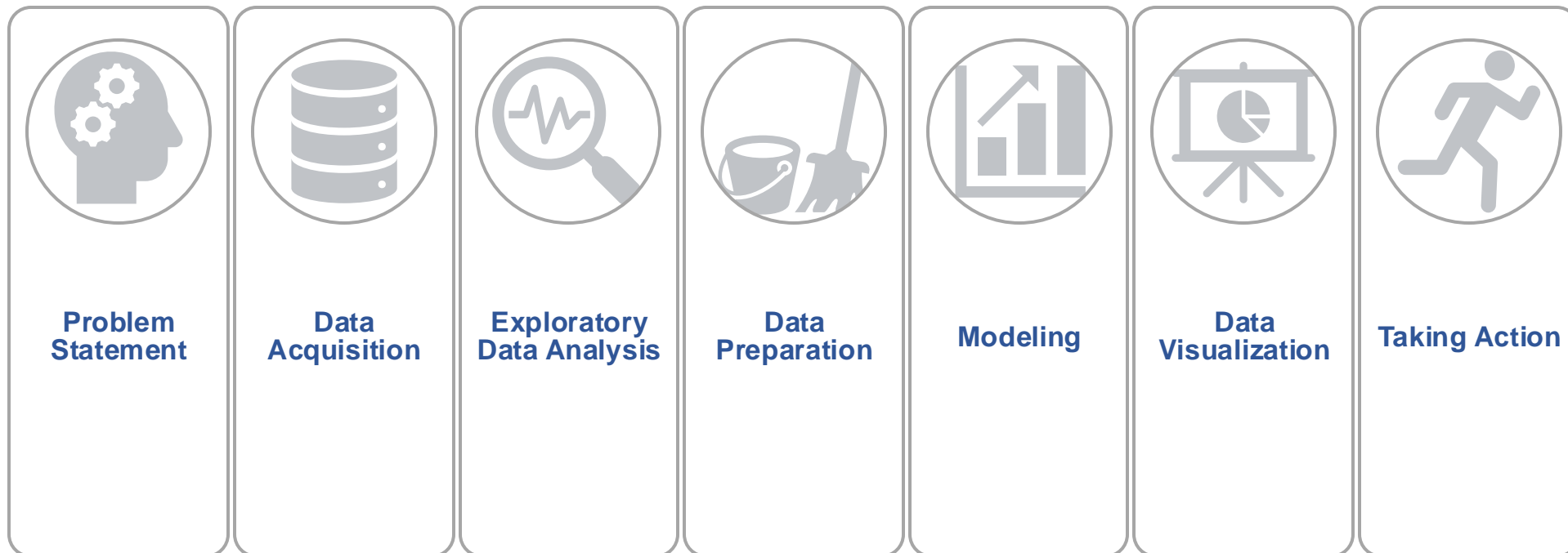




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Data Science Process





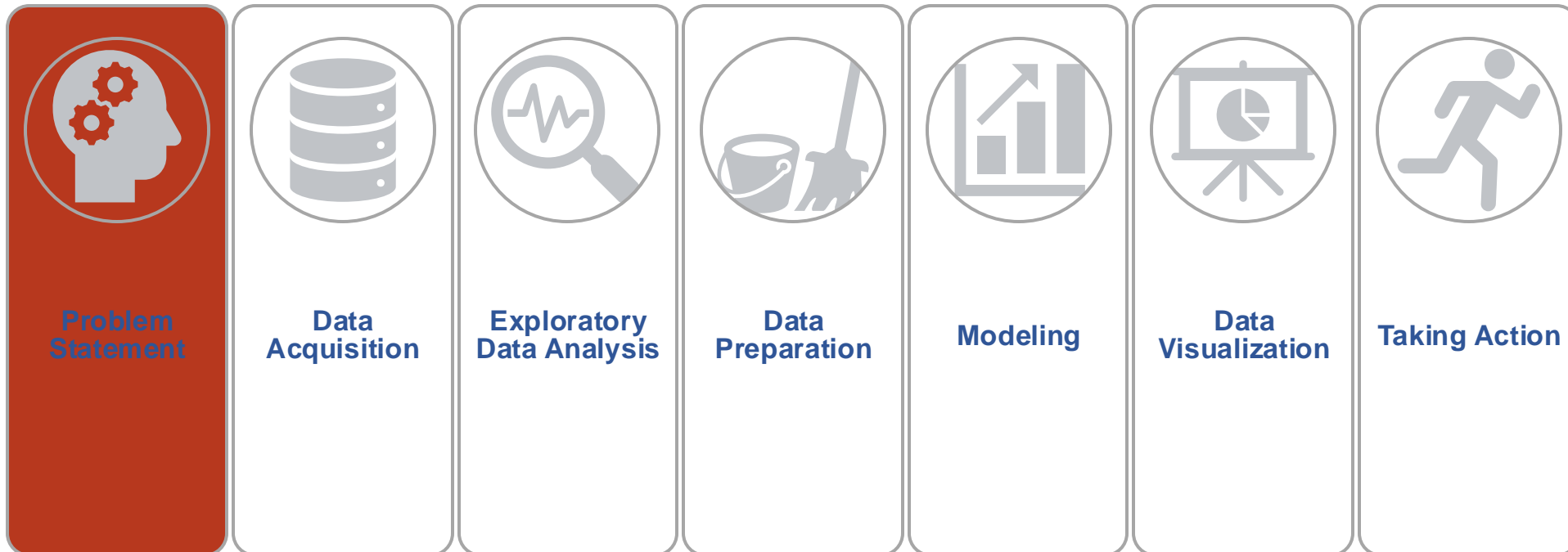
7 Step Data Science Process

Navigate through a data science project using the seven-step data science process:

1. Form a SMART problem statement, understanding what data science can and cannot do
2. Acquire useful data that can assist in solving the problem statement
3. Explore data and analyze preliminary findings to leverage initial insights from the data
4. Prepare data for use in machine learning pipelines
5. Understand basic machine learning model concepts
6. Render compelling visualizations to communicate data-driven narratives to your colleagues
7. Apply the insights gained from your data science project to your work

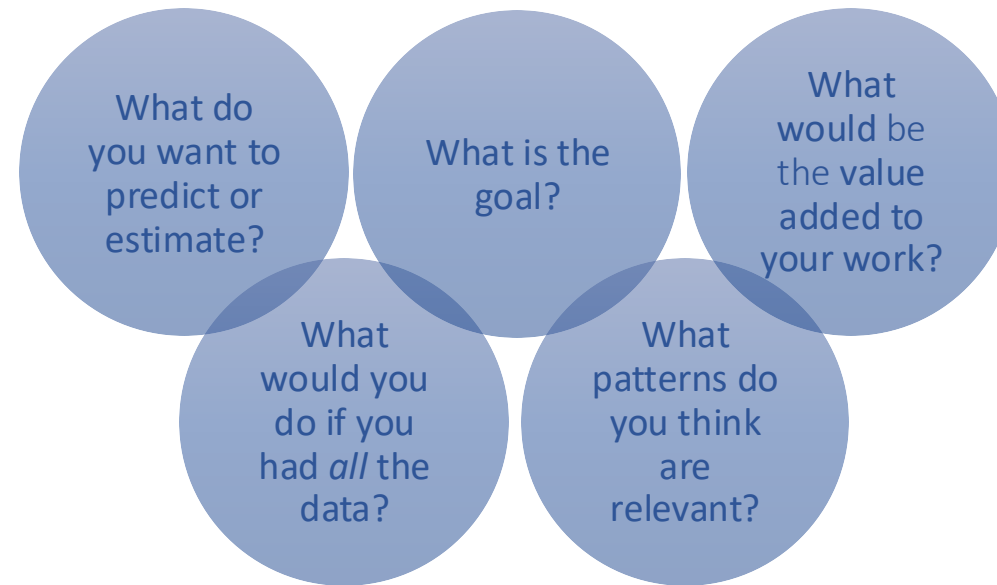


Problem Statement



What Questions Can Data Science Answer?

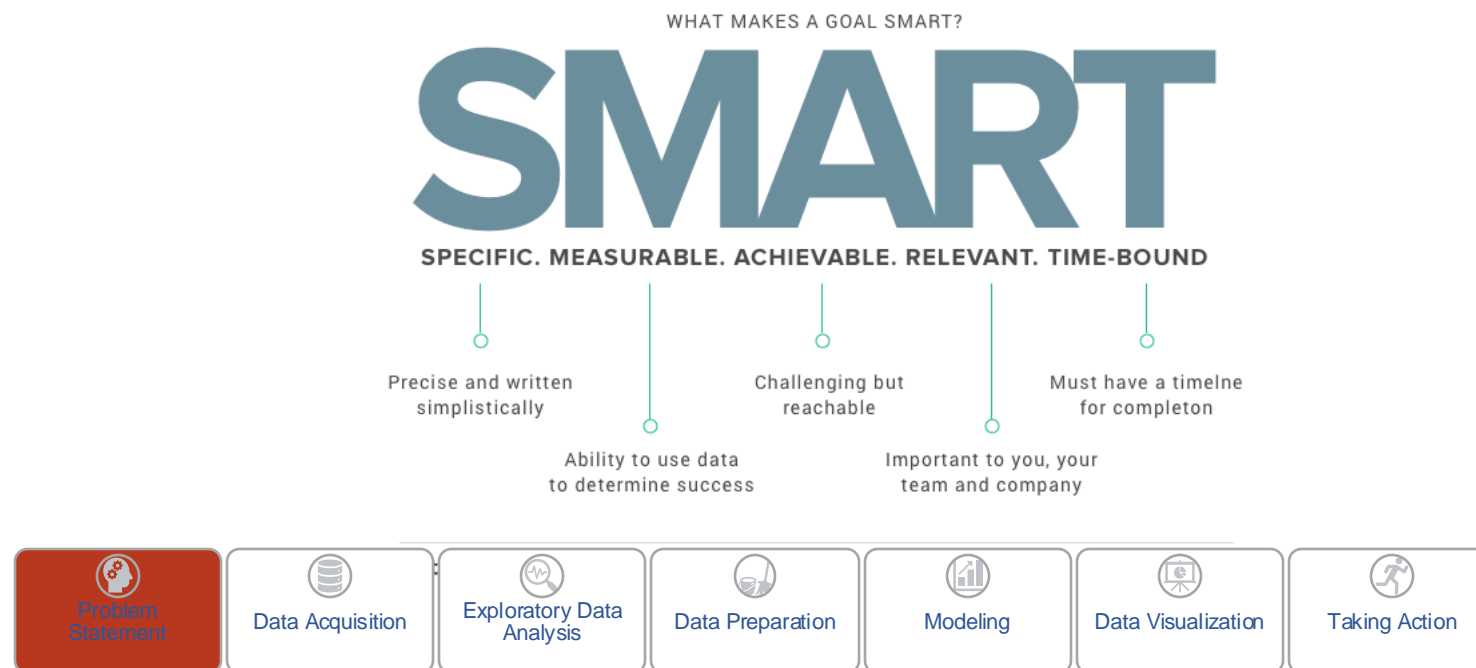
- Data science can't answer just any question
- Questions must be structured and attainable
- A few questions to ask yourself to help you get started:





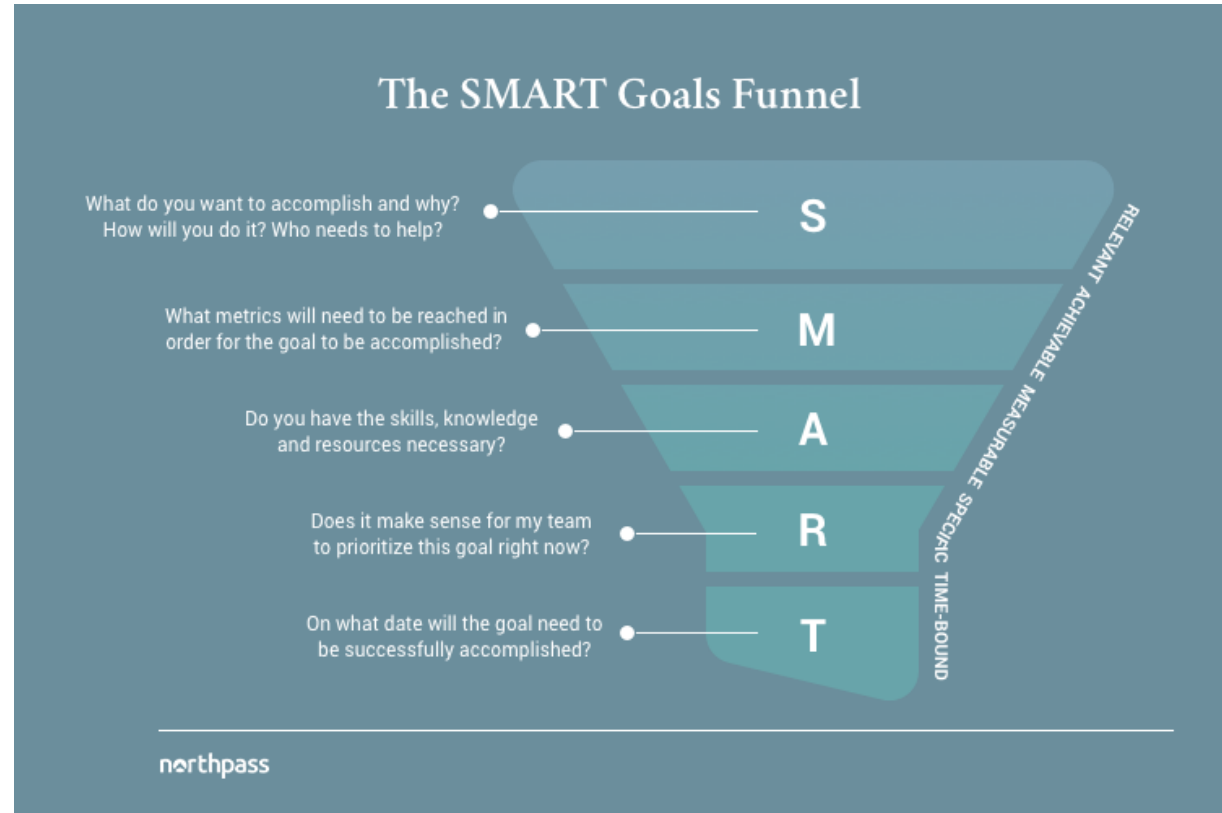
Creating SMART Problem Statements

- When developing your problem statements, think through whether the question is SMART!
- Although SMART goals are not necessarily specific to data science, we can use this methodology to make sure we create attainable problem statements





The SMART Goals Funnel



Problem Statement



Data Acquisition



Exploratory Data Analysis



Data Preparation



Modeling



Data Visualization

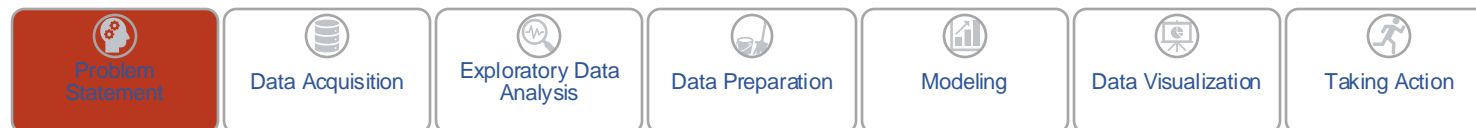


Taking Action

Example – SMART Goals

Healthcare Objective

- Researchers seek a data-driven approach to better understand the factors that are most strongly associated with chronic kidney disease.
- The aim of this project is to develop models using clinical patient data to accurately predict chronic kidney disease.



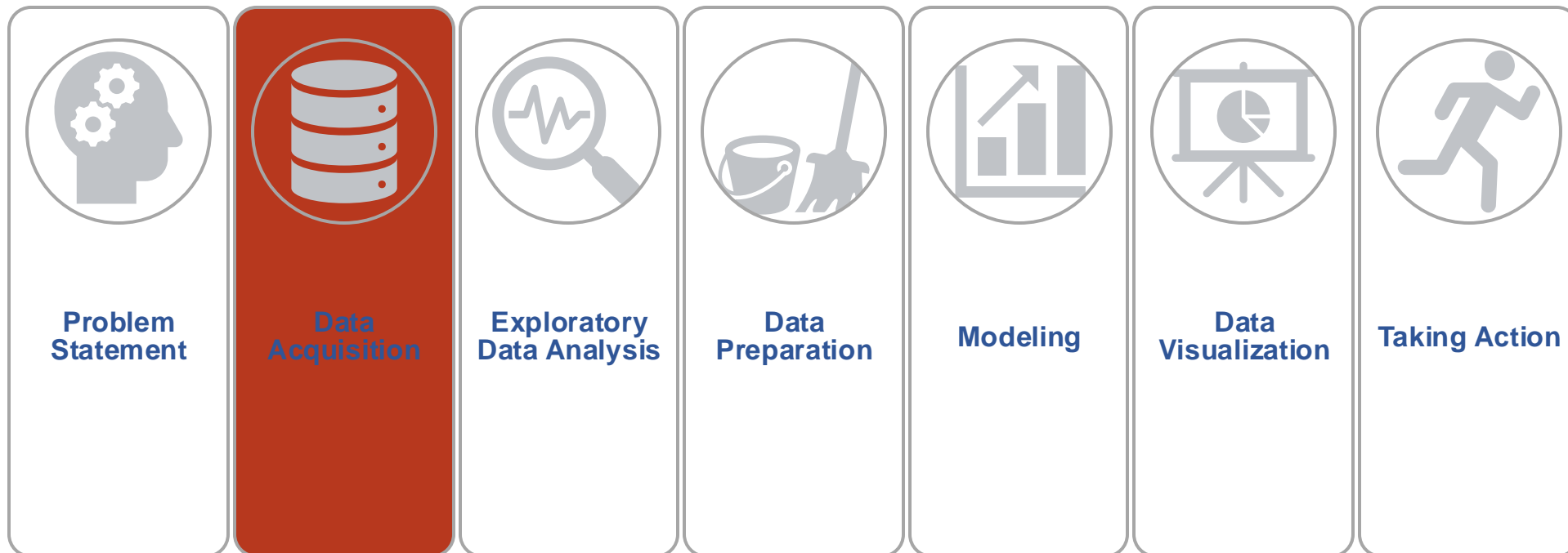
Example – SMART Goals

- S** – We will train machine learning models using clinical patient data to predict who's at greatest risk for developing chronic kidney disease.
- M** – Success will be measured by the model's accuracy – targeting at least 90%.
- A** – By leveraging existing data sets and proven analytics capabilities, we'll work with resources readily available to the NIH.
- R** – The models will help researchers and medical providers make objective, data-driven healthcare decisions by highlighting insights that may be currently overlooked.
- T** – The models will be developed, validated, and ready for deployment within 6 months, with a prototype ready for review in 3 months.



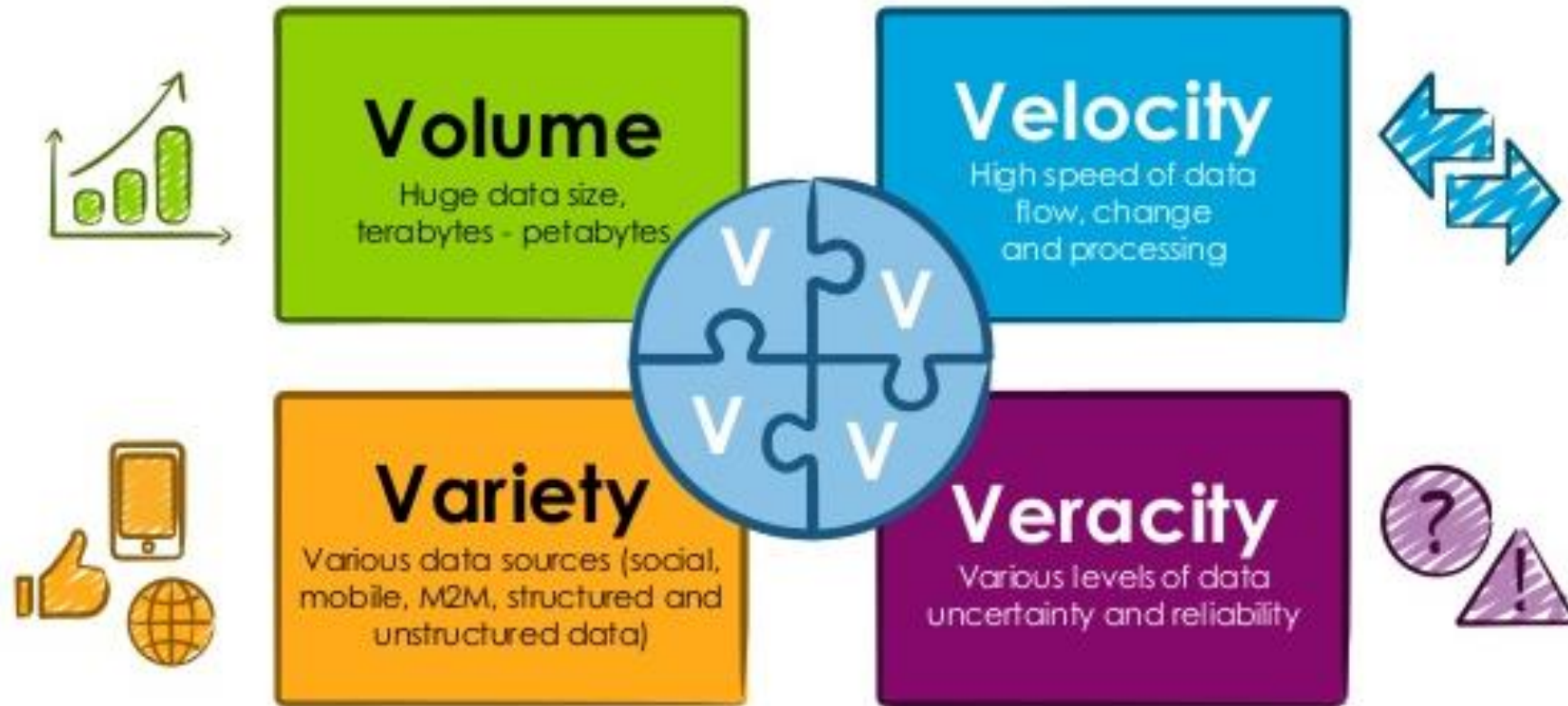


Data Acquisition





The Four Vs of Big Data

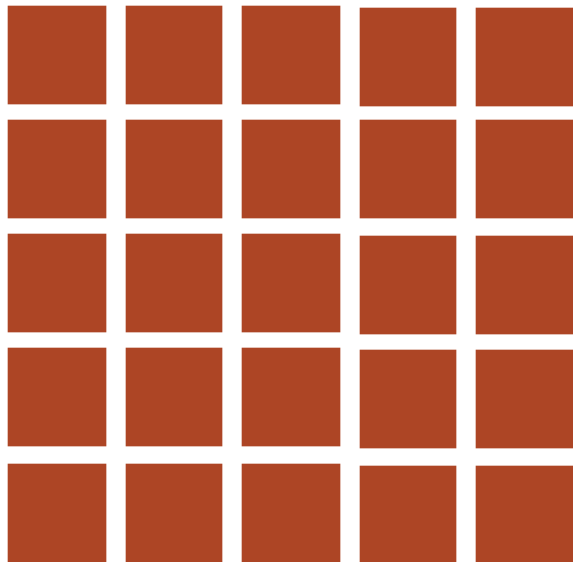


- Problem Statement
- Data Acquisition**
- Exploratory Data Analysis
- Data Preparation
- Modeling
- Data Visualization
- Taking Action

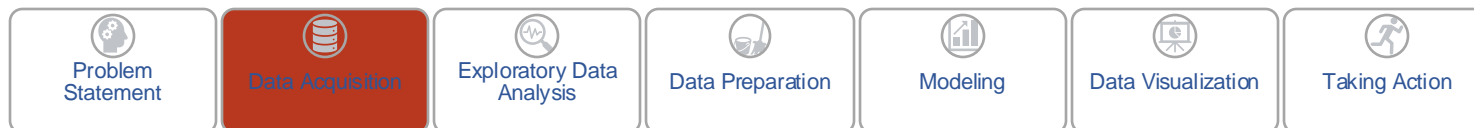


Structured vs Unstructured Data

Structured Data

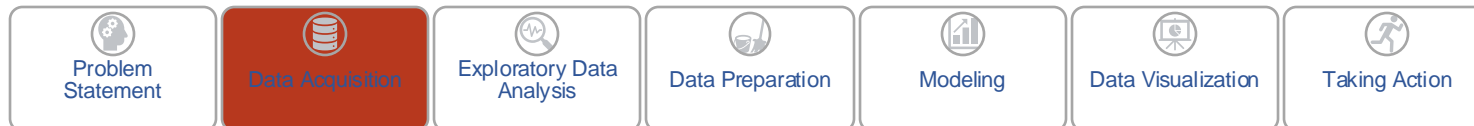
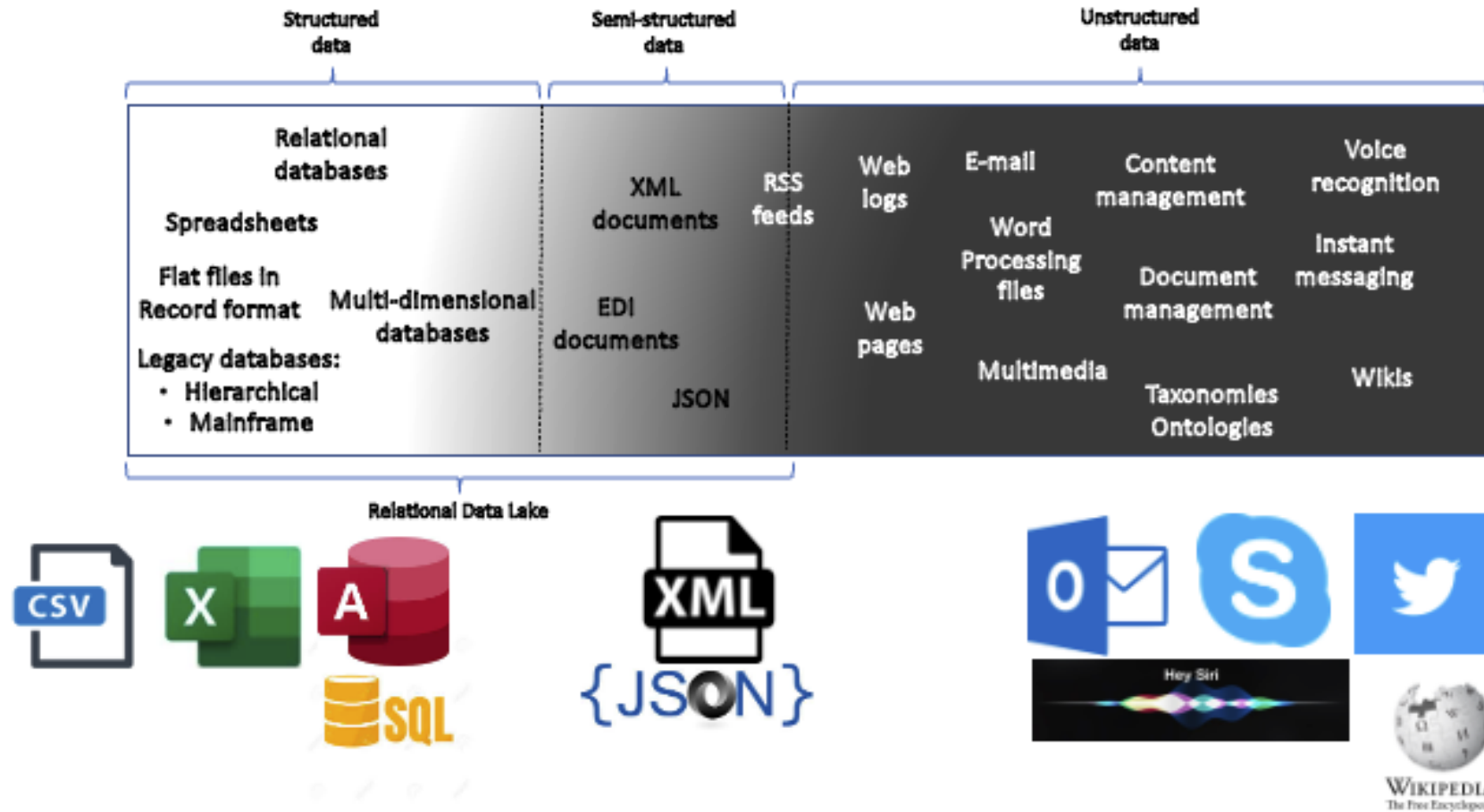


Unstructured Data





Data Acquisition: Data Structures



Example – Kidney Disease Data

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
1	id	age	bp	sg	al	su	rbc	pc	pcc	ba	bgr	bu	sc	sod	pot	hemo	pcv	wc	rc	htn	dm	cad	appet	pe	ane	classification
2	0	48	80	1.02	1	0		normal	notpresent	notpresent	121	36	1.2			15.4	44	7800	5.2	yes	yes	no	good	no	no	ckd
3	1	7	50	1.02	4	0		normal	notpresent	notpresent			18	0.8		11.3	38	6000		no	no	no	good	no	no	ckd
4	2	62	80	1.01	2	3	normal	normal	notpresent	notpresent	423	53	1.8			9.6	31	7500		no	yes	no	poor	no	yes	ckd
5	3	48	70	1.005	4	0	normal	abnormal	present	notpresent	117	56	3.8	111	2.5	11.2	32	6700	3.9	yes	no	no	poor	yes	yes	ckd
6	4	51	80	1.01	2	0	normal	normal	notpresent	notpresent	106	26	1.4			11.6	35	7300	4.6	no	no	no	good	no	no	ckd
7	5	60	90	1.015	3	0			notpresent	notpresent	74	25	1.1	142	3.2	12.2	39	7800	4.4	yes	yes	no	good	yes	no	ckd
8	6	68	70	1.01	0	0		normal	notpresent	notpresent	100	54	24	104	4	12.4	36			no	no	no	good	no	no	ckd
9	7	24		1.015	2	4	normal	abnormal	notpresent	notpresent	410	31	1.1			12.4	44	6900	5	no	yes	no	good	yes	no	ckd
10	8	52	100	1.015	3	0	normal	abnormal	present	notpresent	138	60	1.9			10.8	33	9600	4	yes	yes	no	good	no	yes	ckd
11	9	53	90	1.02	2	0	abnormal	abnormal	present	notpresent	70	107	7.2	114	3.7	9.5	29	12100	3.7	yes	yes	no	poor	no	yes	ckd
12	10	50	60	1.01	2	4		abnormal	present	notpresent	490	55	4			9.4	28			yes	yes	no	good	no	yes	ckd
13	11	63	70	1.01	3	0	abnormal	abnormal	present	notpresent	380	60	2.7	131	4.2	10.8	32	4500	3.8	yes	yes	no	poor	yes	no	ckd
14	12	68	70	1.015	3	1		normal	present	notpresent	208	72	2.1	138	5.8	9.7	28	12200	3.4	yes	yes	yes	poor	yes	no	ckd
15	13	68	70						notpresent	notpresent	98	86	4.6	135	3.4	9.8				yes	yes	yes	poor	yes	no	ckd
16	14	68	80	1.01	3	2	normal	abnormal	present	present	157	90	4.1	130	6.4	5.6	16	11000	2.6	yes	yes	yes	poor	yes	no	ckd
17	15	40	80	1.015	3	0		normal	notpresent	notpresent	76	162	9.6	141	4.9	7.6	24	3800	2.8	yes	no	no	good	no	yes	ckd
18	16	47	70	1.015	2	0		normal	notpresent	notpresent	99	46	2.2	138	4.1	12.6				no	no	no	good	no	no	ckd
19	17	47	80						notpresent	notpresent	114	87	5.2	139	3.7	12.1				yes	no	no	poor	no	no	ckd
20	18	60	100	1.025	0	3		normal	notpresent	notpresent	263	27	1.3	135	4.3	12.7	37	11400	4.3	yes	yes	yes	good	no	no	ckd
21	19	62	60	1.015	1	0		abnormal	present	notpresent	100	31	1.6			10.3	30	5300	3.7	yes	no	yes	good	no	no	ckd
22	20	61	80	1.015	2	0	abnormal	abnormal	notpresent	notpresent	173	148	3.9	135	5.2	7.7	24	9200	3.2	yes	yes	yes	poor	yes	yes	ckd
23	21	60	90						notpresent	notpresent		180	76	4.5		10.9	32	6200	3.6	yes	yes	yes	good	no	no	ckd
24	22	48	80	1.025	4	0	normal	abnormal	notpresent	notpresent	95	163	7.7	136	3.8	9.8	32	6900	3.4	yes	no	no	good	no	yes	ckd

Data Source: [UC Irvine Machine Learning Repository](#)





Example – Kidney Disease Data

Column Name	Description	Data Type
age	Age	Numeric
bp	Blood Pressure	Numeric
sg	Specific Gravity	Numeric
al	Albumin	Numeric
su	Sugar	Numeric
rbc	Red Blood Cells	Categorical
sc	Serum Creatinine	Numeric
...
classification	Chronic Kidney Disease (yes/no)	Binary (Categorical)

Source: [UC Irvine Machine Learning Repository](#)



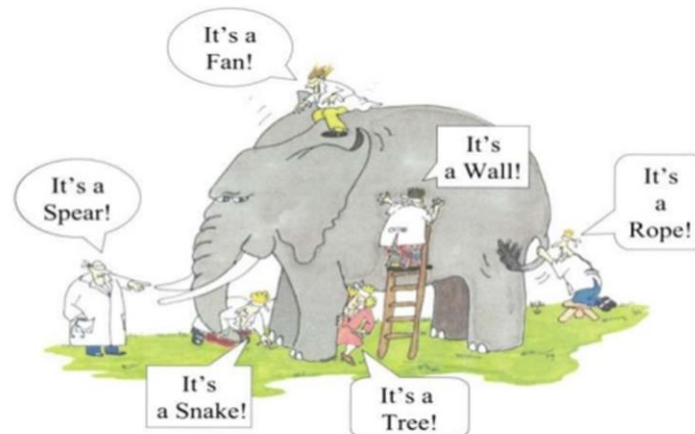


Exploratory Data Analysis



Understand Your Data!

- It's time to sit down and analyze the many intricacies of the dataset
- It's important to look for different insights to understand your data as a whole



BIG DATA

Arnon Rotem-Gal-Oz

Director of Technology Research, Amdocs

The blind men and the elephant. Poem by John Godfrey Saxe (Cartoon originally copyrighted by the authors; G. Renee Guzlas, artists http://www.nature.com/ki/journal/v62/n5/fig_tab/4493262f1.htm)



Types of Analytics

Four types of analytics:

- **Descriptive:** What happened?
- **Diagnostic:** Why did it happen?
- **Predictive:** What will happen?
- **Prescriptive:** How can we make this happen?



Types of Discovery

Class Discovery

- Find the categories of objects (population segments), events, and behaviors in your data



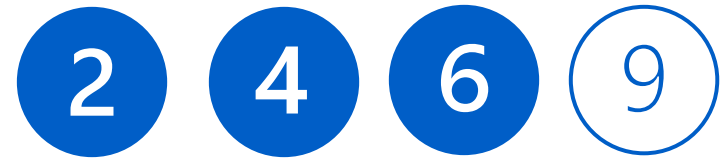
Correlation Discovery

- Find trends, patterns, and dependencies in data that reveal the governing principles or behavioral patterns (the object's "DNA")



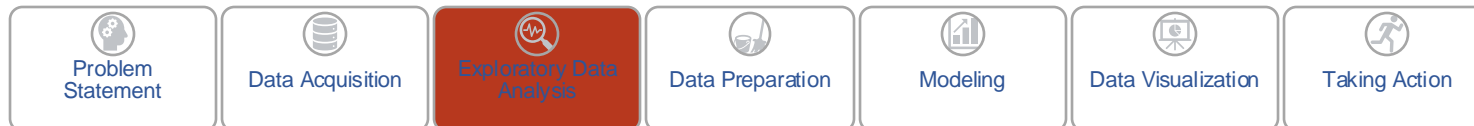
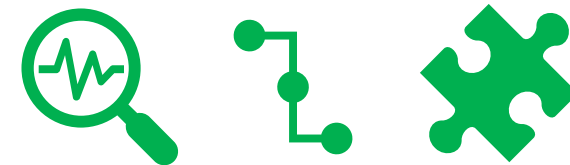
Outlier Discovery

- Find the new, surprising, unexpected one-in-a-million object, event, or behavior



Association Discovery

- Find both the typical (usual) and the atypical (unusual, interesting) data associations, links, or connections in your domain



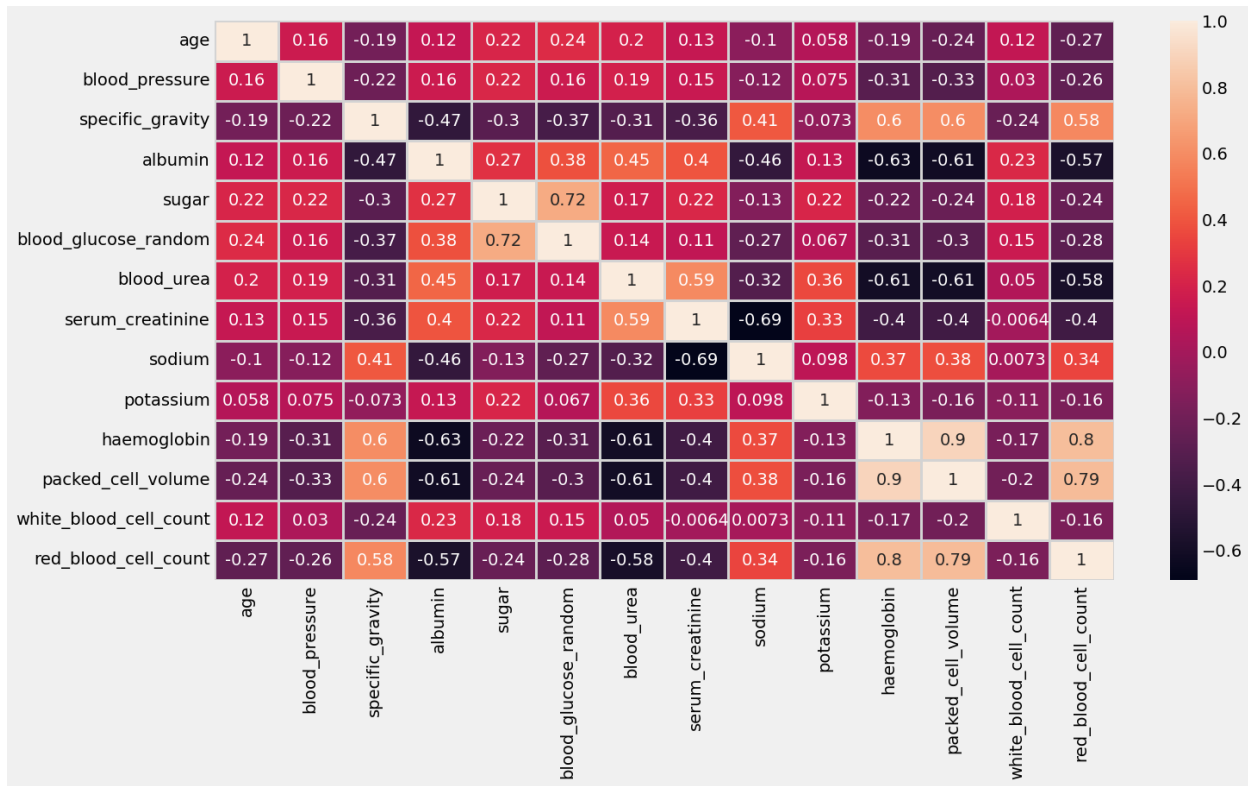


Example – Correlation Heatmap

```
# heatmap of data

plt.figure(figsize = (15, 8))

sns.heatmap(df[num_cols].corr(), annot = True, linewidths = 2, linecolor = 'lightgrey')
plt.show()
```

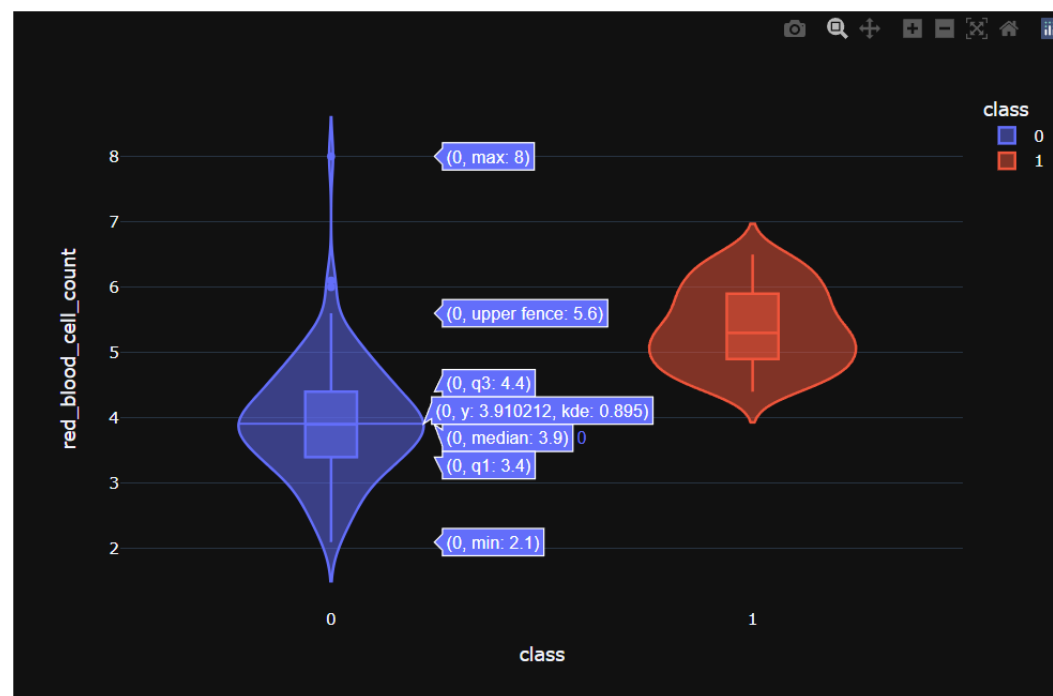




Example – Violin Distribution Plot

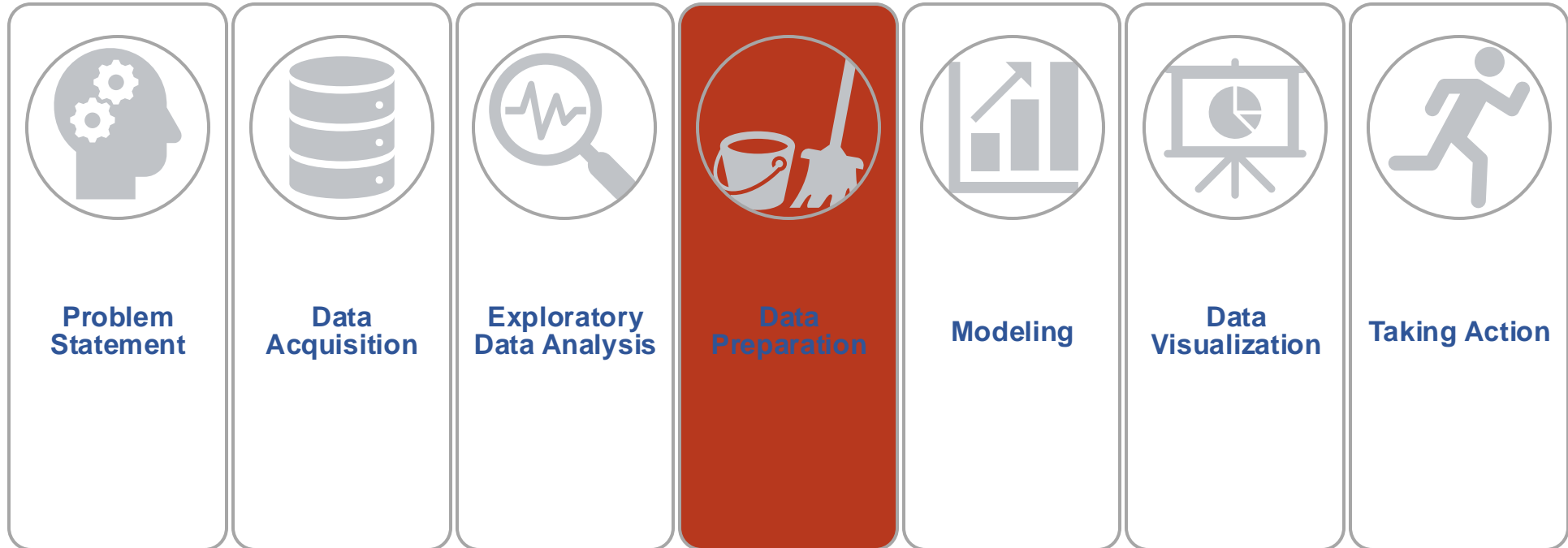
```
import plotly.express as px

fig = px.violin(df, y= 'red_blood_cell_count', x= 'class', color= 'class', box = True, template = 'plotly_dark')
fig.show()
```





Data Preparation

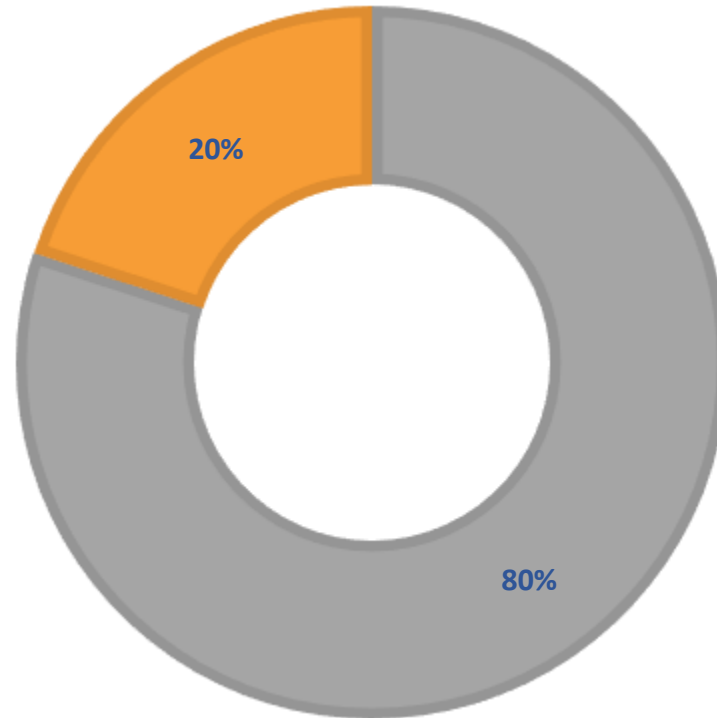




Real World Data Is Messy

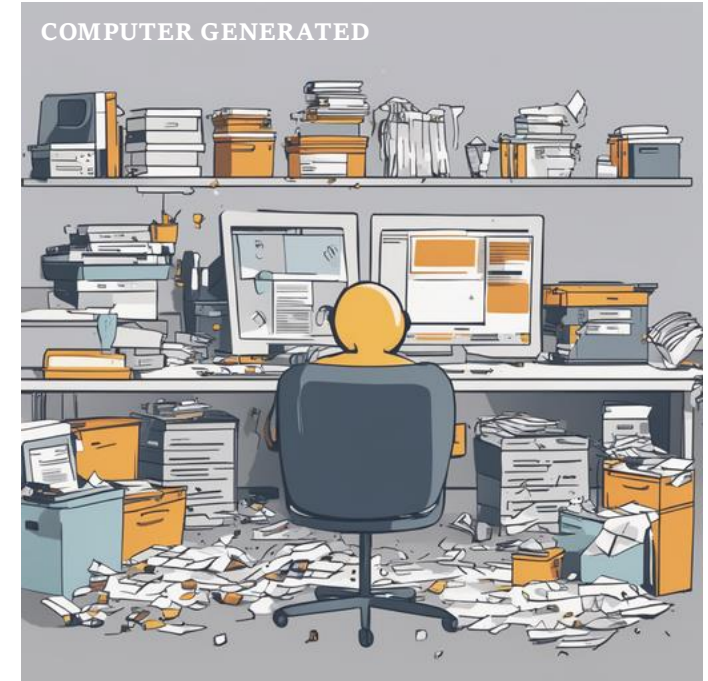
DATA SCIENTIST'S WORKLOAD

■ Data Preparation ■ Everything else



Dirty Data

- Dirty data is everywhere!
 - Any data with typos or errors
 - Missing data
 - Null fields
 - Different labels for the same item
 - Duplicate entries
 - Entries that don't match up with another dataset
 - So much more!
- These data entries can skew the outcome of your models





Example – Missing Values

```
# checking for null values  
df.isna().sum().sort_values(ascending = False)
```

red_blood_cells	152
red_blood_cell_count	131
white_blood_cell_count	106
potassium	88
sodium	87
packed_cell_volume	71
pus_cell	65
haemoglobin	52
sugar	49
specific_gravity	47
albumin	46
blood_glucose_random	44
blood_urea	19
serum_creatinine	17
blood_pressure	12
age	9

Garbage In, Garbage Out

- Concept that the quality of information coming out can only be as good as the quality of information that went in
- In other words, the condition of the data going into a model is the ceiling of the condition of the outcoming data



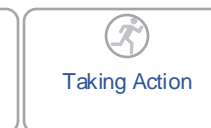
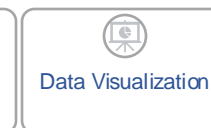
Feature Engineering

- Using domain knowledge to adjust the dataset and use it properly for the chosen model and question
- Applications of feature engineering:
 - Imputation
 - Handling Outliers
 - Binning
 - Scaling
 - Log Transformation
 - One-Hot Encoding
 - Grouping Operations
 - Feature Split
 - Extracting Date

BEFORE

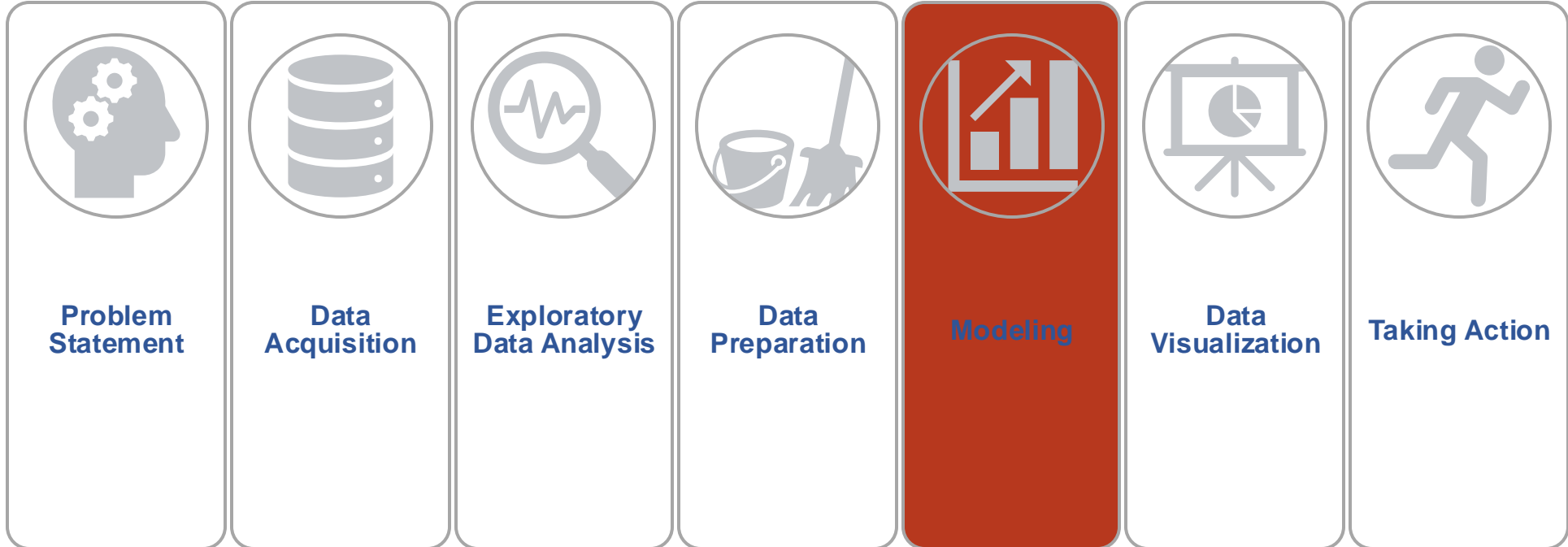


AFTER



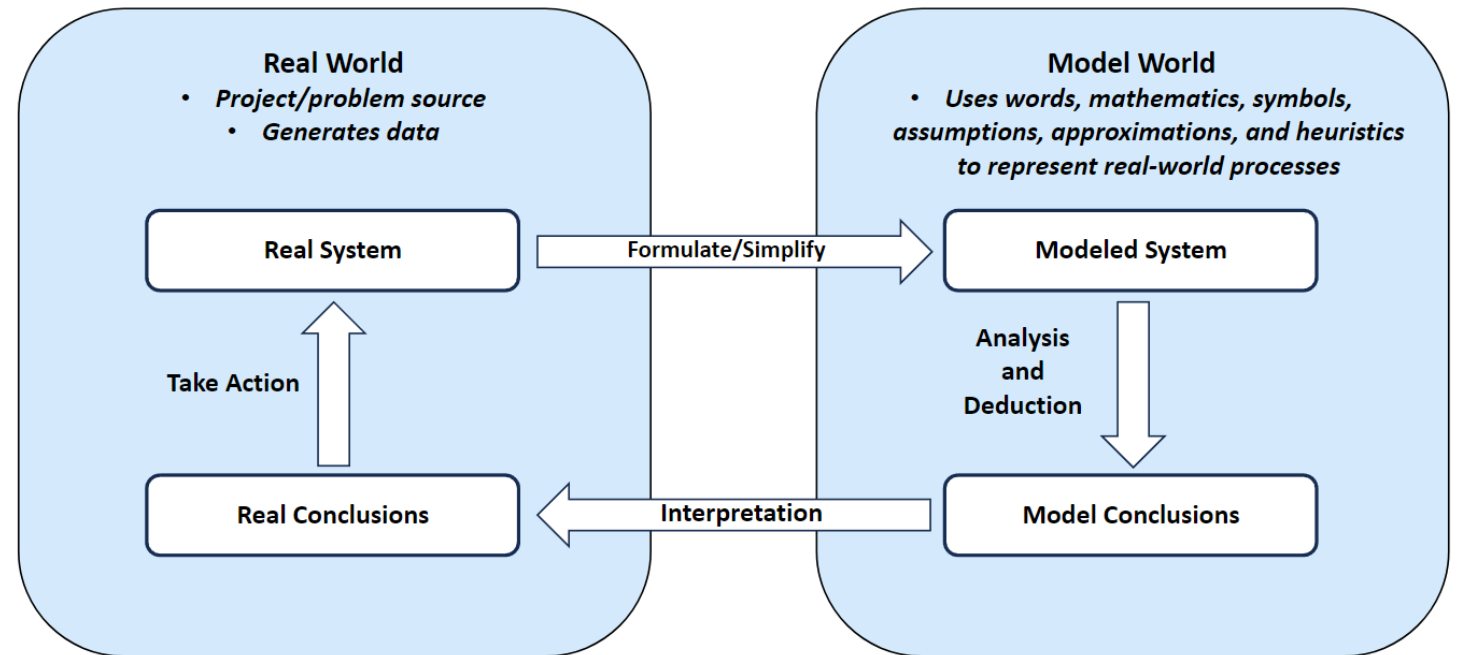


Modeling



What Is a Model?

- A model is a representation of a real-world process.
- Models use simplifying assumptions to make problems more tractable (e.g., for analyses and computational purposes).
- **Goal:** Balance representing the real world to a high fidelity with the level of simplification imposed.



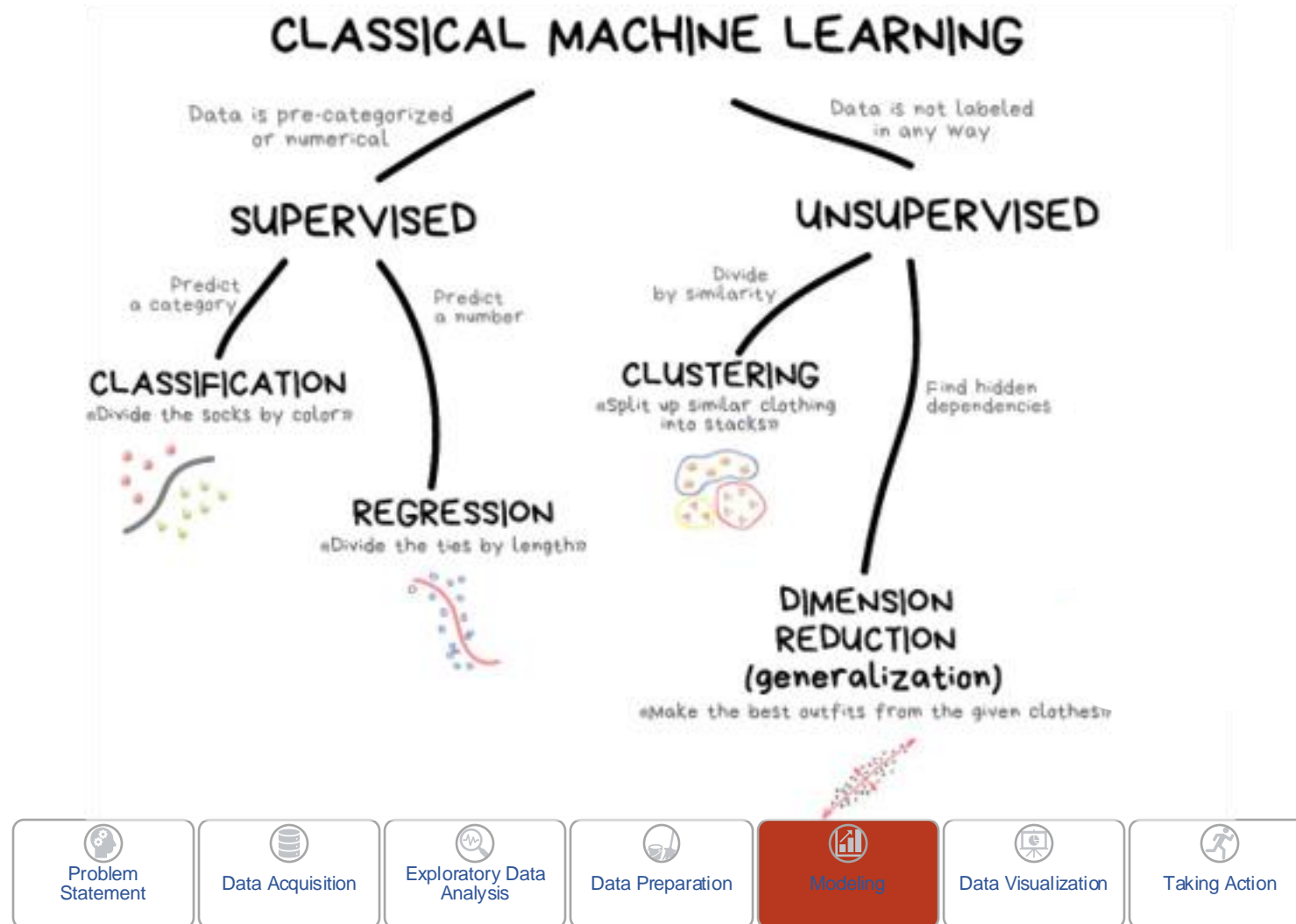
What Is a Machine Learning Model?

- A machine learning (ML) model is a program or system that learns patterns from data.
- ML models use discovered patterns to make predictions or decisions without being explicitly programmed for specific tasks.
- A helpful analogy is to think of ML as akin to baking, as illustrated in the correspondence table at right.
- The computer's goal is to determine the "best" way to mix data together to achieve a desired outcome.

Machine Learning	Baking
Data <ul style="list-style-type: none"> • Human provided 	Ingredients to be mixed together (e.g., flour, sugar, butter, etc.)
Model parameters <ul style="list-style-type: none"> • Computer determines these 	Quantities of ingredients used in recipe (e.g., 3 cups sugar, 4 tbsp butter, etc.)
Desired model output <ul style="list-style-type: none"> • Human provided 	Tasty treat (e.g., cake, cookie, biscuit, etc.)



Types of Machine Learning



Supervised Learning

- Step 1: Provide the machine learning algorithm **categorized or “labeled”** input and output data to learn from
- Step 2: Feed the machine **new, unlabeled information** to see if it tags new data appropriately. If not, continue refining the algorithm



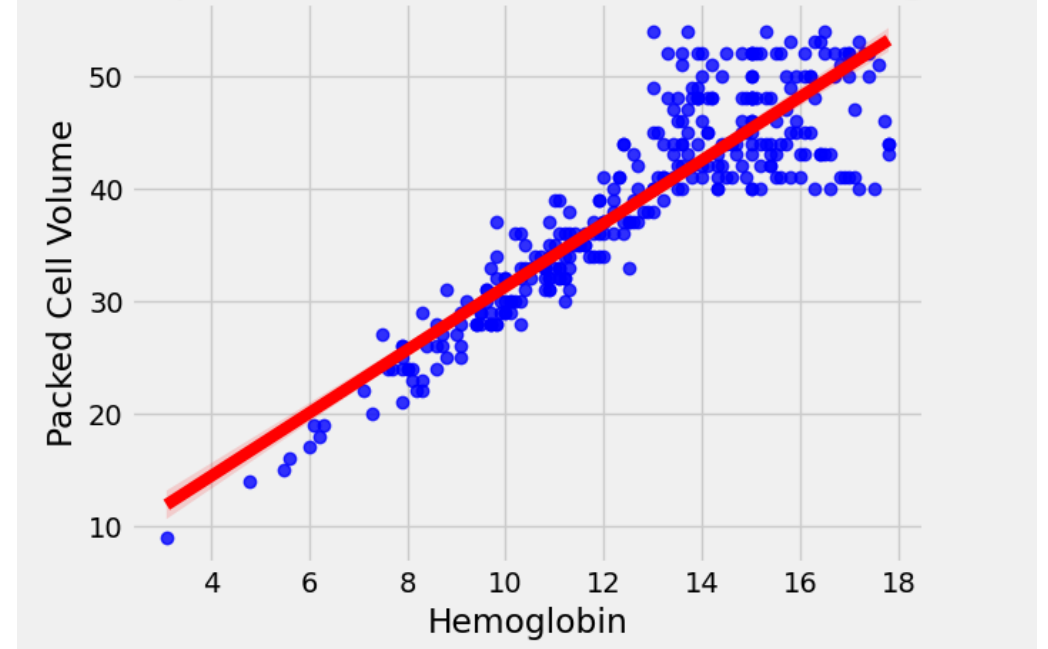
Regression

Regression is the task of predicting a continuous numeric value.

Examples:

- Predicting packed cell volume using hemoglobin measurements.
- Predicting house price using square footage.
- Forecasting the price of a stock.

Scatterplot of Packed Cell Volume vs. Hemoglobin



Problem Statement



Data Acquisition



Exploratory Data Analysis



Data Preparation



Modeling



Data Visualization

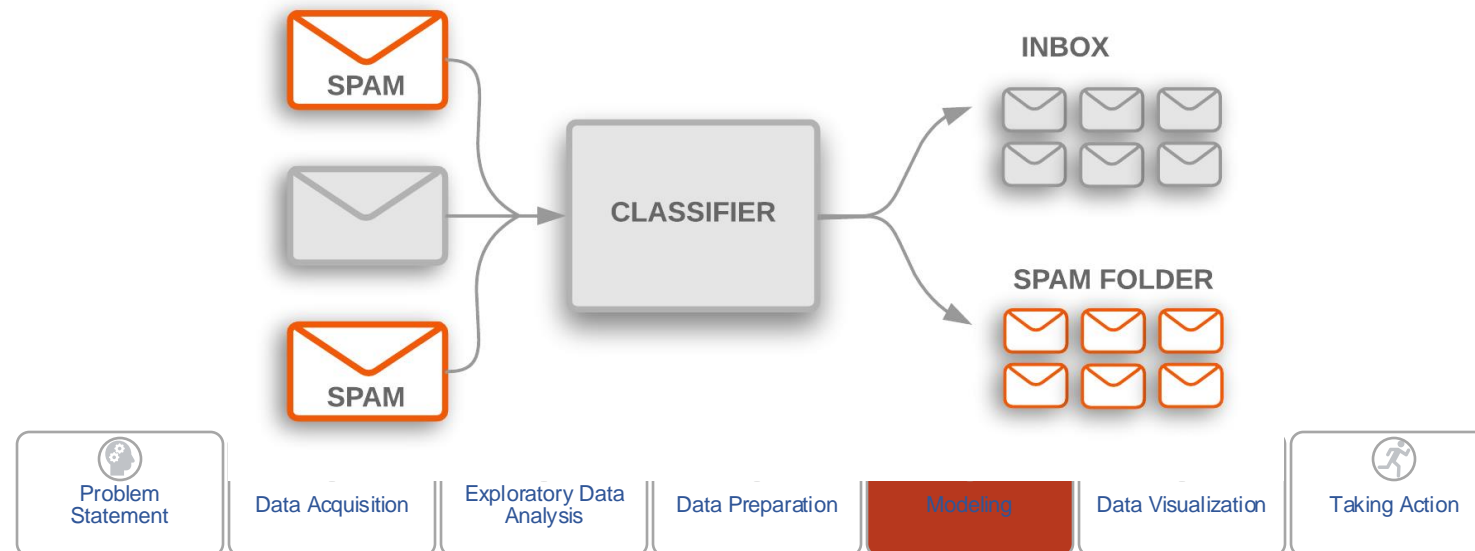


Taking Action

Classification

Classification is the task of predicting a discrete class label.

- Data is labeled into one of two or more classes.
- **Examples:**
 - Classifying a patient as at risk for chronic kidney disease or not
 - Labeling emails as spam or not spam.



Unsupervised Learning

- Step 1: Provide the machine learning algorithm **uncategorized, unlabeled input** data to see what pattern it finds
- Step 2: Observe and **learn from the patterns** the machine identifies

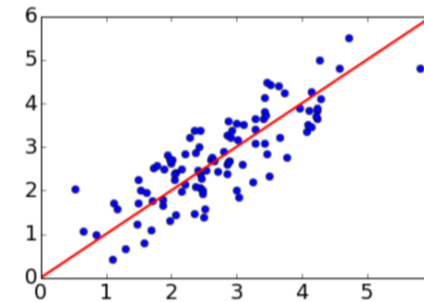


Dimensionality Reduction

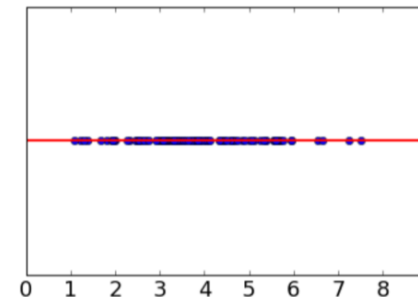
Dimensionality reduction is the process of reducing the number of input features in a dataset while retaining as much important information as possible.

- Dimensionality reduction often helps ML algorithms detect patterns in high-dimensional datasets.
- **Example:** A photograph reduces a 3-dimensional subject to a 2-dimensional representation while maintaining many important features.

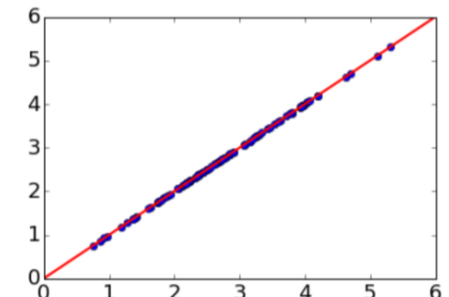
Projecting 2-dimensional data onto a 1-dimensional line, preserving maximum variance in the data



Projection onto \mathbb{R} :



Projection onto a 1-d line in \mathbb{R}^2 :



Problem Statement



Data Acquisition



Exploratory Data Analysis



Data Preparation



Modeling



Data Visualization

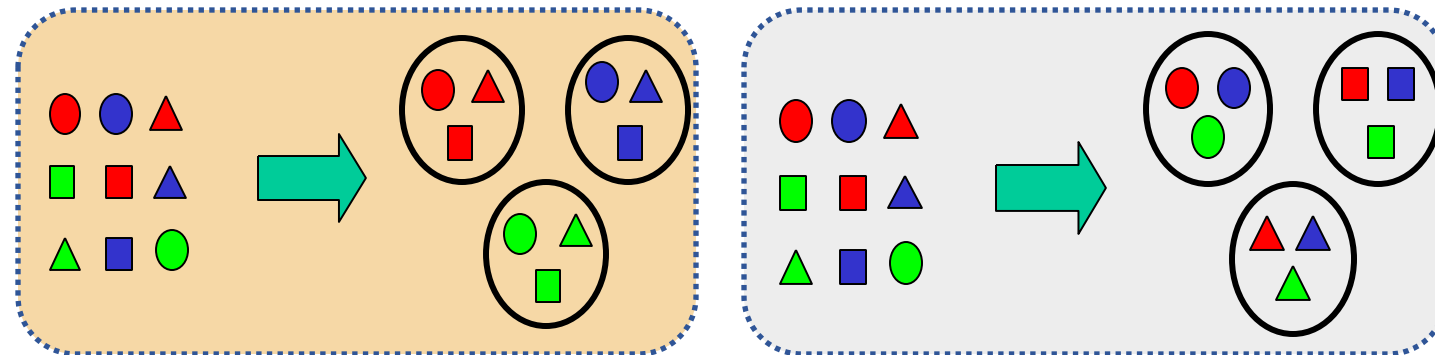


Taking Action

Clustering

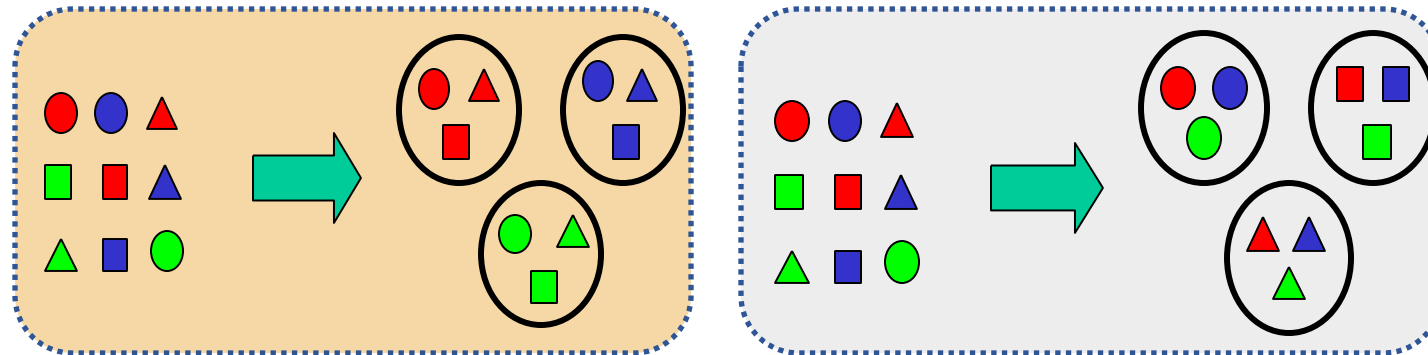
Clustering is the process of partitioning data into subsets (segments or clusters) such that data points most similar to one another are grouped together.

- The computer groups together data it sees as similar and separates dissimilar ones.
- Data scientists and SMEs work together to identify similar characteristics, patterns, or behaviors among the subsets identified by the algorithm.



Clustering Challenges

- No prior knowledge of either the number or semantic meaning of the clusters.
- The same dataset can lead to different clusters.
 - Selecting different features can change the resulting clusters.

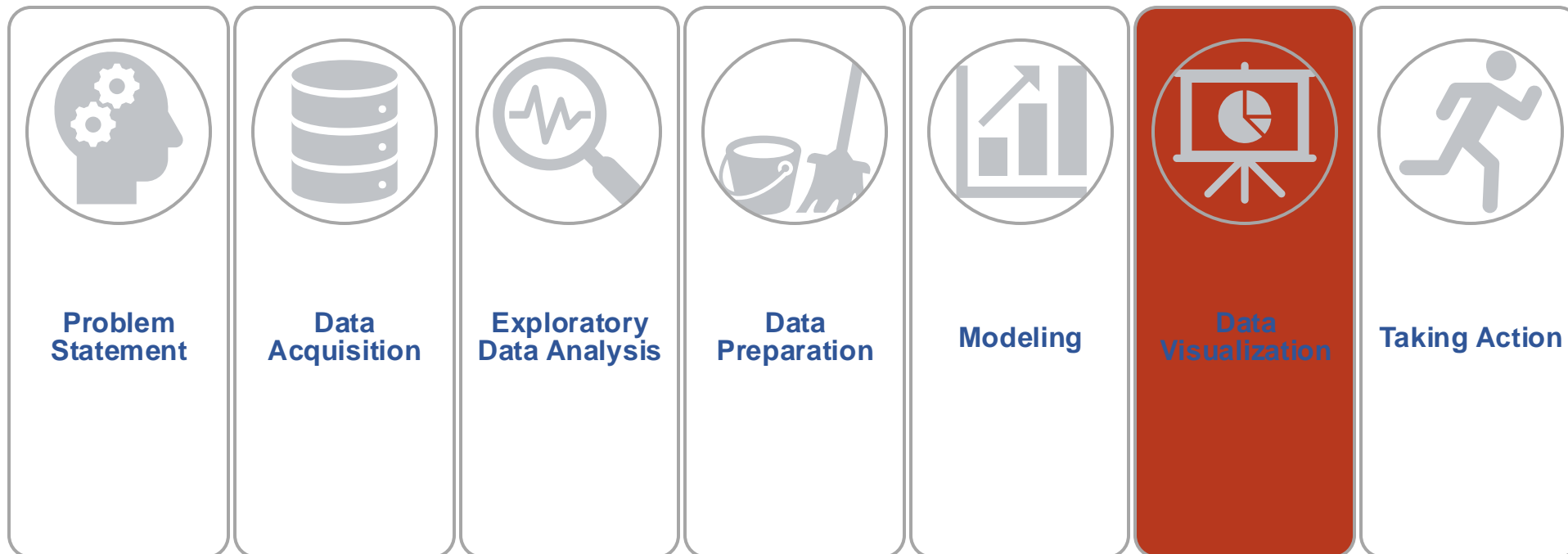




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Visualizing and Communicating Results



Why Visualization Is Important

- Visualizations can express aspects of the data that numbers alone cannot demonstrate
- They can tell a story about the results



BEFORE DATA VISUALIZATION

- Scattered data
- Multiple stakeholder dependencies
- Difficulties In information absorption



AFTER DATA VISUALIZATION

- Better information absorption
- Actionable insights
- Singular view of scattered data

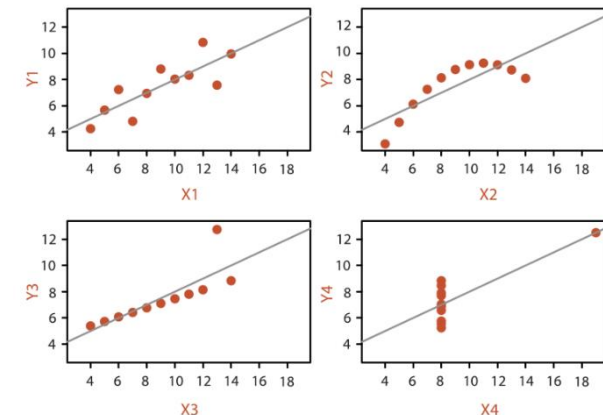


Aren't Statistics Enough?

- All these plots have the same:
 - Mean
 - Variance
 - Correlation
- But looking at the visualization, you can see that they do not look anything alike
- Statistics can sometimes be misleading!
- Without effectively expressing the data, final results may be left up for interpretation

Anscombe's Quartet: Raw Data

	1		2		3		4	
	X	Y	X	Y	X	Y	X	Y
	10.0	8.04	10.0	9.14	10.0	7.46	8.0	6.58
	8.0	6.95	8.0	8.14	8.0	6.77	8.0	5.76
	13.0	7.58	13.0	8.74	13.0	12.74	8.0	7.71
	9.0	8.81	9.0	8.77	9.0	7.11	8.0	8.84
	11.0	8.33	11.0	9.26	11.0	7.81	8.0	8.47
	14.0	9.96	14.0	8.10	14.0	8.84	8.0	7.04
	6.0	7.24	6.0	6.13	6.0	6.08	8.0	5.25
	4.0	4.26	4.0	3.10	4.0	5.39	19.0	12.50
	12.0	10.84	12.0	9.13	12.0	8.15	8.0	5.56
	7.0	4.82	7.0	7.26	7.0	6.42	8.0	7.91
	5.0	5.68	5.0	4.74	5.0	5.73	8.0	6.89
Mean	9.0	7.5	9.0	7.5	9.0	7.5	9.0	7.5
Variance	10.0	3.75	10.0	3.75	10.0	3.75	10.0	3.75
Correlation	0.816		0.816		0.816		0.816	

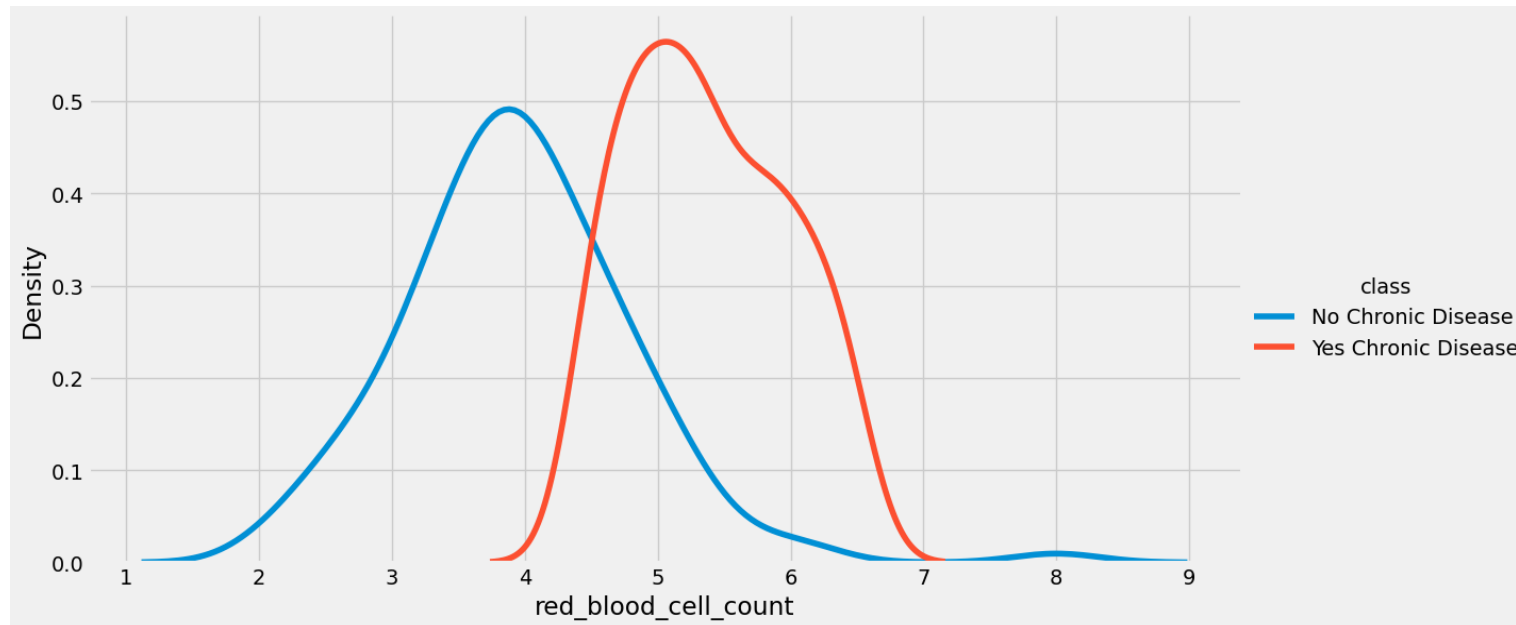




Example – Red Blood Cell Count Distribution

```
import seaborn as sns

grid = sns.FacetGrid(df, hue="class", height = 6, aspect=2)
grid.map(sns.kdeplot, 'red_blood_cell_count')
grid.add_legend(labels = ['No Chronic Disease', 'Yes Chronic Disease'])
```



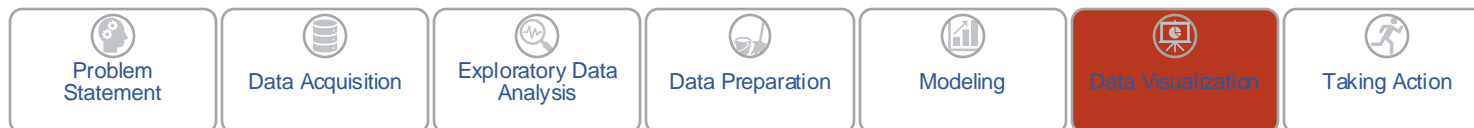


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Visualization Tools: Open Source

Language		 python™	
Example of Library			

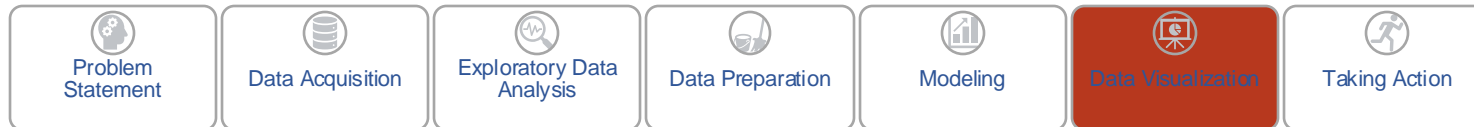
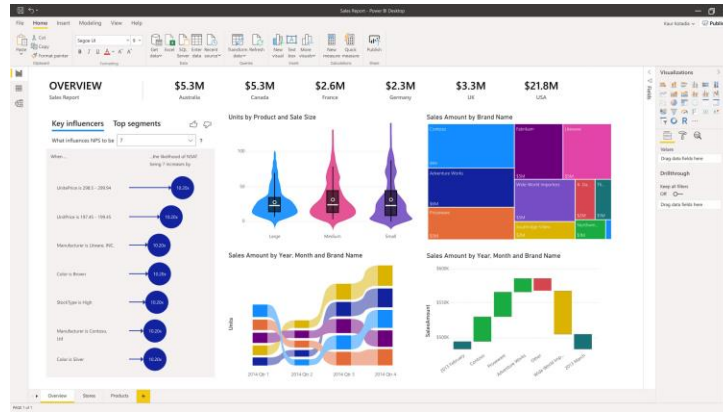
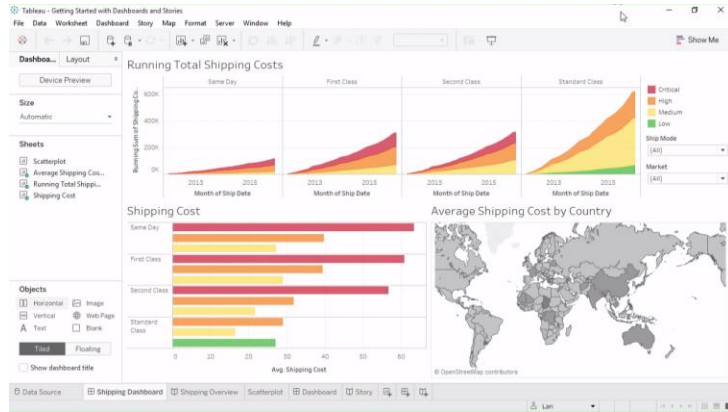




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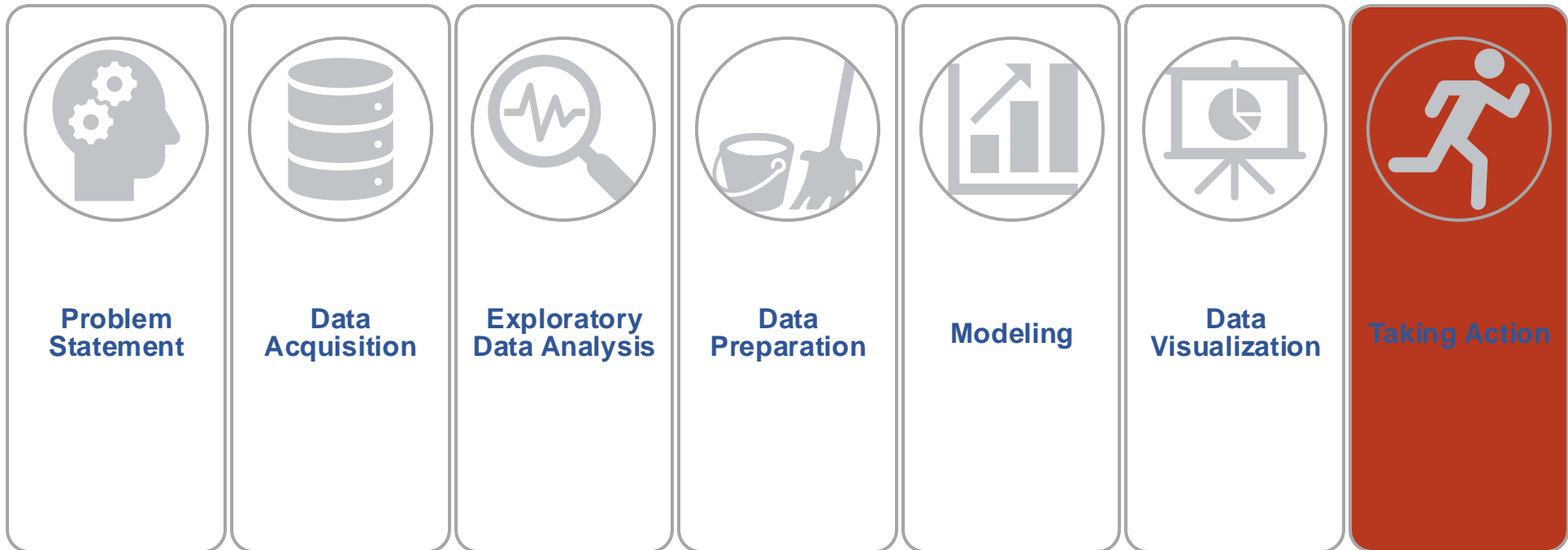
Central Repository

Visualization Tools: Premium





Taking Action





Measuring Model Performance

- Measuring a model's performance is important for users to be able to trust the model outputs
- Model performance not tracked over time can have direct and indirect adverse effects
- Ensure you are tracking appropriate metrics for the given model and dataset
 - Classification
 - Accuracy
 - Precision
 - Recall
 - Regression
 - Mean Absolute Error
 - Mean Squared Error
 - Root Mean Squared Error
 - R- squared





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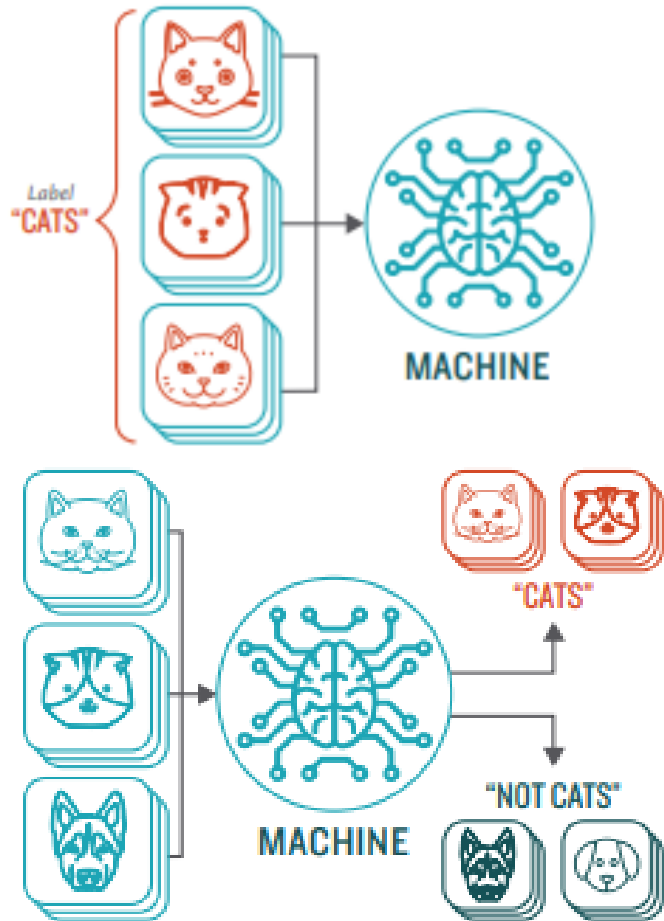
Central Repository

Machine Learning Deep Dive

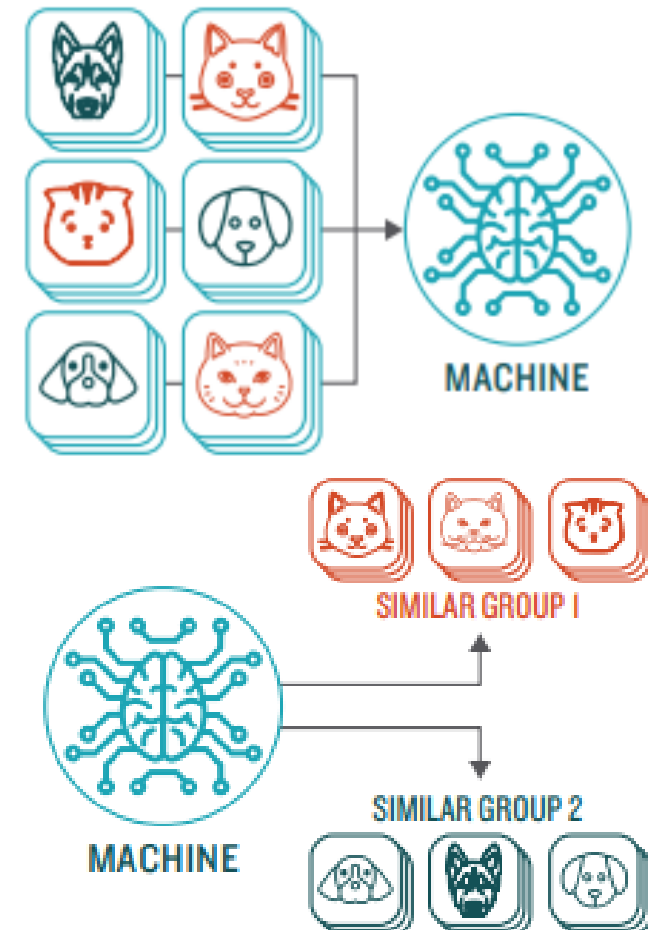


Supervised & Unsupervised Learning

Supervised: labeled data



Unsupervised: unlabeled data



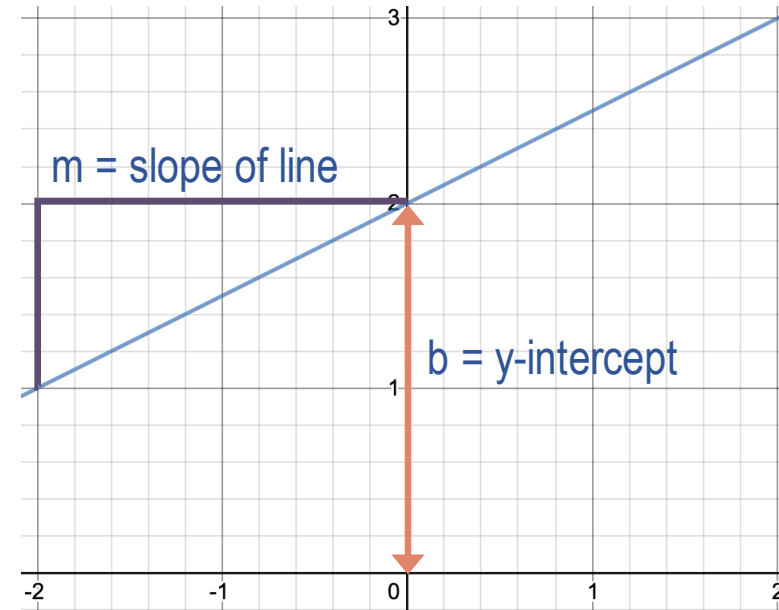
Linear Regression - Equation

$$y = mx + b$$



$$y = \theta_1 X_1 + \theta_0$$

(linear regression)

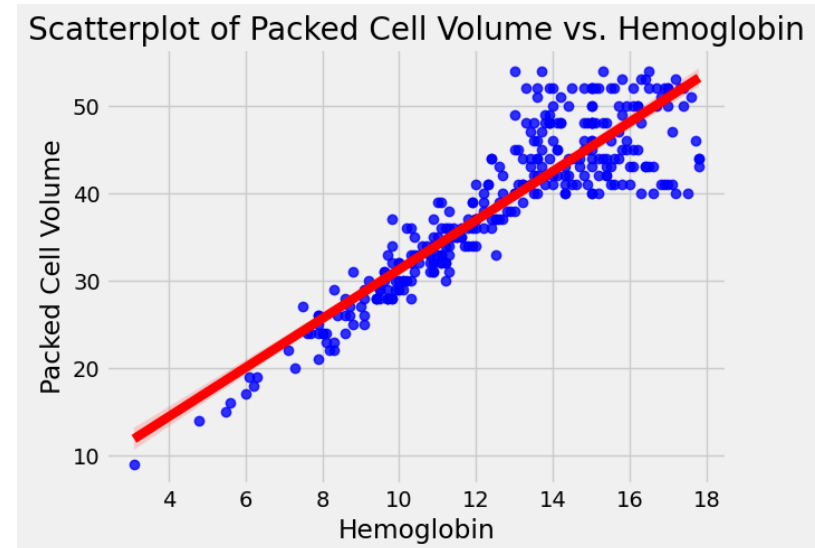


New notation to learn, but the same idea

Linear Regression - Parameters

How do you decide what your θ_1 and θ_0 (the coefficients/parameters) should be?

We could just draw a line
that looks good to us...
But there's a better way to
obtain the regression line of
best fit.

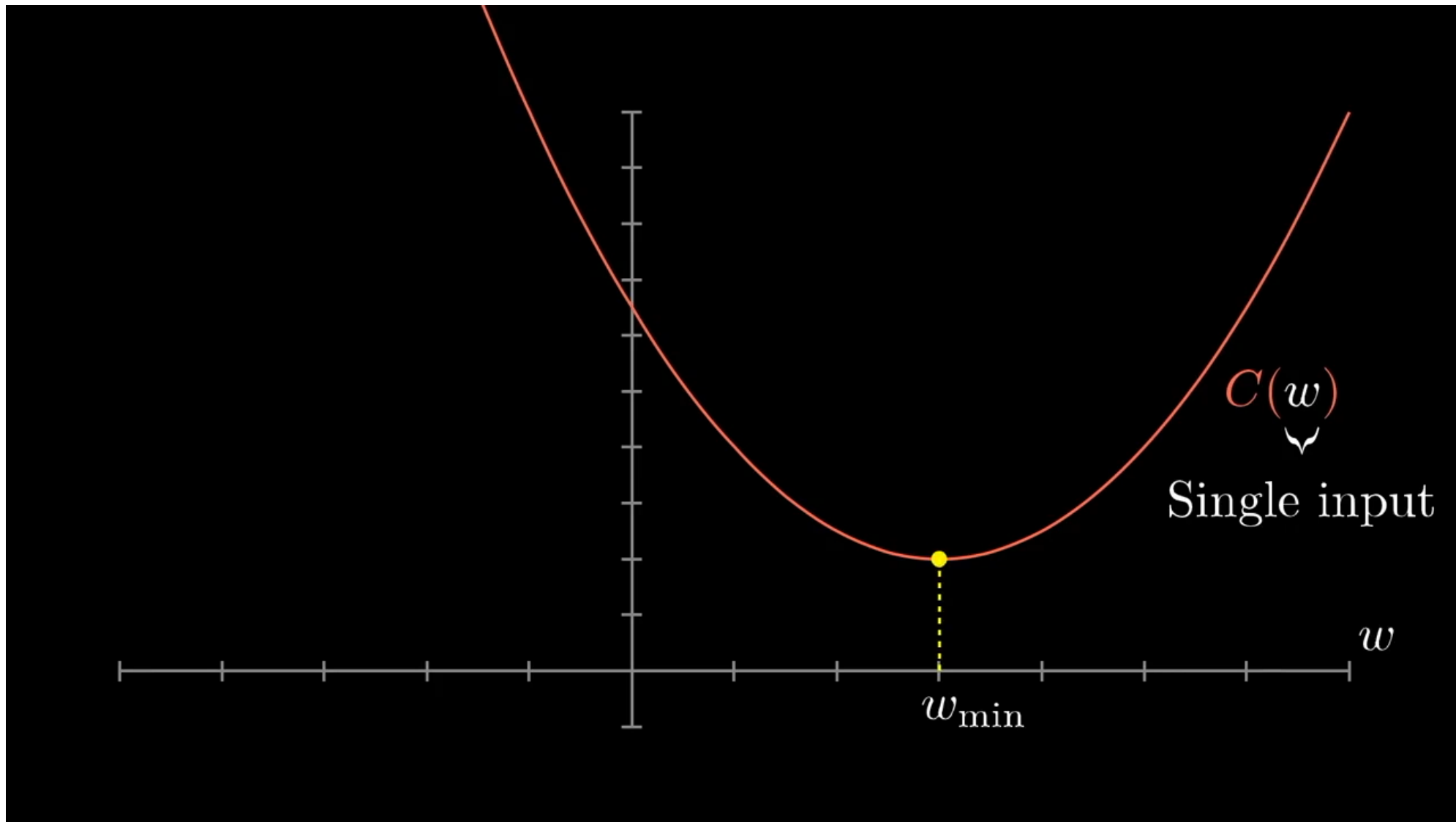


Minimizing our cost function: **least squares estimation**

$$J(\theta) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$



Gradient Descent



Multiple Regression

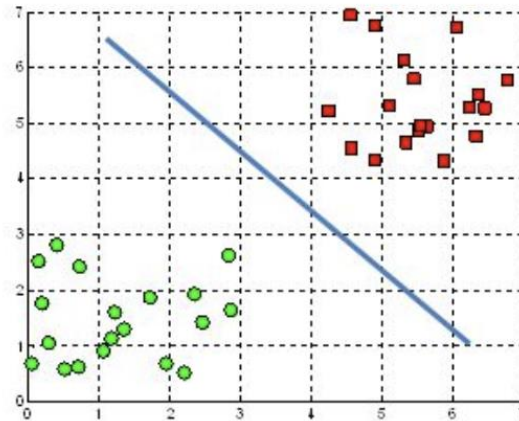
We can extend our regression model to include more features

$$y = \theta_1 X_1 + \theta_2 X_2 + \dots + \theta_n X_n + \theta_0$$

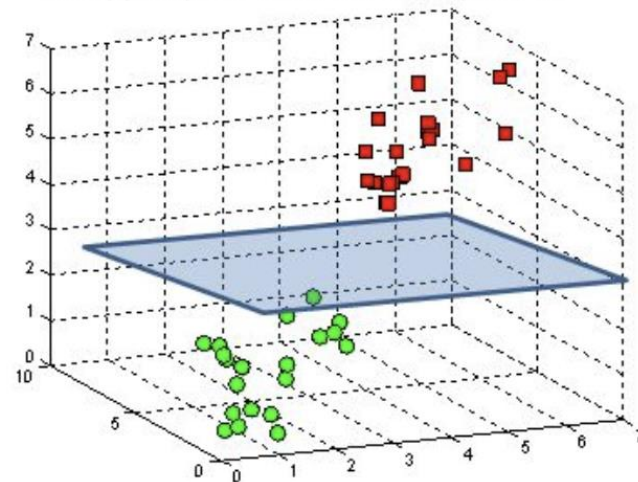
$$\theta_1 \times (\text{Red Blood Cell Count}) + \theta_2 \times (\text{Hemoglobin}) + \dots$$

What would our
model look like with
more features?

A hyperplane in \mathbb{R}^2 is a line



A hyperplane in \mathbb{R}^3 is a plane



Summary: Linear Regression



Pros:

- Simple
- Easy to interpret
- Computationally inexpensive

Cons:

- Oversimplifies many real-world problems
- As the name implies, assumes a linear relationship between model parameters and dependent variables
- Sensitive to outliers



From Linear to Logistic Regression

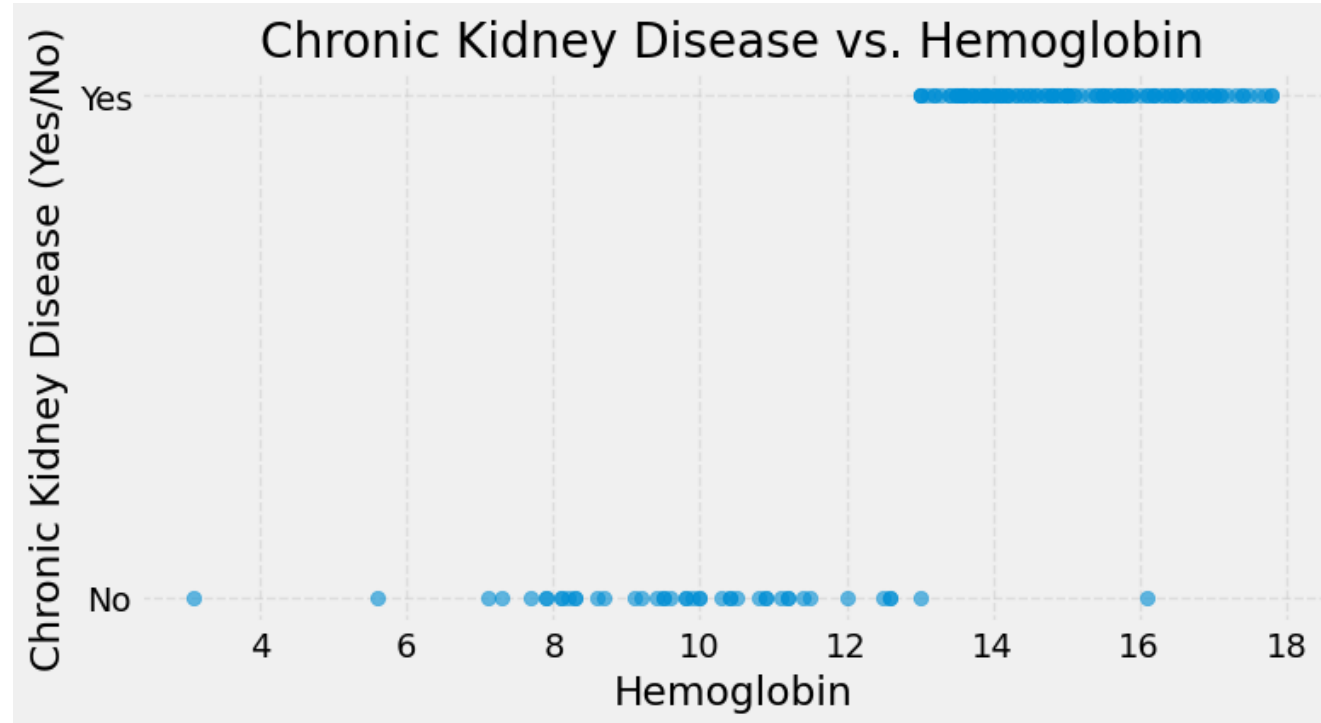
- We used *linear regression* to predict on a quantitative continuous data type
- What if we want to predict a category of data?
 - Nominal – Named categories
 - Ordinal – Categories with implied order
 - Discrete – Finite values
- Using *logistic regression*, we can predict classes of objects.
- What type of data might be involved in predicting whether a patient has chronic kidney disease?





Example - Kidney Disease Detection

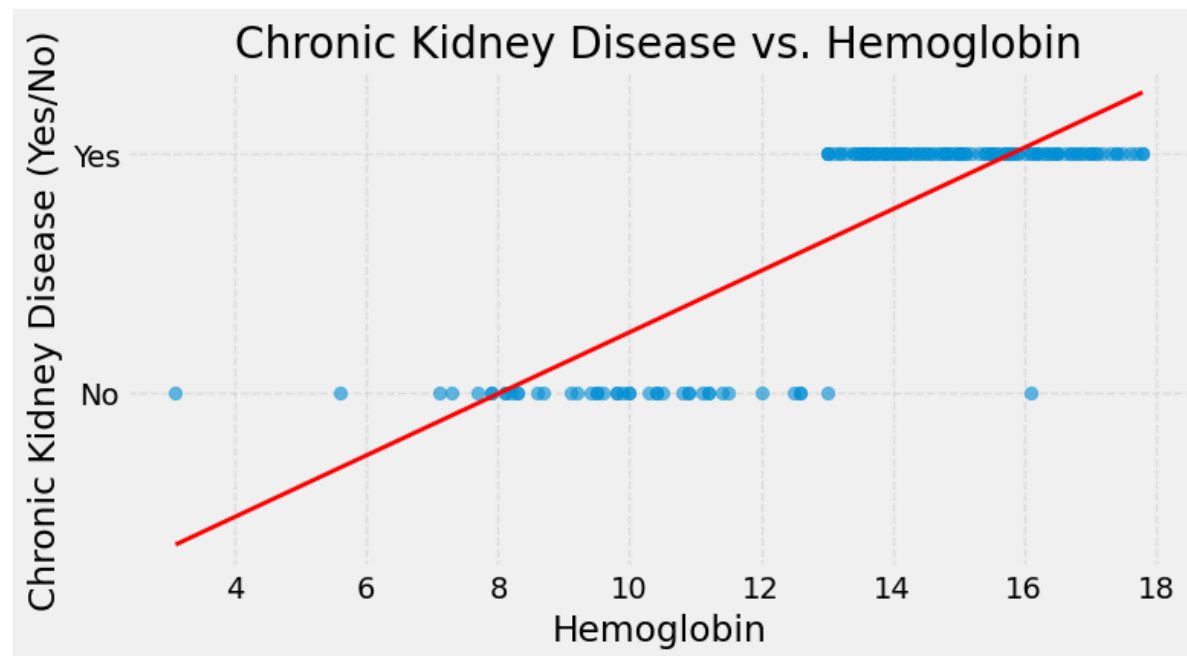
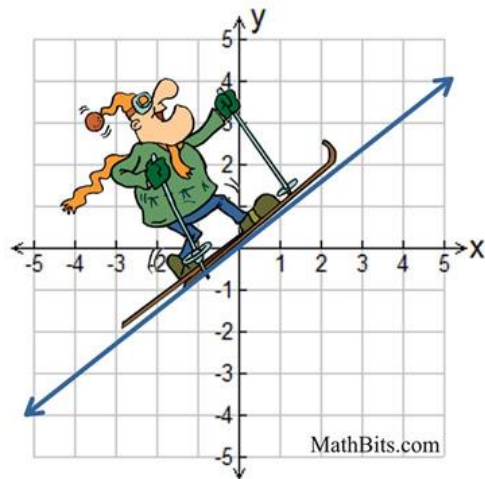
Your data might look something like this:



How would you define boundaries to model this data?

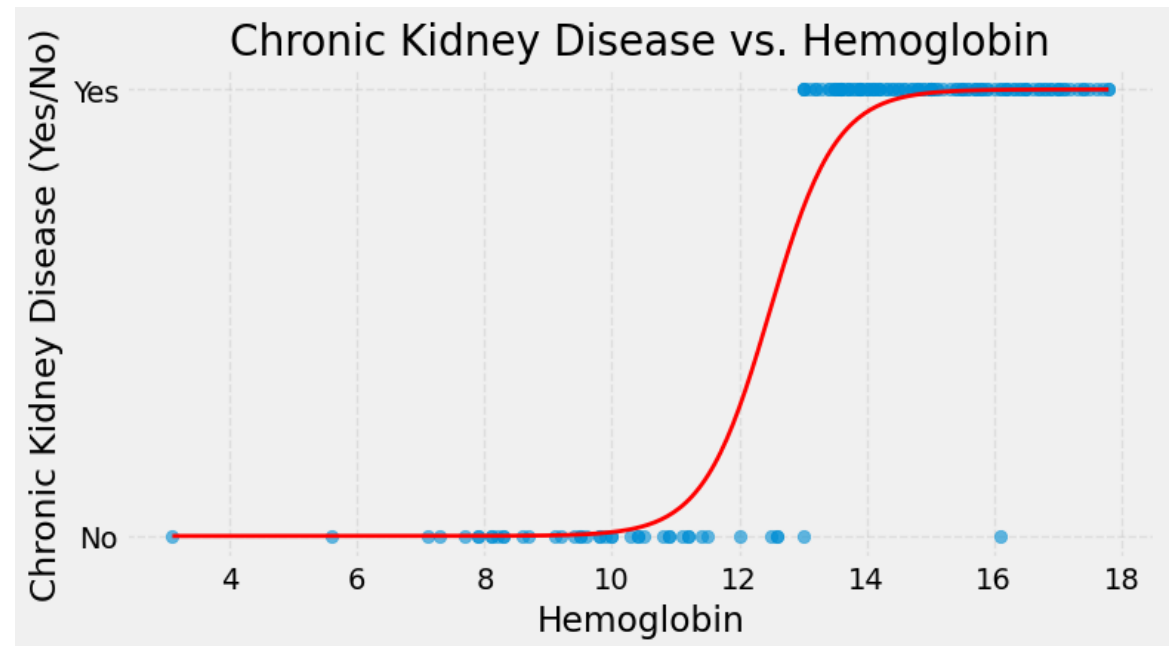
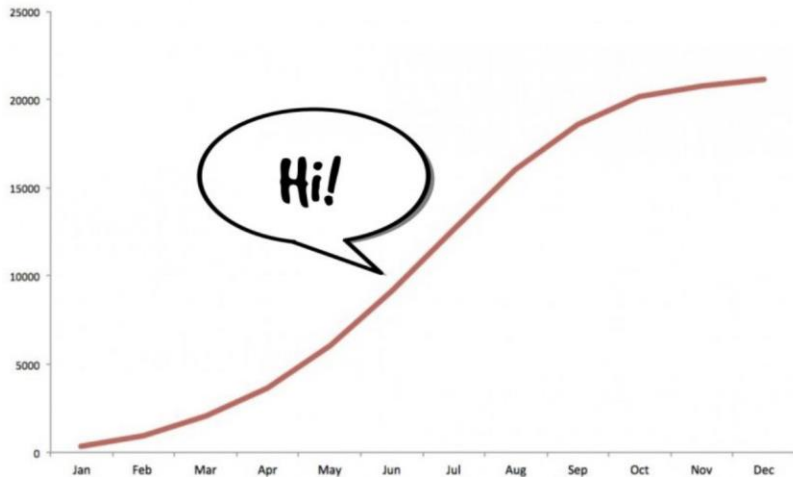
Maybe Something Like This?

- Here is our line of best fit (linear regression):
- What's wrong with this model?



Or Something Like This?

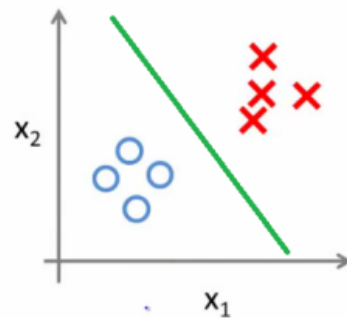
- As you may have ascertained, this is not a linear regression problem.
- An ideal boundary might look more like this:



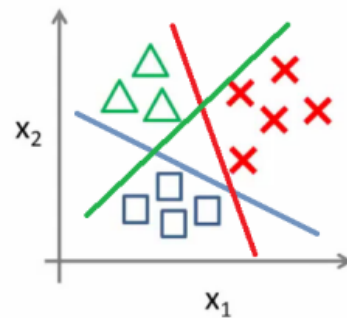
Logistic Regression

- A statistical method for analyzing a dataset that has one or more independent variables that determine an outcome
- Simplistic algorithm, but often makes a good baseline model
- Used to predict a binary outcome (1/0, Yes/No, True/False)
- Allows us to create models for classification problems:
 - What animals are in this image?
 - Is this email spam?
 - Disease predicted?

Binary classification:



Multi-class classification:



Binary
Classification



- Spam
- Not spam

Multiclass
Classification



- Dog
- Cat
- Horse
- Fish
- Bird
- ...

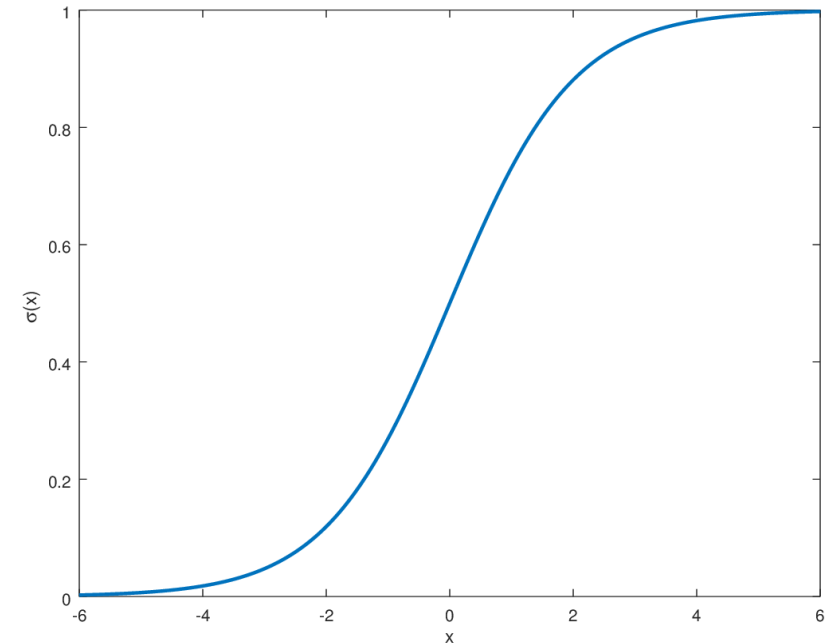
Logistic Regression - Equation

- Logistic regression is just linear regression with one additional step

$$y = \theta_1 X_1 + \theta_0$$

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

All values become
constrained between 0 and 1





Summary: Logistic Regression



Pros:

- Easy to interpret
- Quick to train
- Provides probabilities as outputs

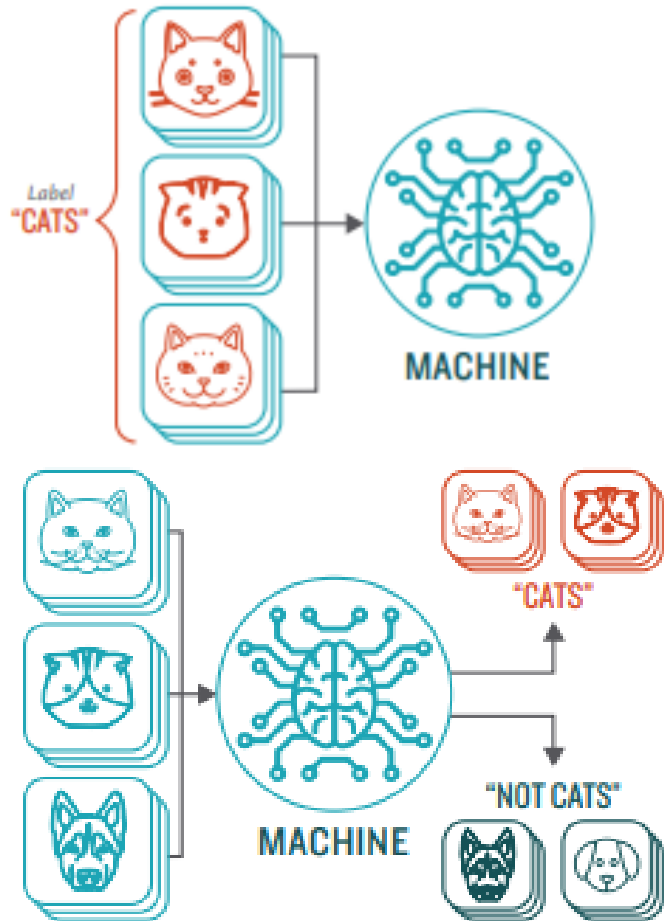
Cons:

- Poor performance in large feature spaces
- Cannot handle large amounts of categorical variables well
- In practice, it's typically only applied to binary classification outcomes

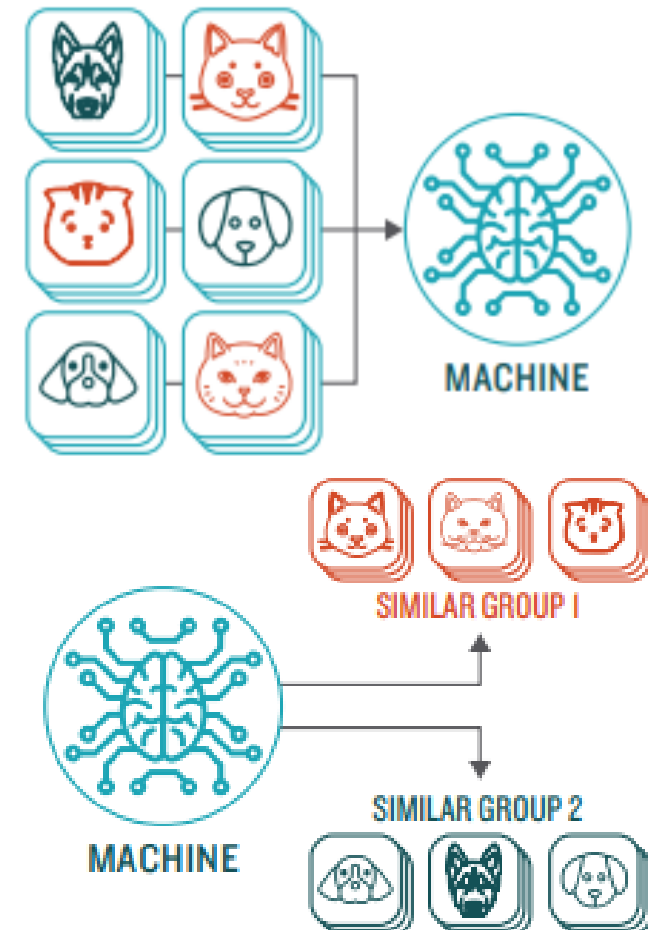


Supervised & Unsupervised Learning

Supervised: labeled data



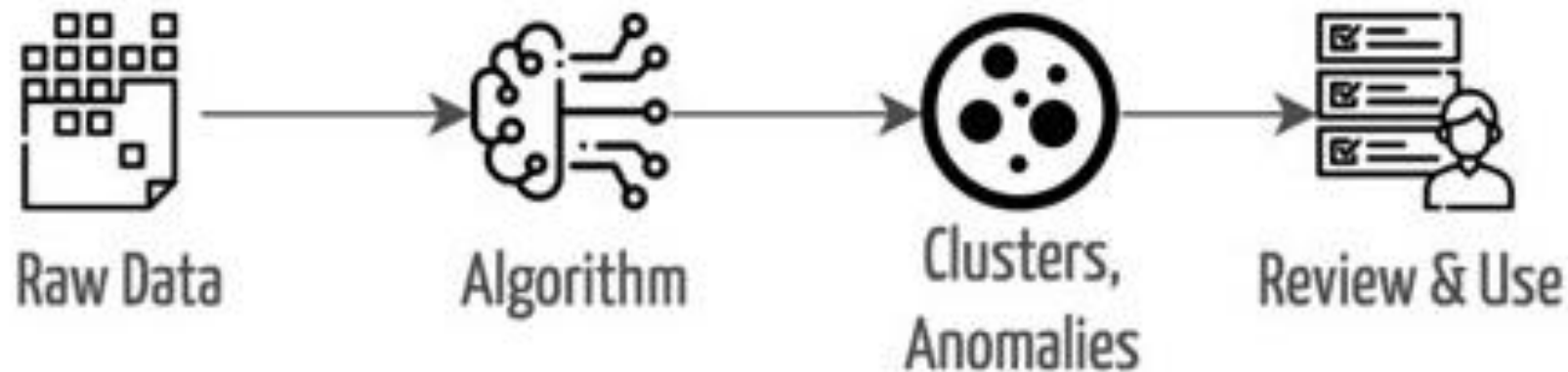
Unsupervised: unlabeled data





Unsupervised Learning - Overview

Uncovering inherent structures, patterns, and relationships hidden in collections of unlabeled data



What Do You Do with Unlabeled Data?

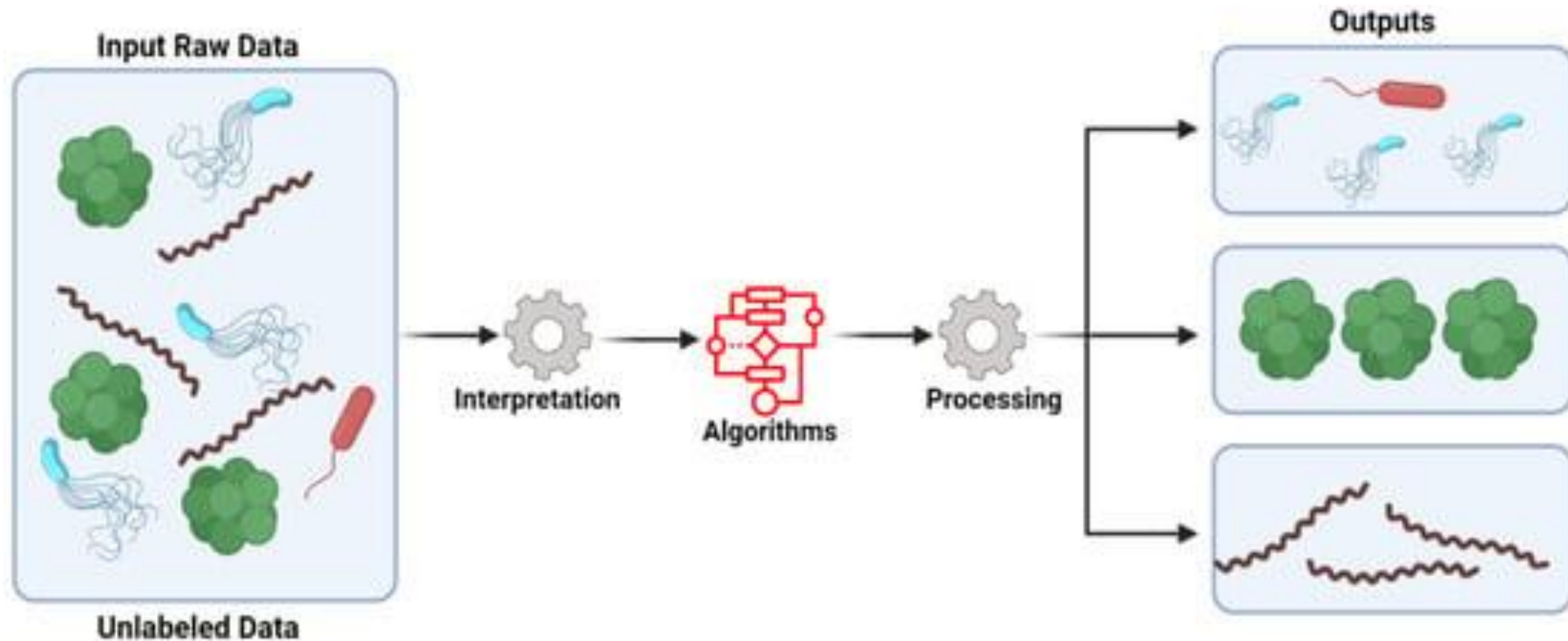
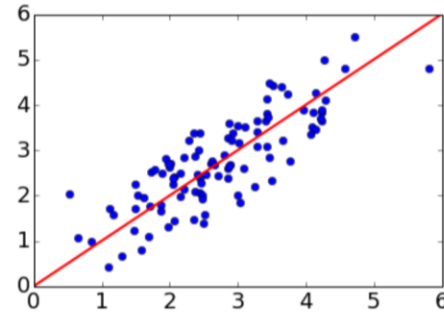


Image Source: [Unsupervised Learning in Precision Medicine | mdpi.com](https://www.mdpi.com)

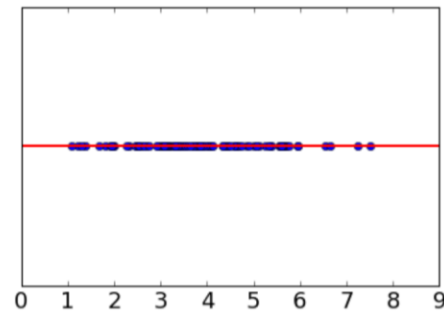


Refresher: Dimensionality Reduction

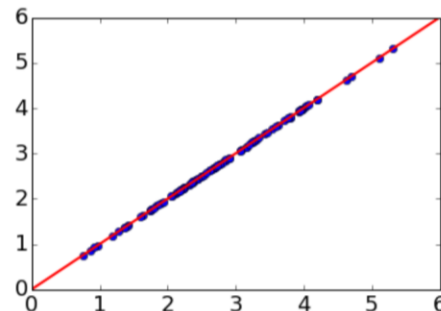
Dimensionality reduction is simply the process of reducing the dimensions of your feature set



Projection onto \mathbb{R} :



Projection onto a 1-d line in \mathbb{R}^2 :





Example – Kidney Disease Data

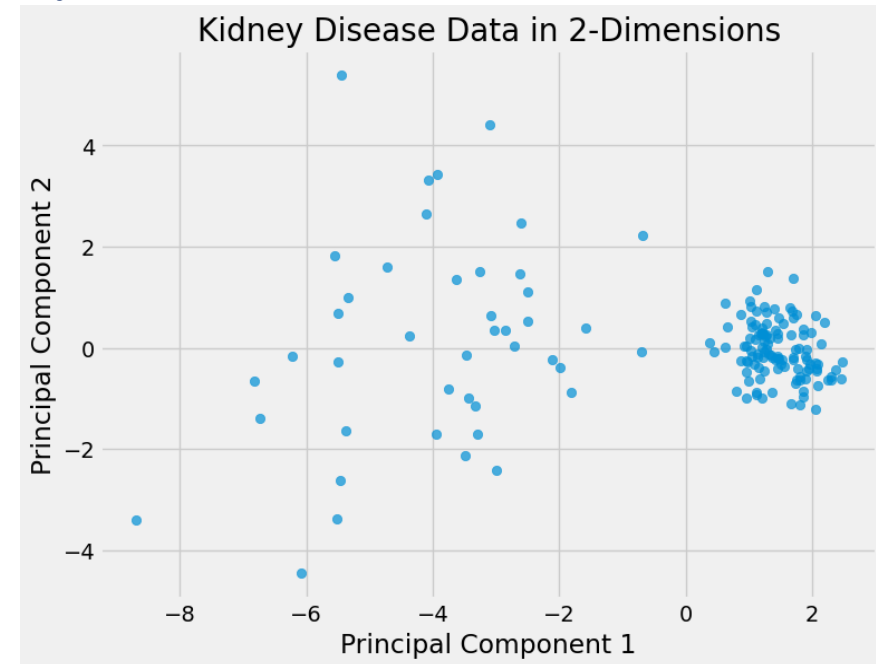
For each patient you find, you have data on the following features:

age = Age	sod = Sodium
pot = Potassium	hemo = Hemoglobin
pcv = Packed Cell Volume	wc = White Blood Cell Count
rc = Red Blood Cell Count	htn = Hypertension
dm = Diabetes Mellitus	cad = Coronary Artery Disease
appet = Appetite	pe = Pedal Edema
ane = Anemia	bp = Blood Pressure
sg = Specific Gravity	al = Albumin
su = Sugar	rbc = Red Blood Cells
pc = Pus Cell	pcc = Pus Cell Clumps
bgr = Blood Glucose Random	bu = Blood Urea
sc = Serum Creatinine	classification = Chronic Disease (Yes/No)

Principal Component Analysis (PCA)

We have a lot of features in our data, so it can be difficult to make sense of the data in this form. We can use principal component analysis (PCA) to reduce our data to two dimensions, which is a great way to visualize feature-rich data.

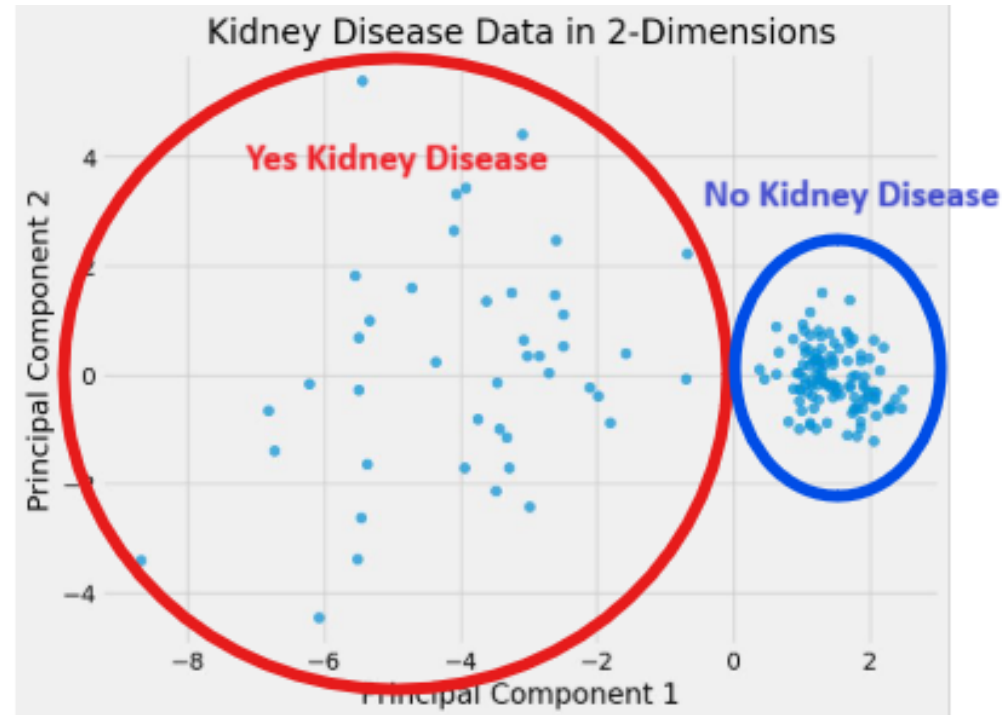
age = Age	sod = Sodium
pot = Potassium	hemo = Hemoglobin
pcv = Packed Cell Volume	wc = White Blood Cell Count
rc = Red Blood Cell Count	htn = Hypertension
dm = Diabetes Mellitus	cad = Coronary Artery Disease
appet = Appetite	pe = Pedal Edema
ane = Anemia	bp = Blood Pressure
sg = Specific Gravity	al = Albumin
su = Sugar	rbc = Red Blood Cells
pc = Pus Cell	pcc = Pus Cell Clumps
bgr = Blood Glucose Random	bu = Blood Urea
sc = Serum Creatinine	classification = Chronic Disease (Yes/No)



But what are these two dimensions now?
 What are these PCA “components” on the X and Y axis?

Which Patients Have Kidney Disease?

- We need a way to assign labels (kidney disease yes/no) to our data
- Clustering techniques (like k-means) provide a possible solution



Summary: PCA



Pros:

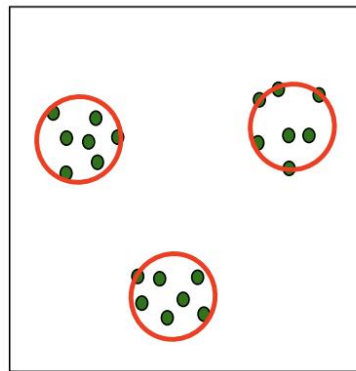
- Prevents overfitting
- Removes correlated features
- Speeds up other machine learning algorithms
- Improves visualization

Cons:

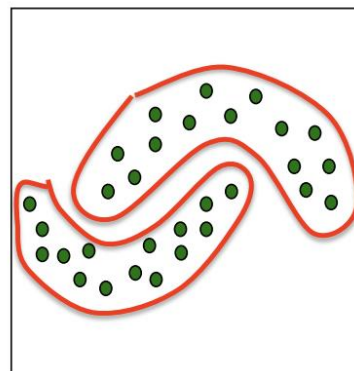
- Difficult to interpret new components
- Can lead to losing information
- Computationally expensive

K-means Clustering

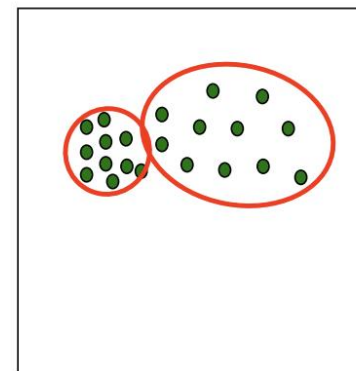
- Clustering describes the process of grouping data into shared characteristics
- The characteristics of a group may vary by data
- K-means takes a data sample as input and outputs the cluster that the new data point belongs to, according to the training that the model went through



Location



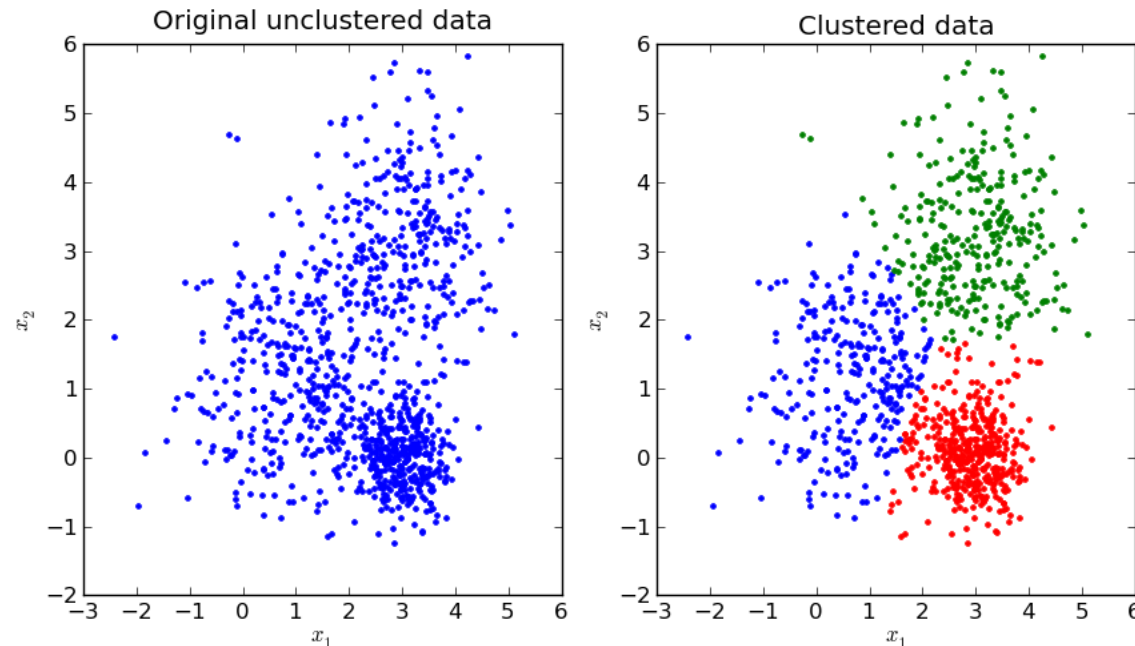
Shape



Density

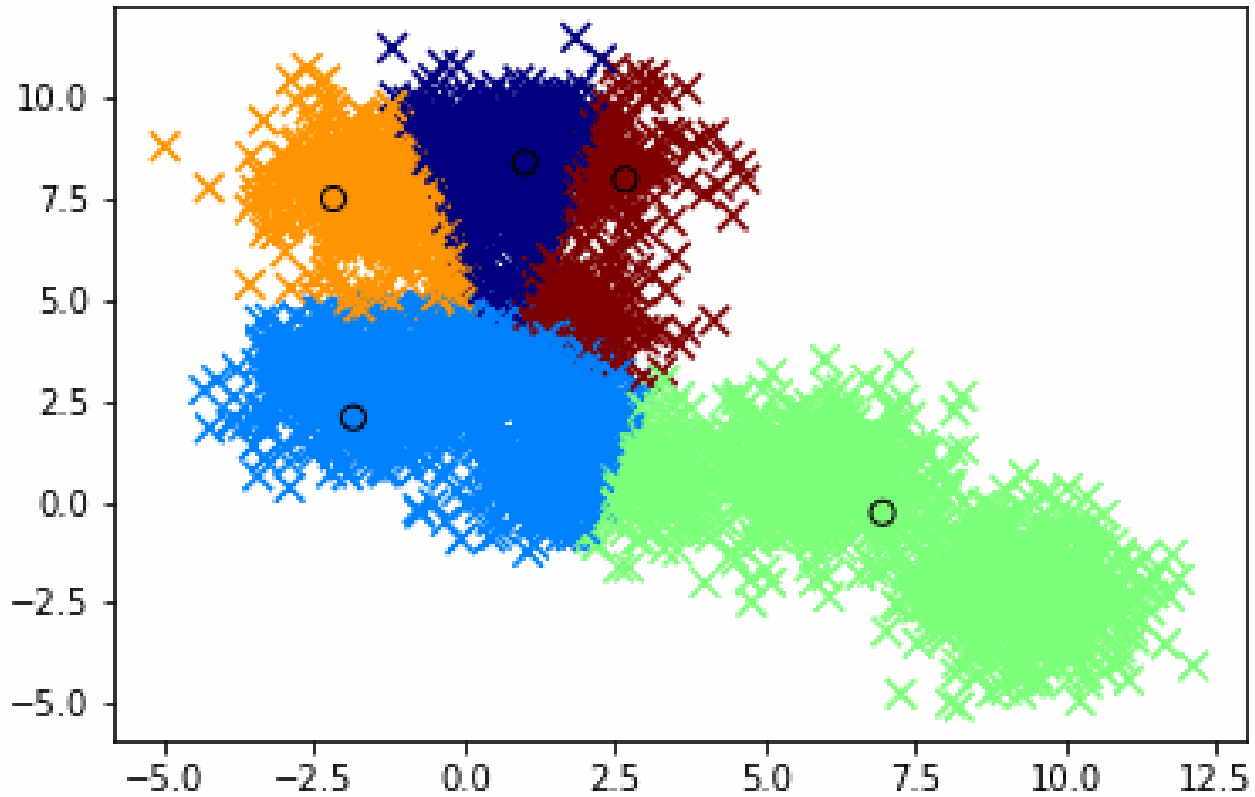
How Does K-means Work?

- An iterative process of clustering or finding groups of data in our dataset that are similar to one another
- Iterates until it reaches the best solution of clusters in our problem space





How Does K-means Work?

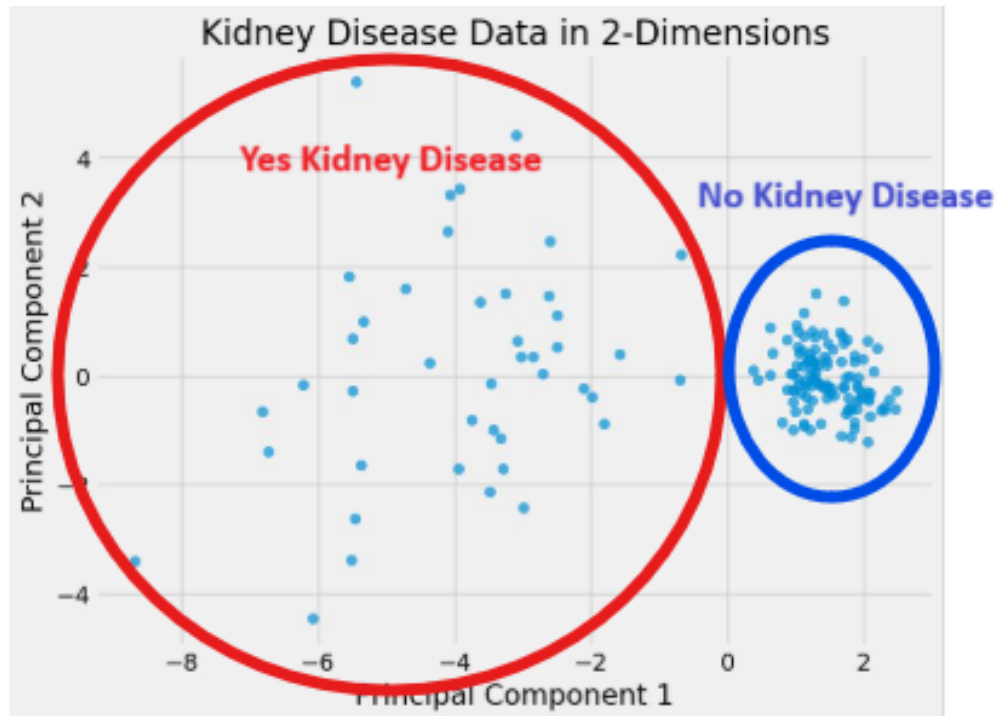


1. Choose k data points to be the initial centroids (cluster centers)
2. Assign each data point to the closest centroid
3. Re-calculate the centroids using the average of the assigned points
4. Iterate (repeat) over steps 2 & 3 until the centroids no longer move (converge)

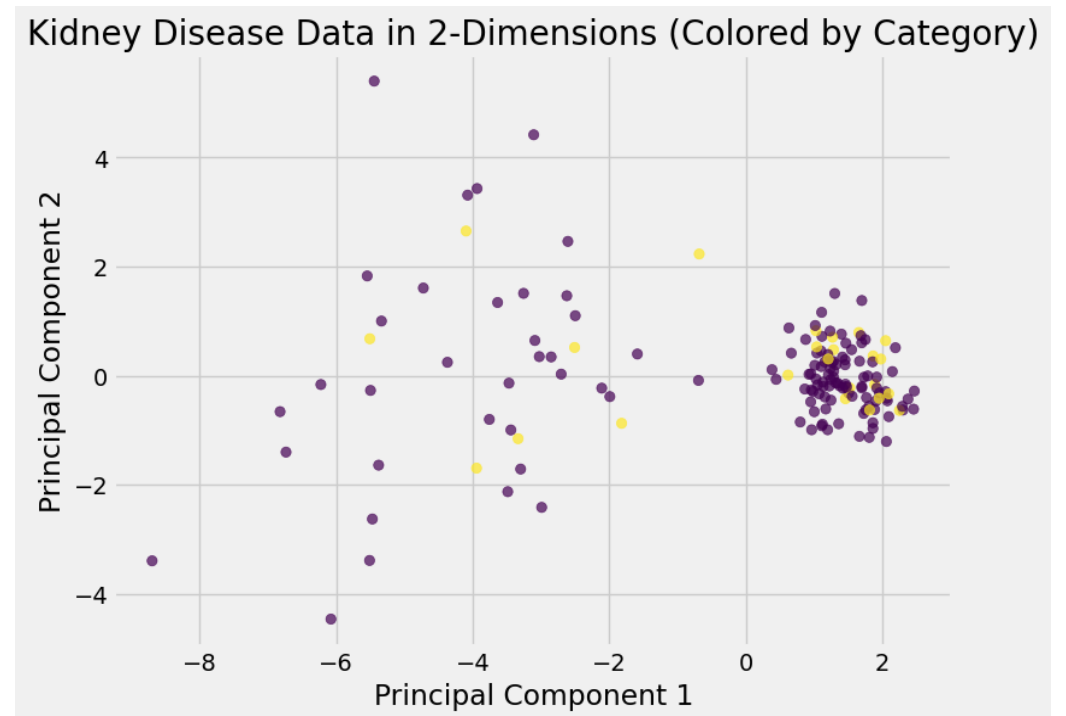


Not a Perfect Solution...

Predicted Unsupervised Labels



Actual Labels





Summary: K-means



Pros:

- Easy to understand and implement
- Computationally inexpensive
- Guarantees convergence

Cons:

- Results are highly variable and dependent on initial values
- Sensitive to outliers
- Struggles with data of varying sizes and densities





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Stretch Break



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Deep Learning Overview

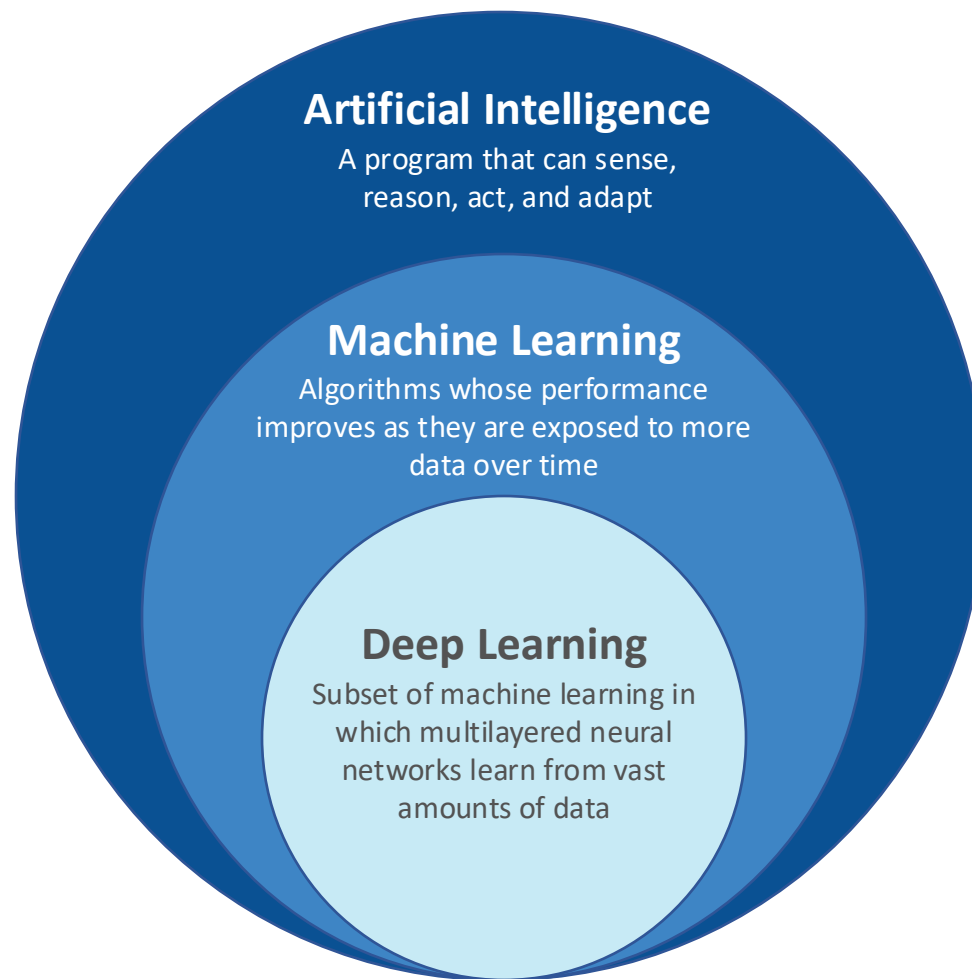




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Deep Learning – Subset of Machine Learning

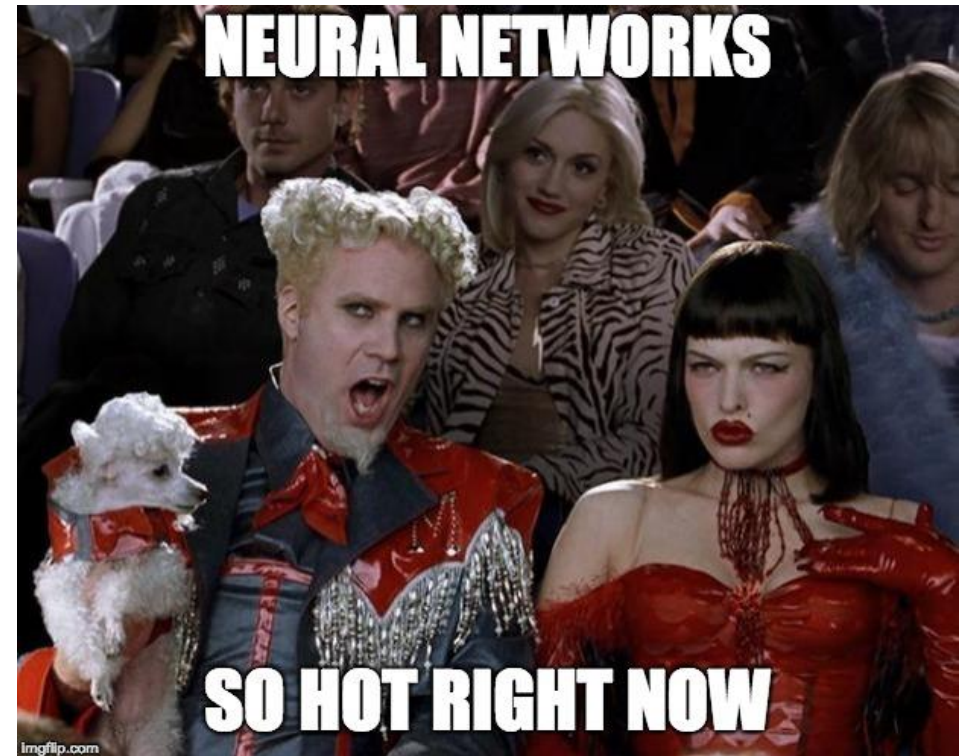




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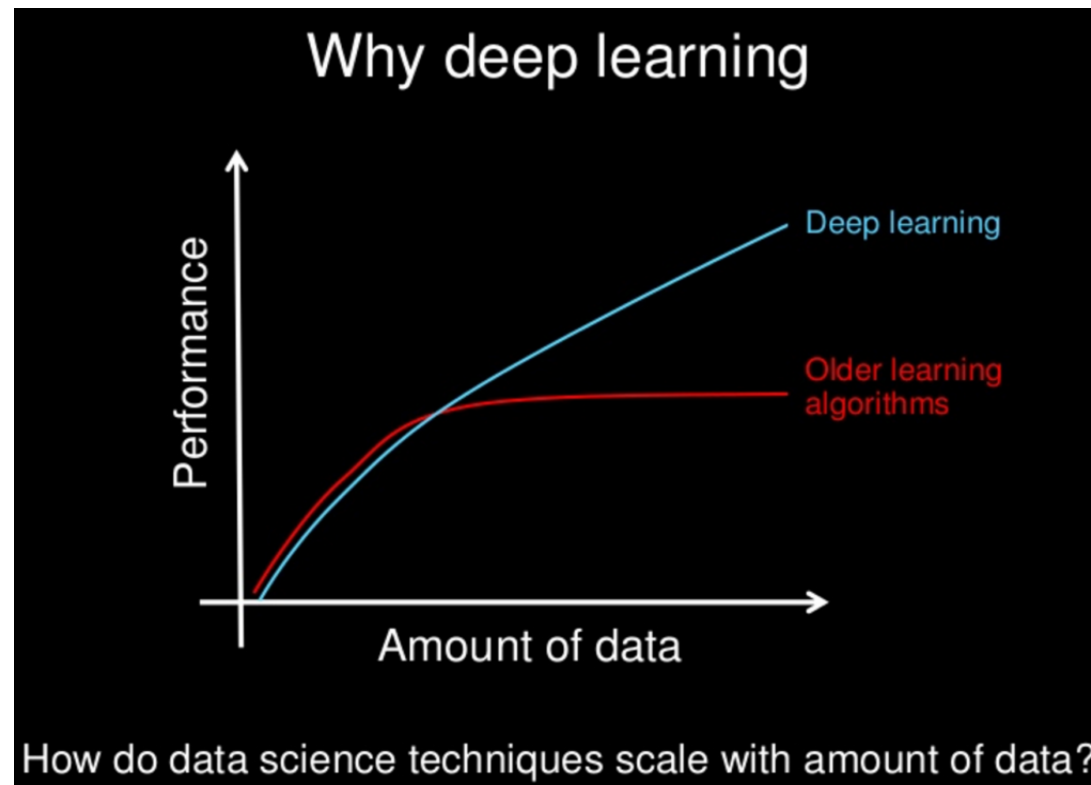
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Neural Networks





Why is Deep Learning So Hot?



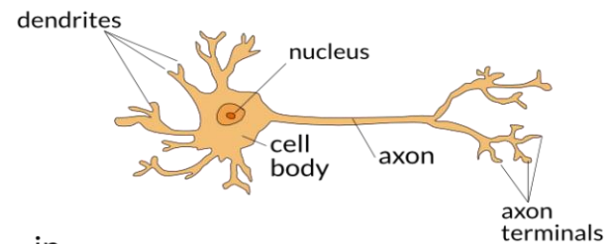


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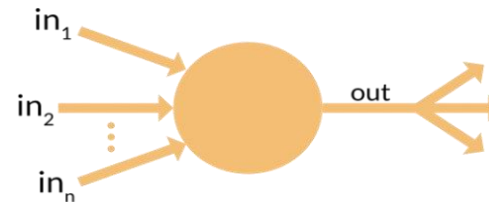
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Deep Learning Inspired Party from Biology

Human neuron



Neural network node

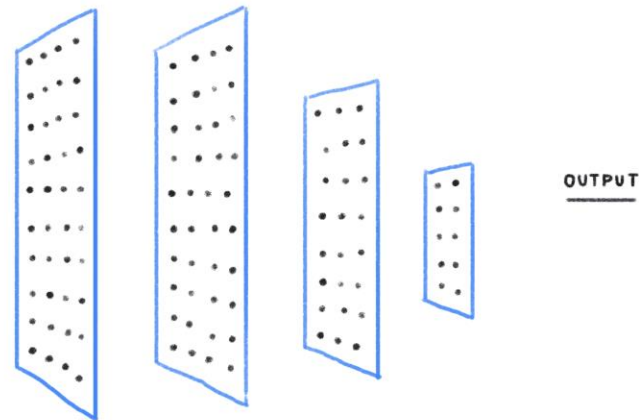


CAT

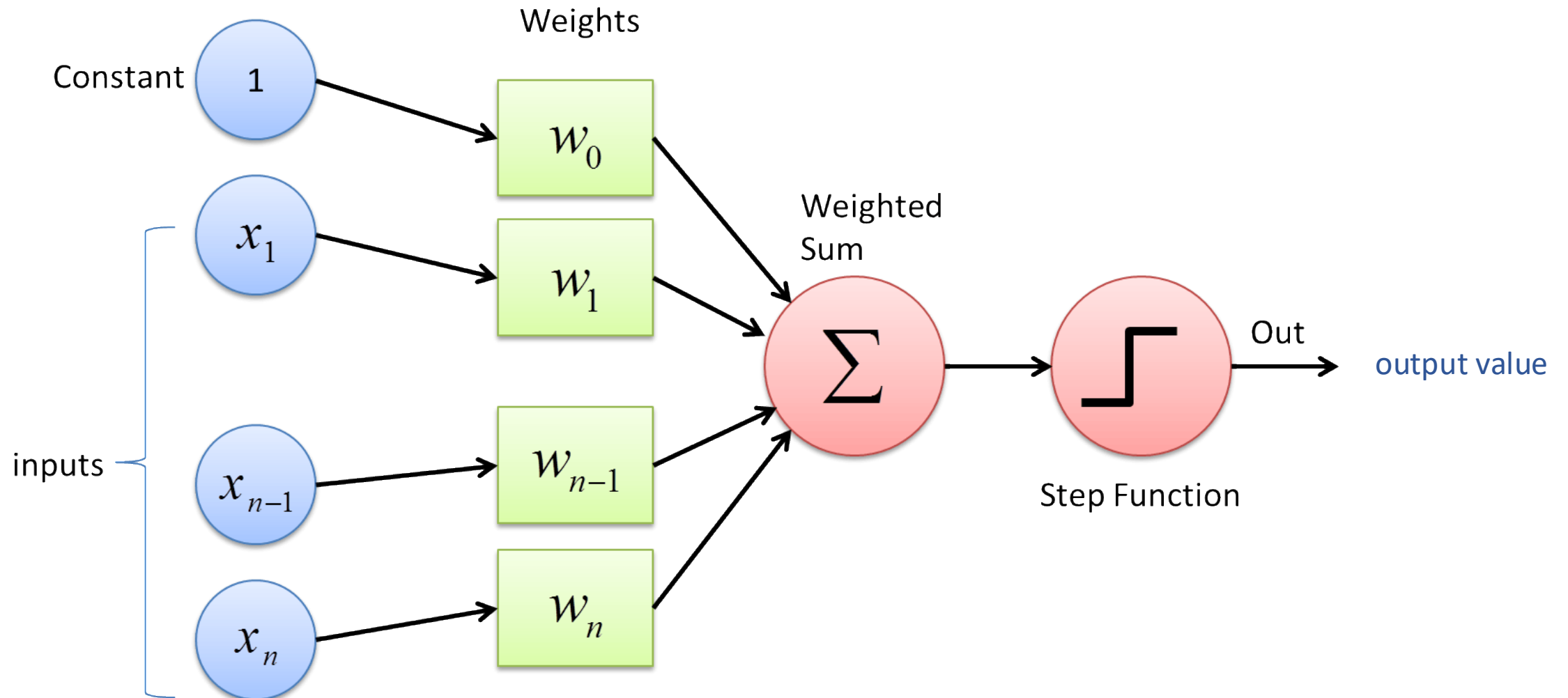


(Labeled
PHOTOS)

DOG

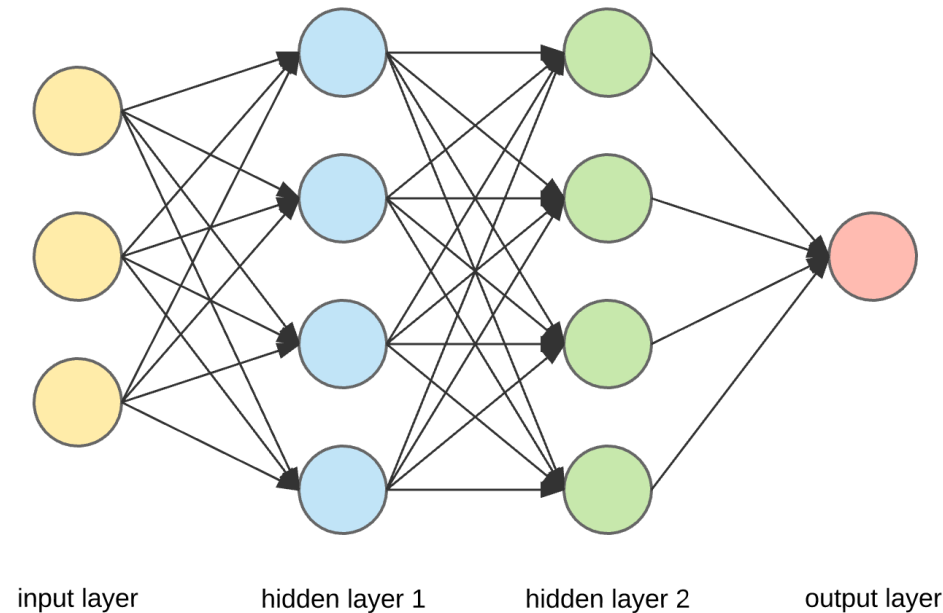


The Perceptron (A Single "Neuron")



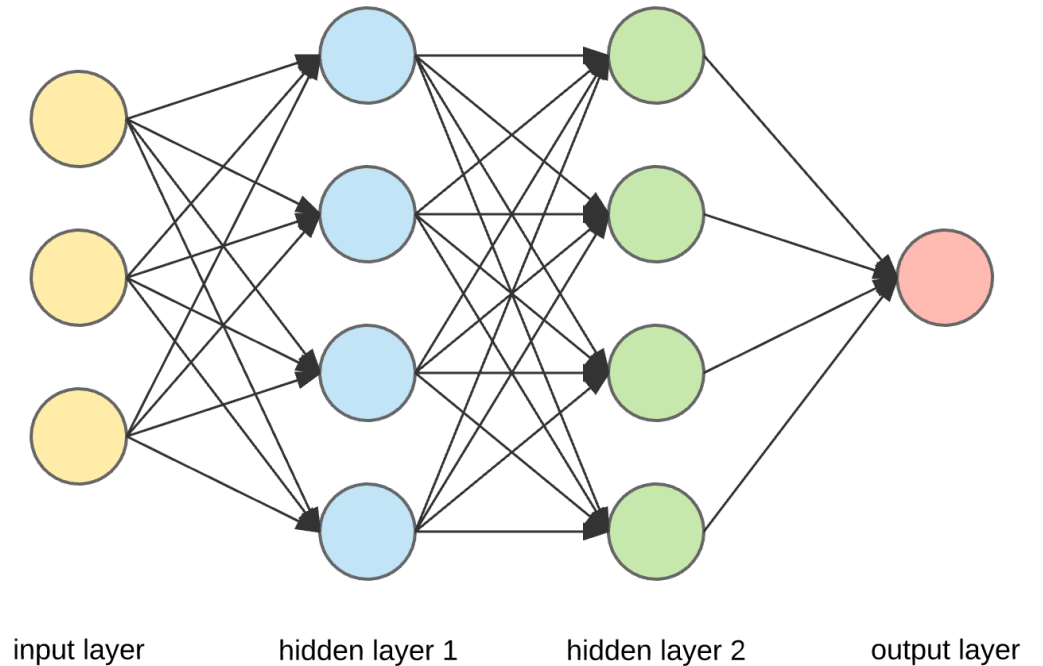
"Feed Forward" Neural Networks

- This is the most basic, vanilla form of neural network that all other neural networks use as a foundation.
- Number of layers and nodes/neurons per layer is a choice made by network's architect(s).
- Each node is essentially a perceptron.



How Neural Networks Learn

- Like we've seen previously, neural networks can use gradient descent to find ideal weights.
- But, they have a special trick called **backpropagation** to calculate the gradients.
- Backpropagation leverages the chain rule, though this goes beyond the scope of this class.





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Neural Networks in Python



TensorFlow



PyTorch



Keras



Summary: Neural Networks



Pros:

- Able to capture more complexity in a model
- Widely applicable to real-world business problems
- Once trained, predictions are fast

Cons:

- Computationally expensive to train
- Needs lots of data
- Can require lots of parameter tweaking and retraining
- Has a "black box" nature





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Specialized DS Topics



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Specialized Topics in Data Science

- **Computer Vision:** Interdisciplinary subfield of AI that enables interpretation and understanding of digital images or videos.
- **Time Series Analysis:** Modeling a sequence of data over an interval of time.
- **Natural Language Processing (NLP):** Interdisciplinary subfield of AI that enables interpretation and understanding of natural language data (e.g., text and speech).



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Computer Vision



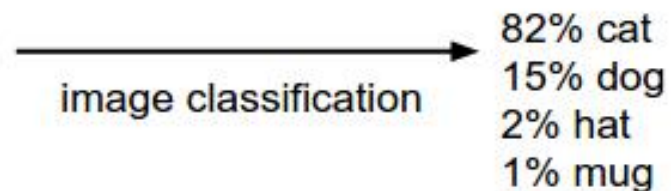


How Does a Computer Understand Image Data?



08	02	22	97	38	15	00	40	00	75	04	05	07	78	52	12	50	77	91	22
49	49	99	40	17	81	18	57	60	87	17	40	98	43	69	45	04	56	62	00
81	49	31	73	55	79	14	29	93	71	40	67	55	08	30	03	49	13	36	65
92	70	95	23	04	60	11	42	69	24	68	56	01	32	56	71	37	02	36	91
22	31	16	71	51	67	03	89	41	92	36	54	22	40	40	28	66	33	13	80
24	47	33	60	99	03	45	02	44	75	33	53	78	36	84	20	35	17	12	50
52	98	81	28	64	23	67	10	26	38	40	67	59	54	70	66	18	38	64	70
67	26	20	68	02	62	12	20	95	63	94	39	63	08	40	91	66	49	94	21
24	55	58	05	66	73	99	26	97	17	78	78	96	83	14	88	34	89	63	72
21	36	23	09	75	00	76	44	20	45	35	14	00	61	33	97	34	31	33	95
78	17	53	28	22	75	31	67	15	94	03	80	04	62	16	14	09	53	56	92
16	39	05	42	96	35	31	47	55	58	88	24	00	17	54	24	36	29	85	57
86	56	00	48	35	71	89	07	05	44	44	37	44	60	21	58	51	54	17	58
19	80	81	68	05	94	47	69	28	73	92	13	86	52	17	77	04	89	85	40
04	52	08	83	97	35	99	16	07	97	57	32	16	26	26	79	33	27	98	66
02	56	68	87	57	62	20	72	03	46	33	67	46	55	12	32	63	93	53	69
04	42	16	73	38	35	39	11	24	94	72	18	08	46	29	32	40	62	76	36
20	69	36	41	72	30	23	88	34	05	89	69	82	67	59	85	74	04	36	16
20	73	35	29	78	31	90	01	74	31	49	71	48	58	81	16	23	57	05	54
01	70	54	71	83	51	54	69	16	92	33	48	61	43	52	01	89	17	47	48

What the computer sees



Computer Vision Tasks

Classification



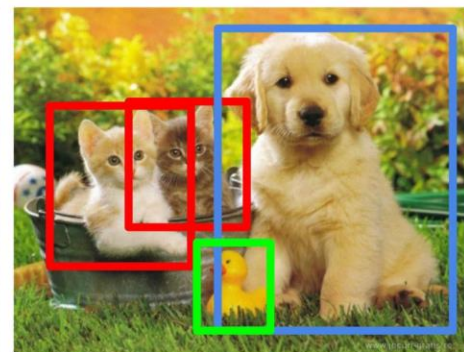
CAT

**Classification
+ Localization**



CAT

Object Detection



CAT, DOG, DUCK

**Instance
Segmentation**



CAT, DOG, DUCK

Single object

Multiple objects

Computer Vision: MNIST Dataset

The problem:

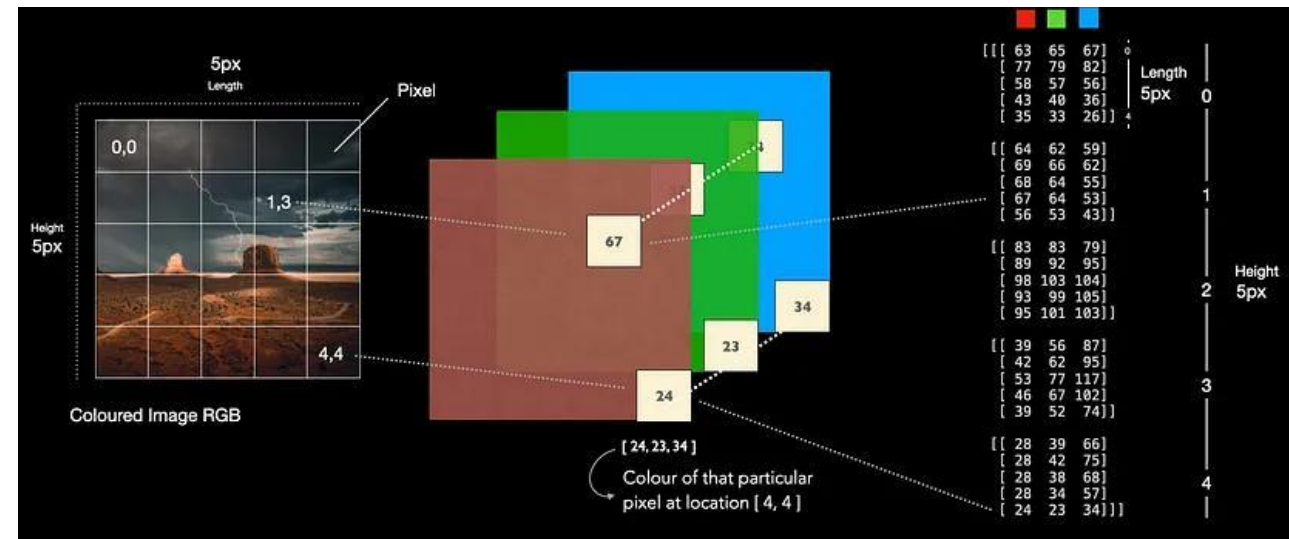
Given a collection of images of handwritten digits, determine which single-digit value was written.

0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9



Computer Vision: MNIST Dataset

- How do computers make sense of images?
- They convert them into a grid of pixel values.
- For example, in a color image, each pixel has a coordinate location on the image and an intensity value associated with the red-green-blue (RGB) color model.



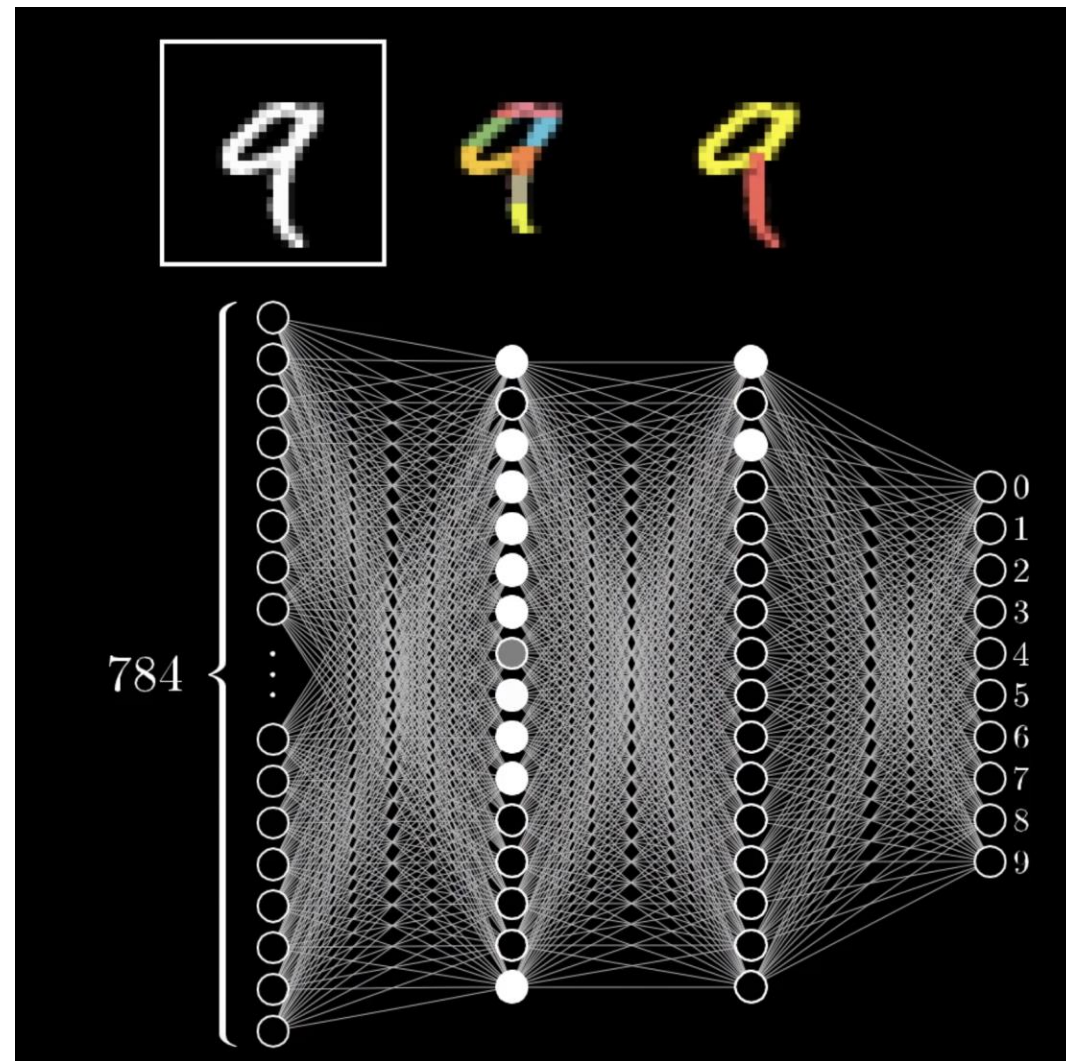
Computer Vision: MNIST Dataset



Computer Vision: MNIST Dataset

Conceptually, we can imagine each hidden layer of neurons acting to identify more and more complex features:

- 0th layer (the input layer) is the numeric pixel data of our image.
- 1st layer learns to look for vertical and horizontal lines.
- 2nd layer learns to put the lines together to form loops.
- 3rd layer (output layer) puts all of it together to decide what number the computer is "seeing."





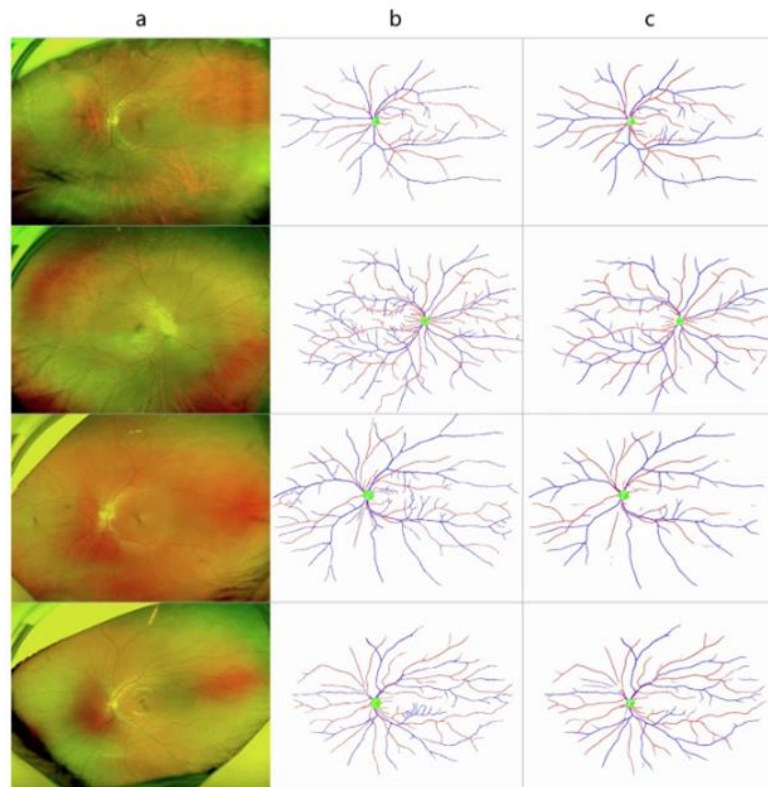
Computer Vision Isn't Perfect



IN CS, IT CAN BE HARD TO EXPLAIN
THE DIFFERENCE BETWEEN THE EASY
AND THE VIRTUALLY IMPOSSIBLE.



Example – Computer Vision for Renal Function



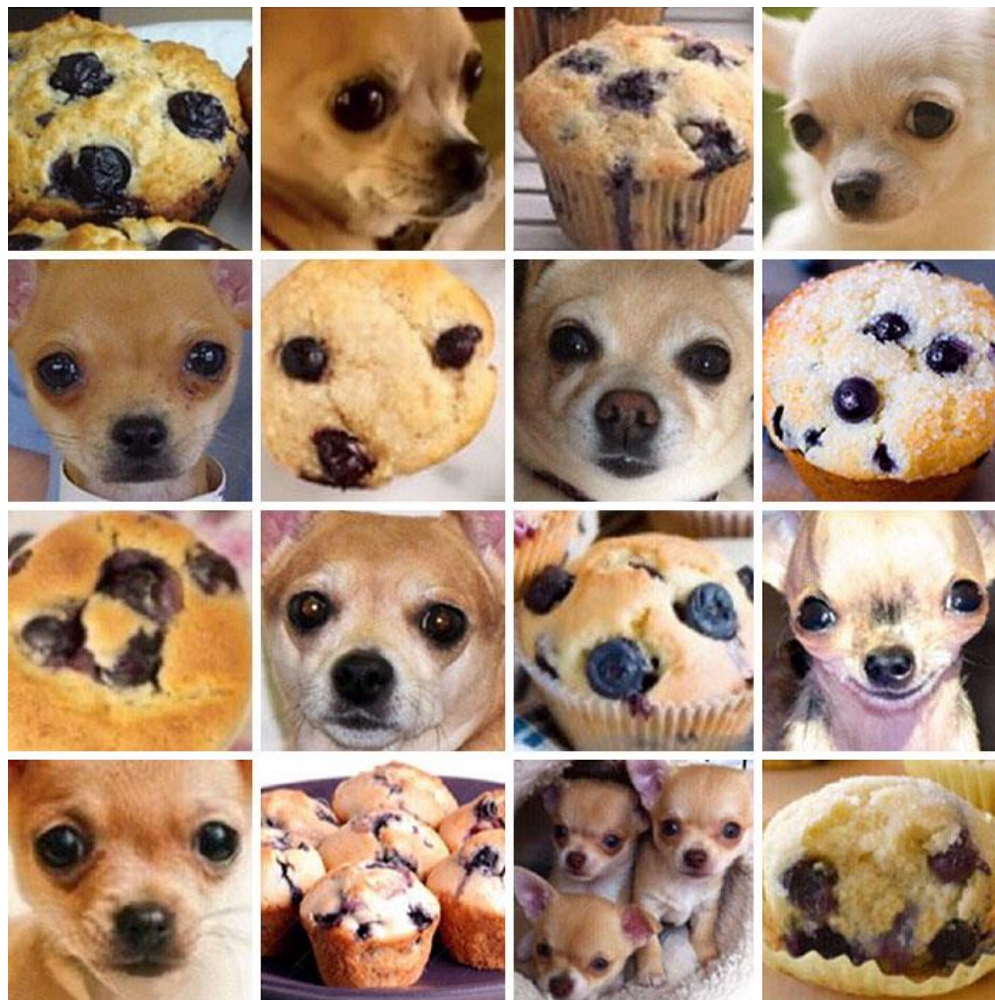
Four UWF images (a) and the segmentation results from experienced ophthalmology experts (b) and the segmentation model (c) were randomly selected for representation. The automatic segmentation of the optic disc and the vessels were very close to the doctor's annotation.



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Difficult Use Case: Chihuahua or Muffin?





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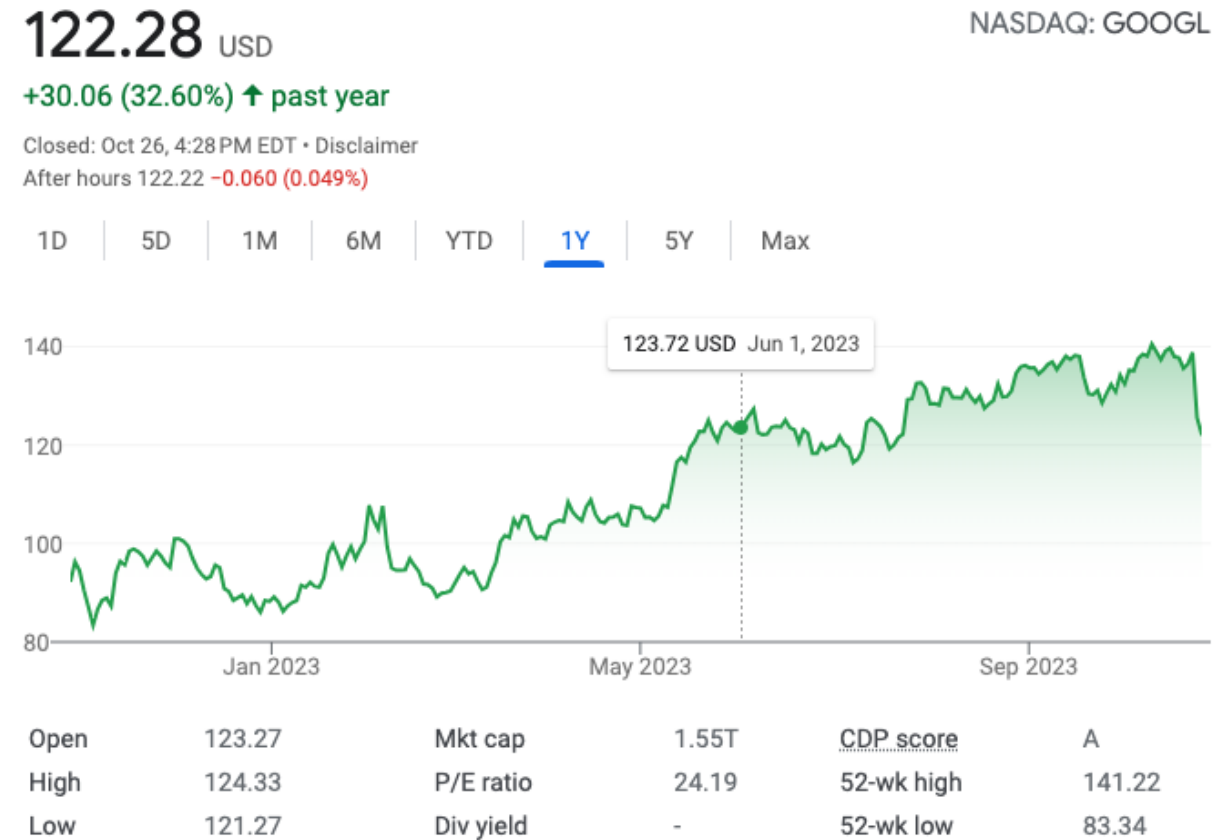
Time Series Analysis





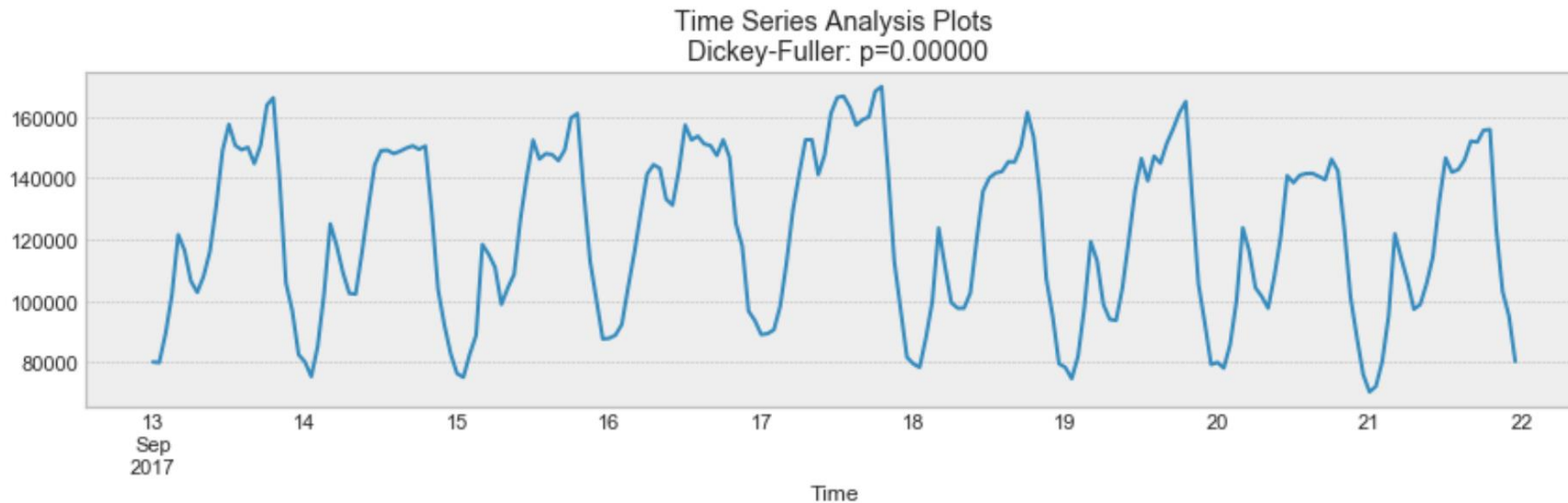
Time Series

- Time series data are commonly encountered in everyday life.
- Time series data is periodically captured for a given time period.
- Examples include financial prices, weather, home energy usage, height measured over time, etc.
- Stock prices and market indices are common examples.



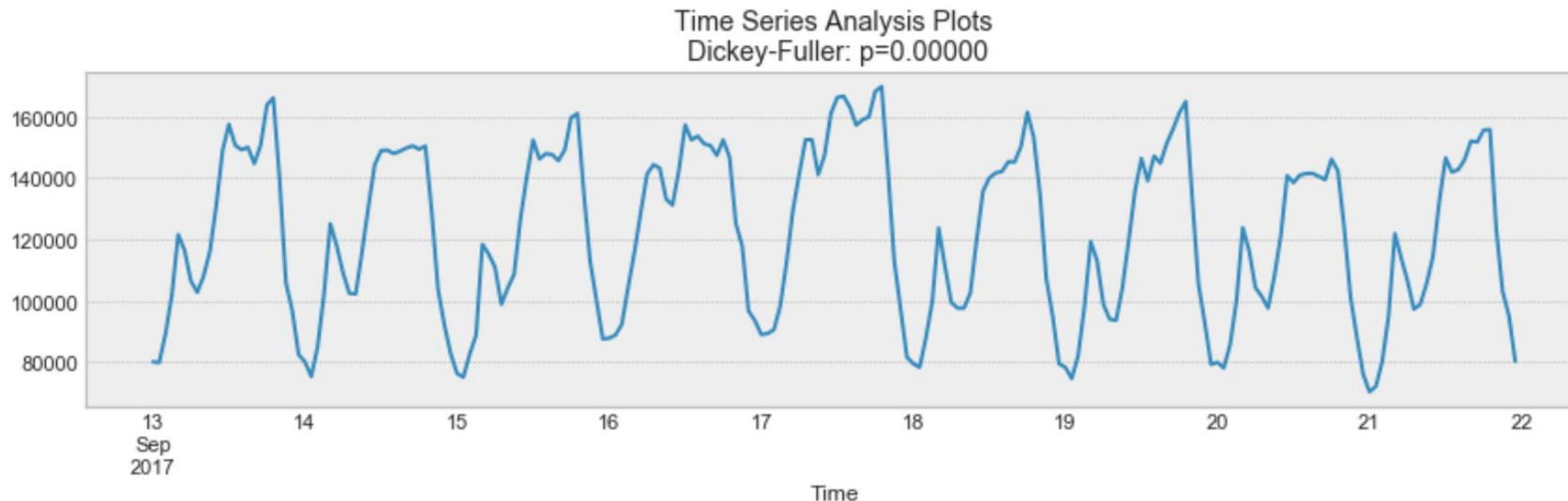
Seasonality in Time Series Data

- Periodic fluctuations in the graph.
- Trends that reoccur over time.
- Example: energy consumption is high during the day and low at night.



Stationarity

- A time series is stationary when its statistical properties do not change overtime (e.g., constant mean and variance).
- Stationary time series are ideal for modeling.
- The plot from the slide before is considered stationary.



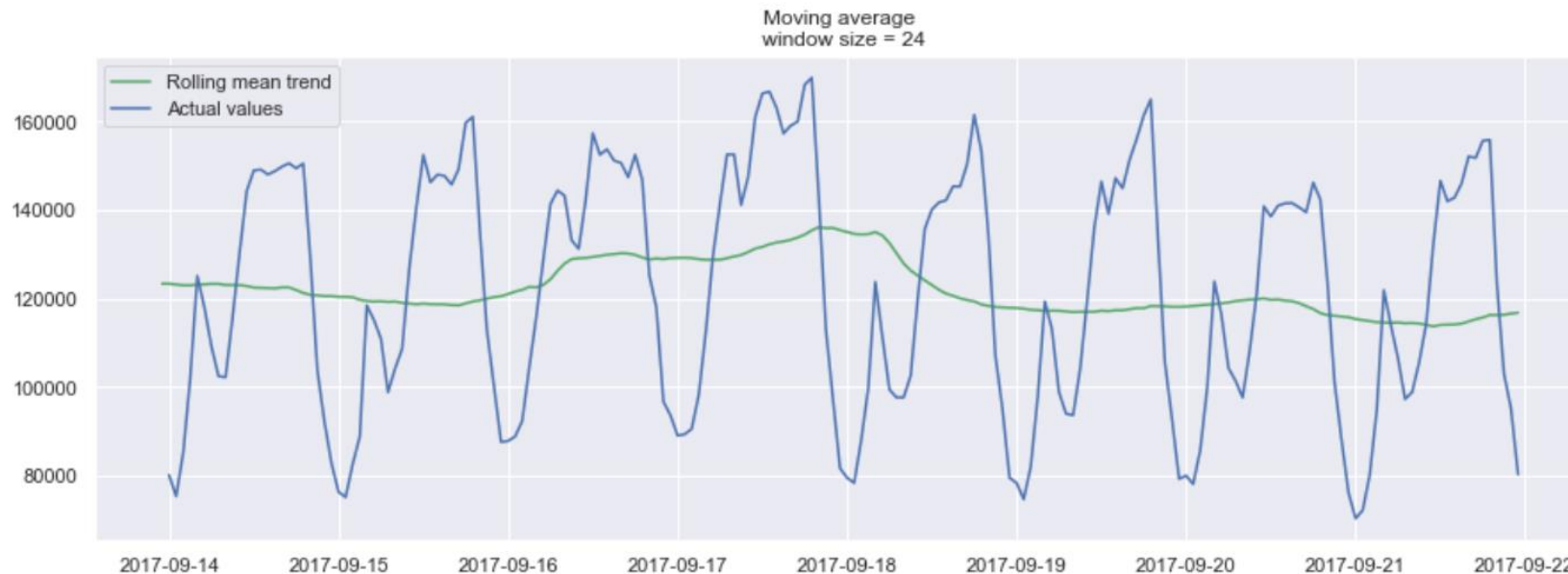


Smoothing Methods

- Smoothing methods reduce the effects of the random variation that comes from seasonality.
- These methods reveal the underlying trends in the data.
- Forecasts are weighted averages of past observations.
- There are two groups of smoothing methods:
 - Averaging Methods
 - Exponential Smoothing Methods

Moving Averages

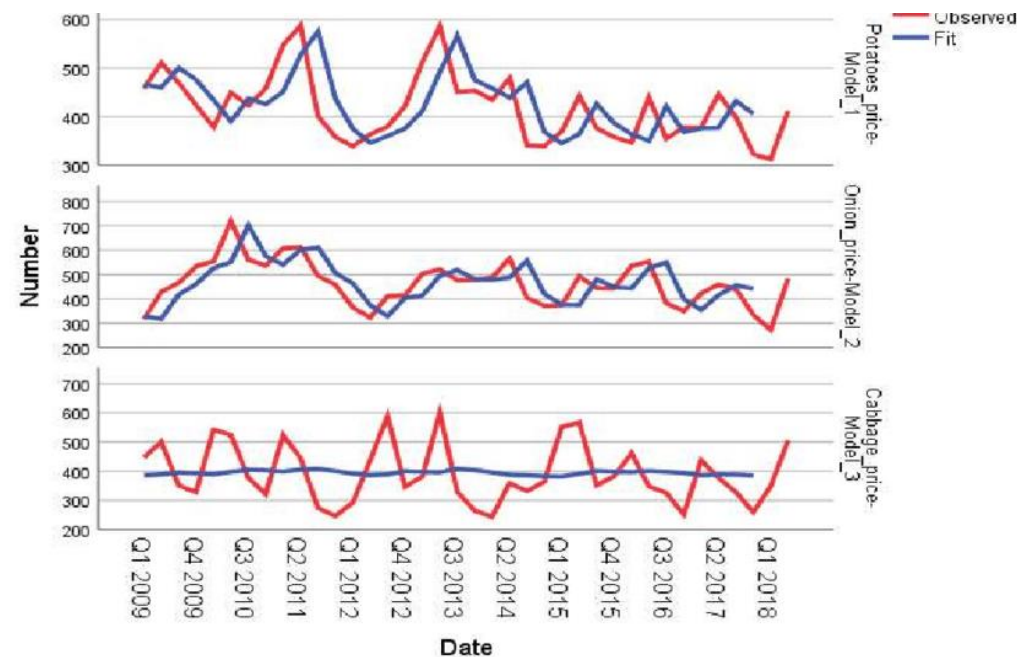
- Also known as rolling means.
- A naïve way to evaluate the intricacies of the data.
- The next observation is the mean of a given window or all past observations.
- A window applies the moving average model to smooth the time series and highlight different trends.





Exponential Smoothing Methods

- Use this method for data sets that are more irregular where there is no seasonality or trends.
- Calculated as a weighted average from the previous level and the current observation.

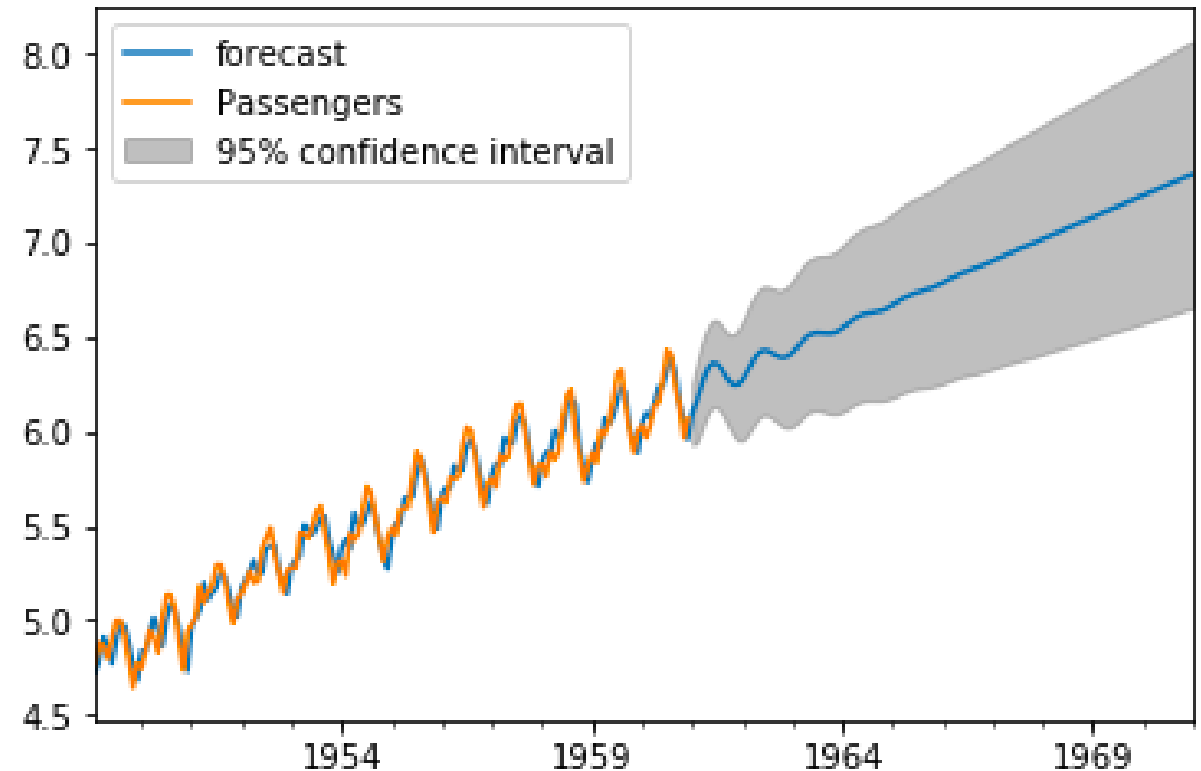




ARIMA Model

ARIMA models in time series forecasting predict future values based on historical data and patterns.

- AR: Autoregression
 - Linear relationship with previous data
 - lag observations – parameter p
- I: Integrated
 - making the time series stationary
 - differencing order – parameter d
- MA: Moving Average
 - uses the moving average for previous data
 - residual error window size – parameter q



The SARIMA model also accounts for seasonality patterns



Something to Remember about Time Series





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Natural Language Processing (NLP)

Why is it hard?



I'm a huge metal fan!

NLP is hard.



Natural Language Processing

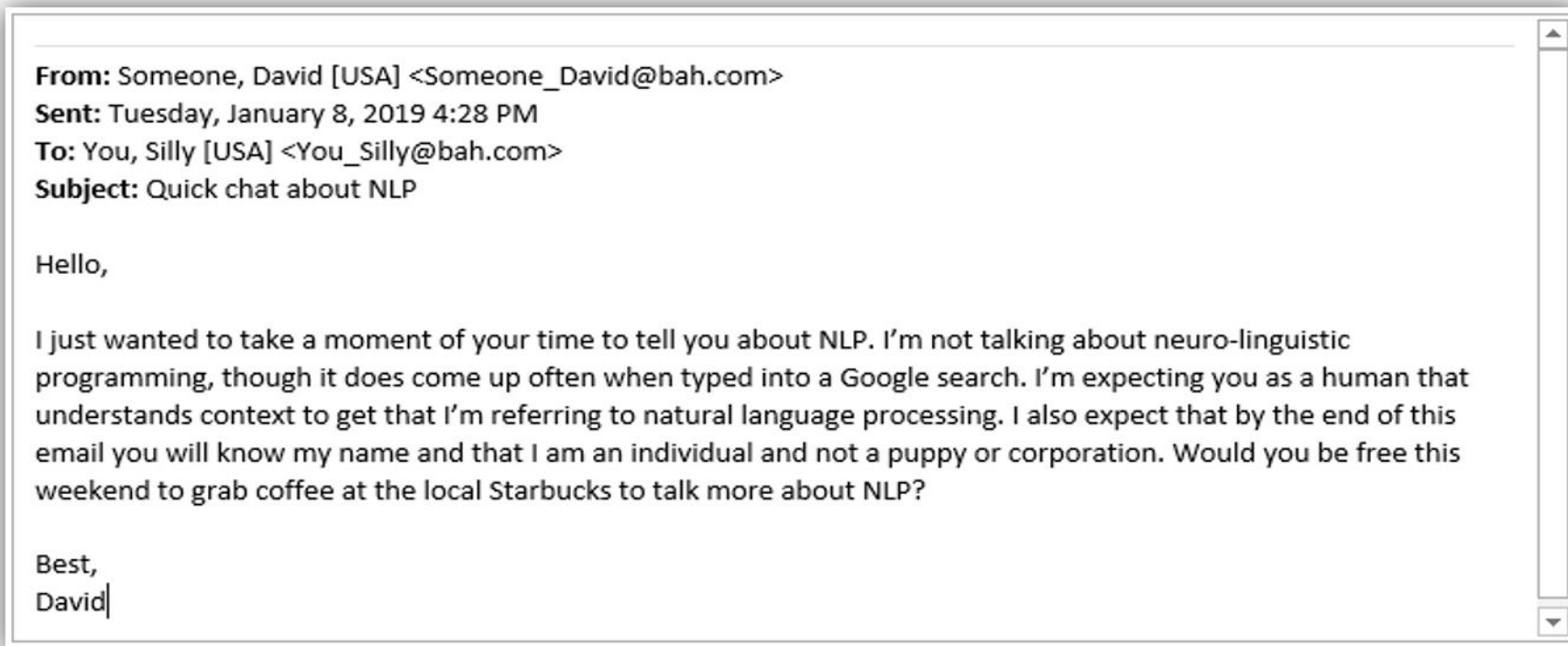
- How can we draw insights from our data when it has a lot of text?
- The focus of NLP is to program computers to process and analyze large amounts of natural language data.
- Many real-world use cases:
 - Machine translation
 - Chatbots
 - Resume filtering





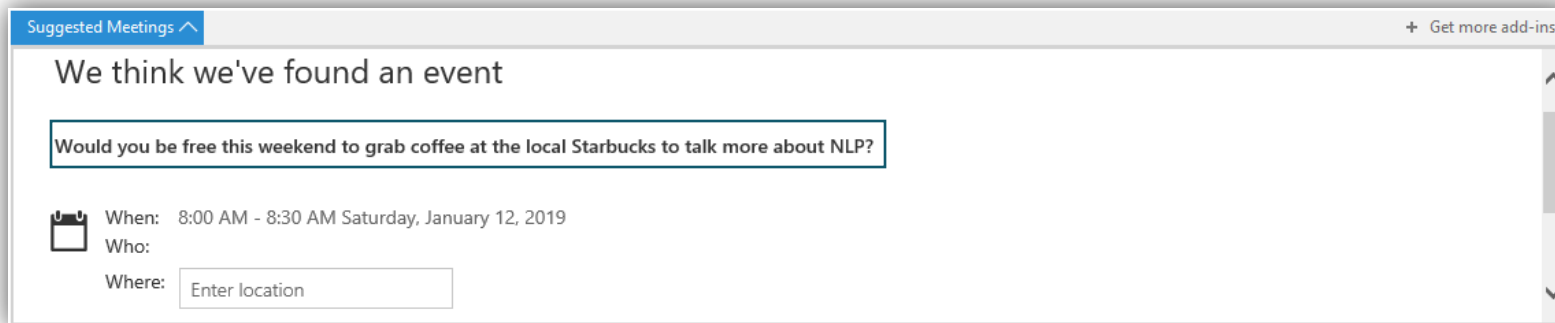
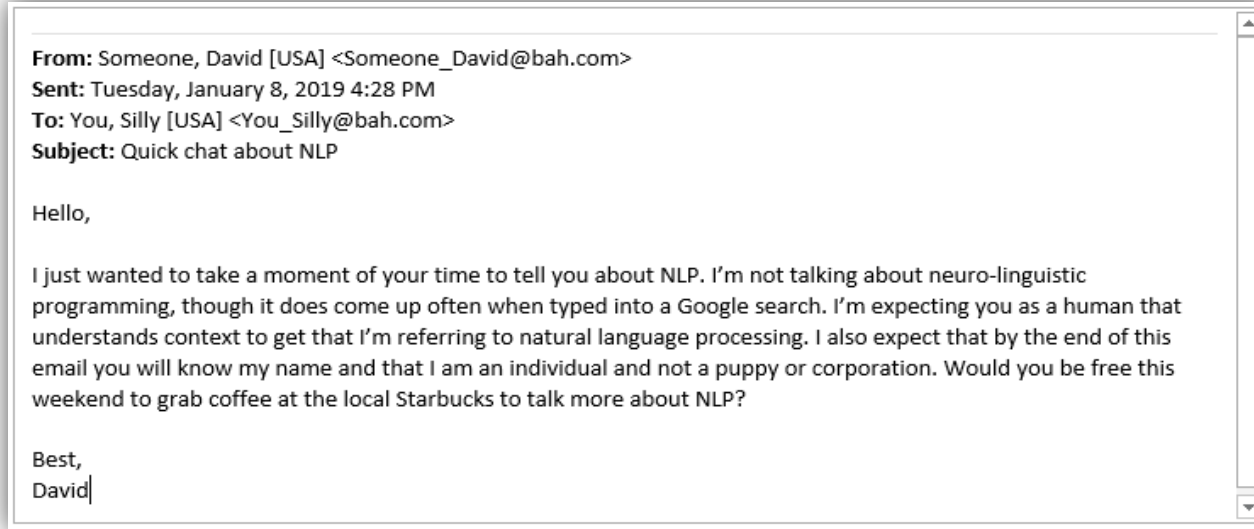
NLP in Outlook

What do you look for when you read an e-mail?





NLP in Outlook



NLP – Count Vectorizer

How do we convert human language to something a computer can understand?

Corpus

Document 1: "Today was
a great, great day."
Document 2: "I like
puppies."

All unique "tokens"

"Today", "was", "a", "great", "day",
"I", "like", "puppies"

count vectorizer

DOC ID	day	great	a	puppies	I	like	was	Today
1	1	2	1	0	0	0	1	1
2	0	0	0	1	1	1	0	0

Word Embeddings / Word Vectors

DOC ID	day	great	a	puppies	I	like	was	Today
1	0	2	1	0	0	0	1	1
2	0	0	0	1	1	1	0	0



[0, 2, 1, 0, 0, 0, 1, 1]

[0, 0, 0, 1, 1, 1, 0, 0]

word vectors

a.k.a.

"word embeddings"

Now, our text is in a representation that our machine learning models can understand.



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Limitations of Count Vectorizers

What is less than ideal with our count vectorizer?



Limitations of Count Vectorizers

What is less than ideal with our count vectorizer?

Count vectorizers treat all occurrences of words equally, so common words (e.g., "the", "a", "of"...) dominate the signal of a vector.



Tf-idf Word Vectorizer

tf-idf = term frequency X inverse document frequency

$$\mathbf{tfidf}_{i,j} = \mathbf{tf}_{i,j} \times \log \left(\frac{\mathbf{N}}{\mathbf{df}_i} \right)$$

$\mathbf{tf}_{i,j}$ = total number of occurrences of i in j

\mathbf{df}_i = total number of documents (speeches) containing i

\mathbf{N} = total number of documents (speeches)

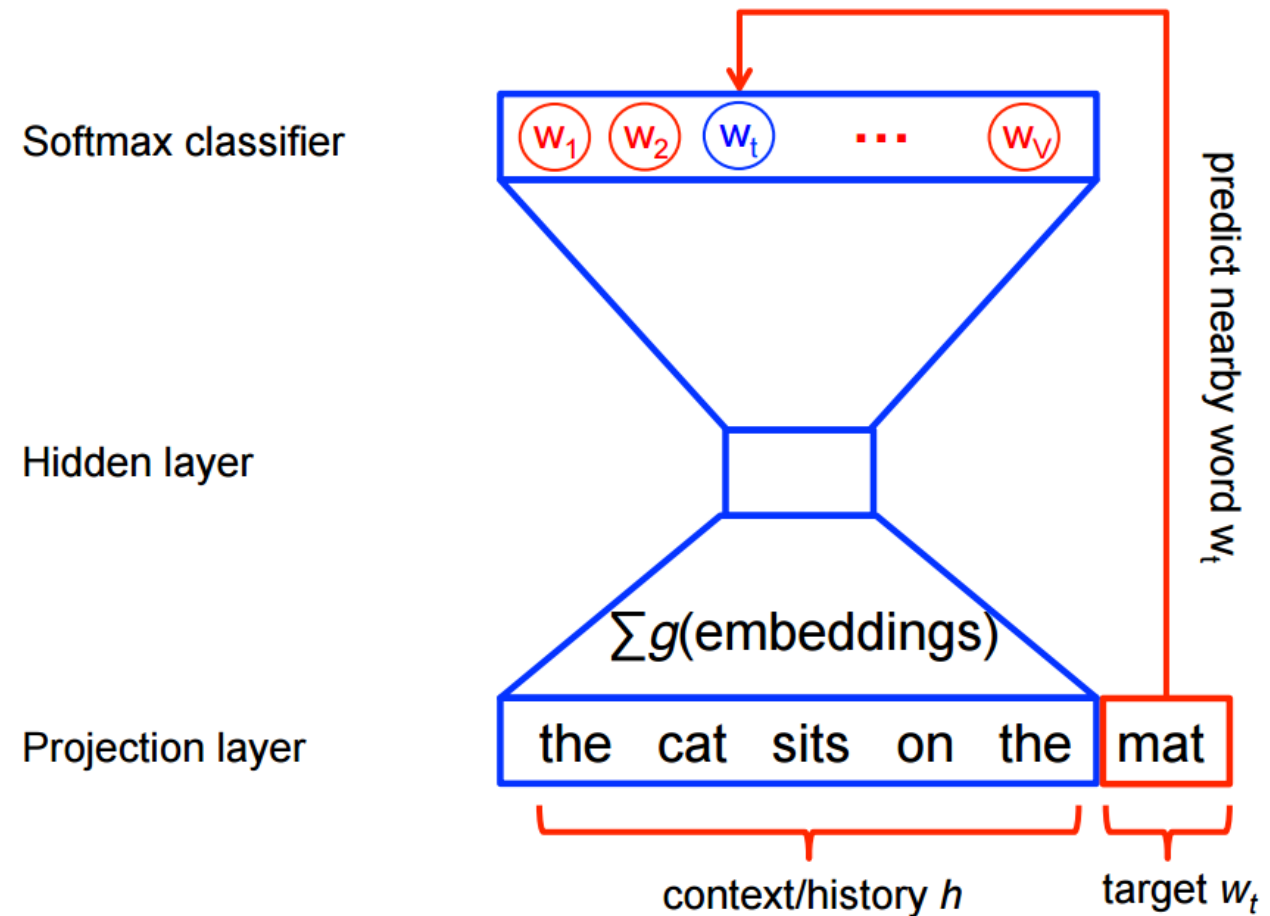
Word2Vec – A More Sophisticated Vector

What's different here?

Instead of creating a vector for each of our documents, we can create a vector for every word in our vocabulary.

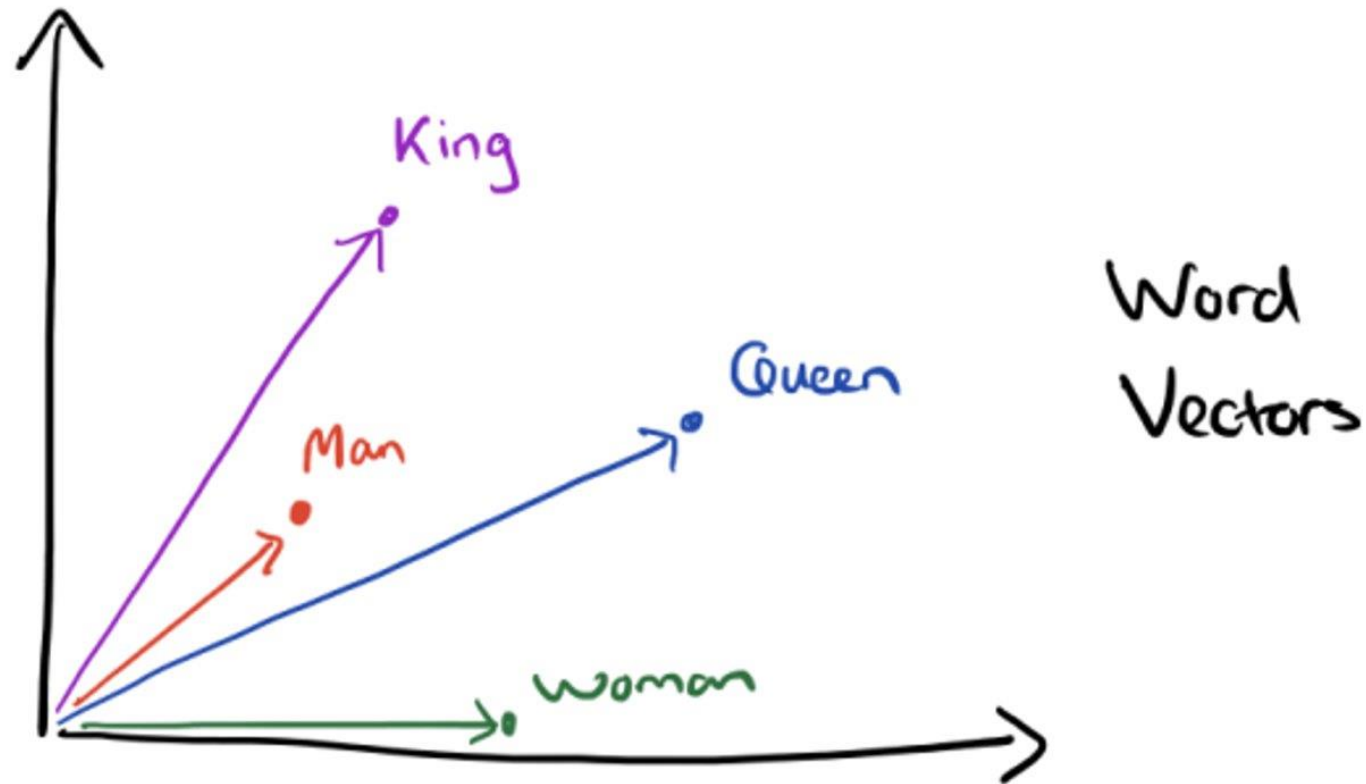
How does it work?

Uses a neural network to predict what word comes next in a sequence, then adjusts the vector for the target word if it was wrong.

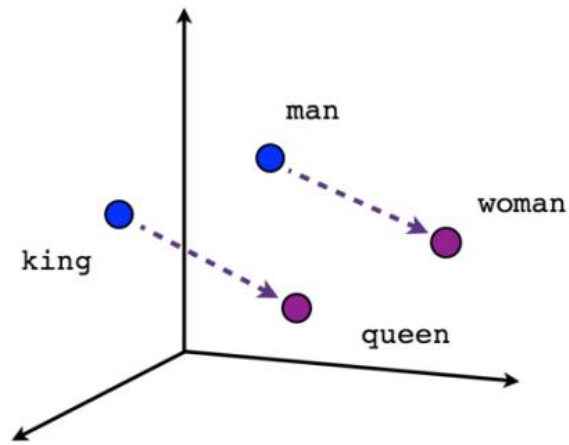


Word2Vec

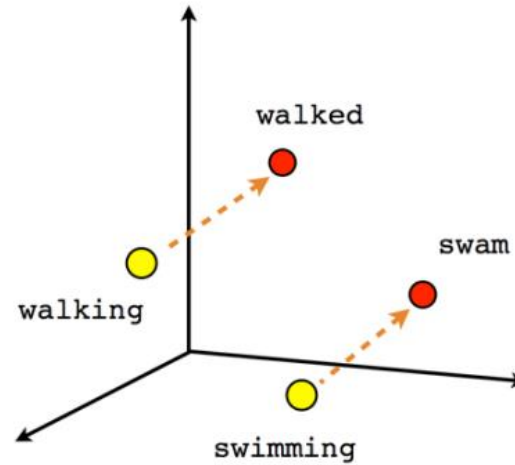
- The result of this strategy of vectorizing words means that individual words that are used in similar contexts are spatially close together.



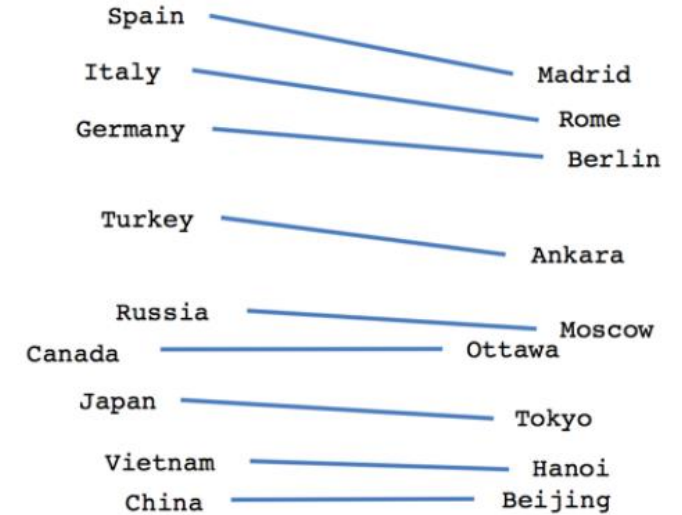
Word2Vec - Examples



Male-Female



Verb tense



Country-Capital



Common Tasks in NLP

Name	Description
Tokenization	Segmenting text into words, punctuation marks, etc.
Part-of-speech (POS) Tagging	Assigning word types to tokens, like verb or noun.
Dependency Parsing	Assigning syntactic dependency labels, describing the relations between individual tokens, such as subject or object.
Lemmatization	Assigning the base forms of words. For example, the lemma of “was” is “be”, and the lemma of “rats” is “rat”.
Sentence Boundary Detection (SBD)	Finding and segmenting individual sentences.
Named Entity Recognition (NER)	Labelling named “real-world” objects, such as persons, companies, or locations.
Entity Linking (EL)	Disambiguating textual entities to unique identifiers in a Knowledge Base.
Similarity	Comparing words, text spans, and documents to determine how similar they are to each other.
Text Classification	Assigning categories or labels to a whole document or parts of a document.
Sentiment Analysis	Allows us to capture meaning or intent in document



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Course Summary



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End of Course Survey



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What Did We Just Learn?

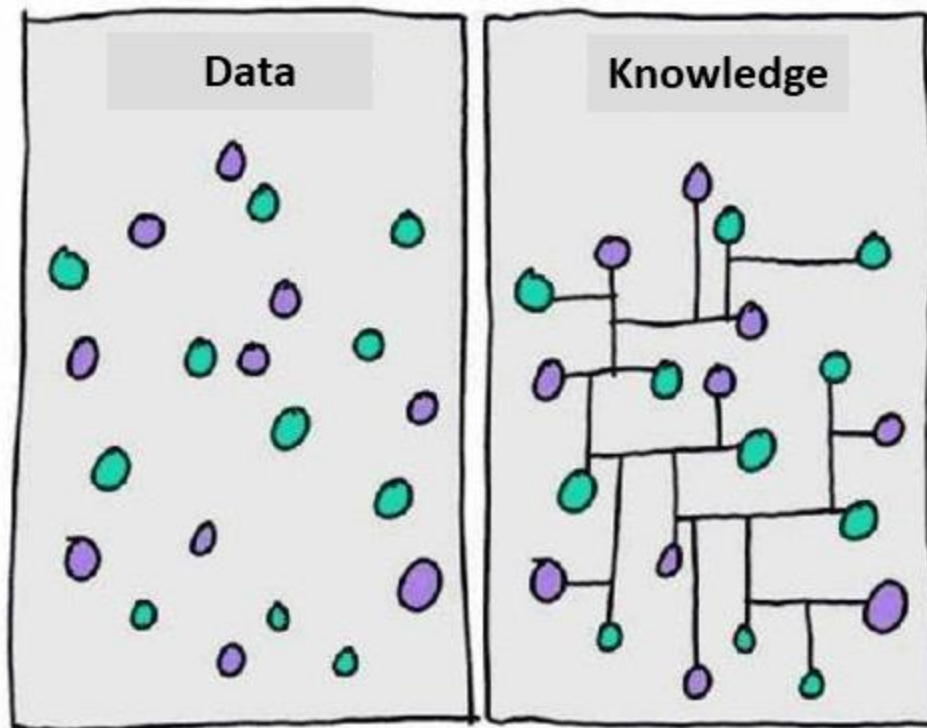




In a Nutshell

Data

Data Science

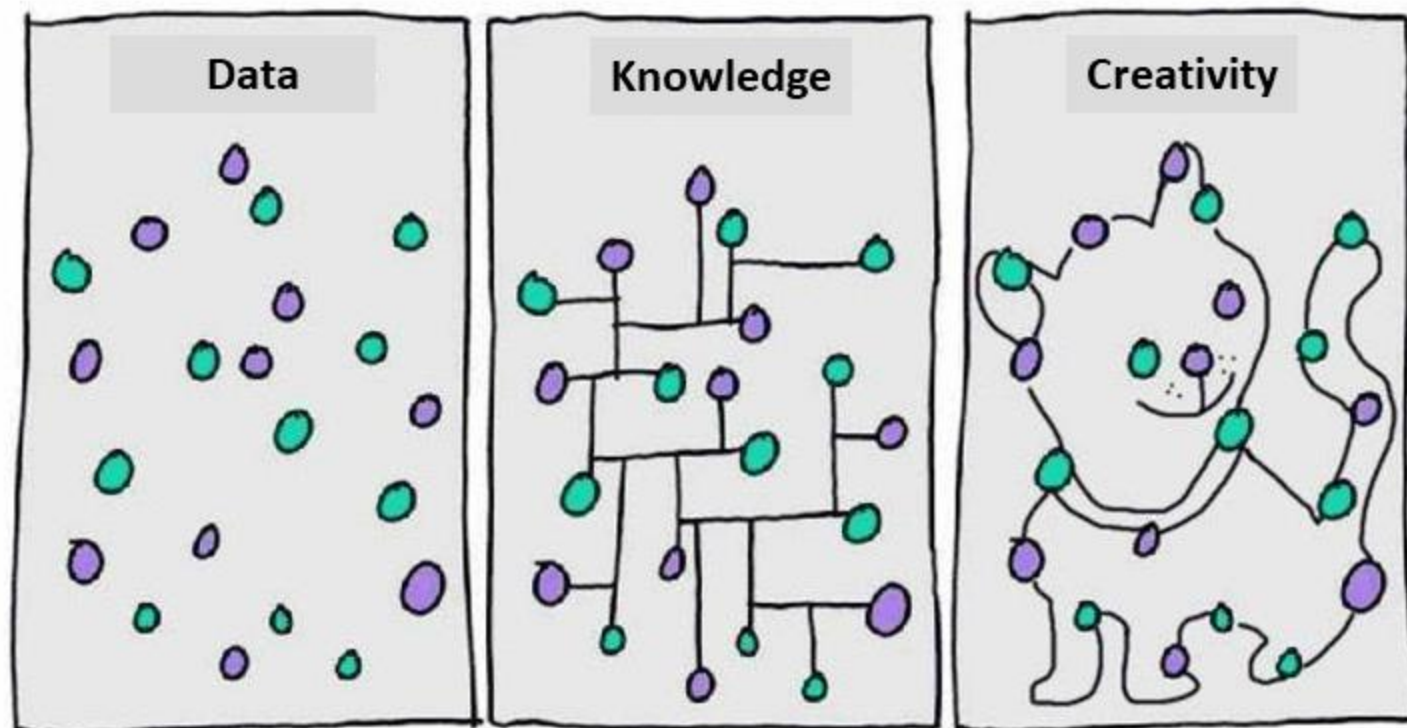


Knowledge is about connecting the dots.
@KirkDBorne



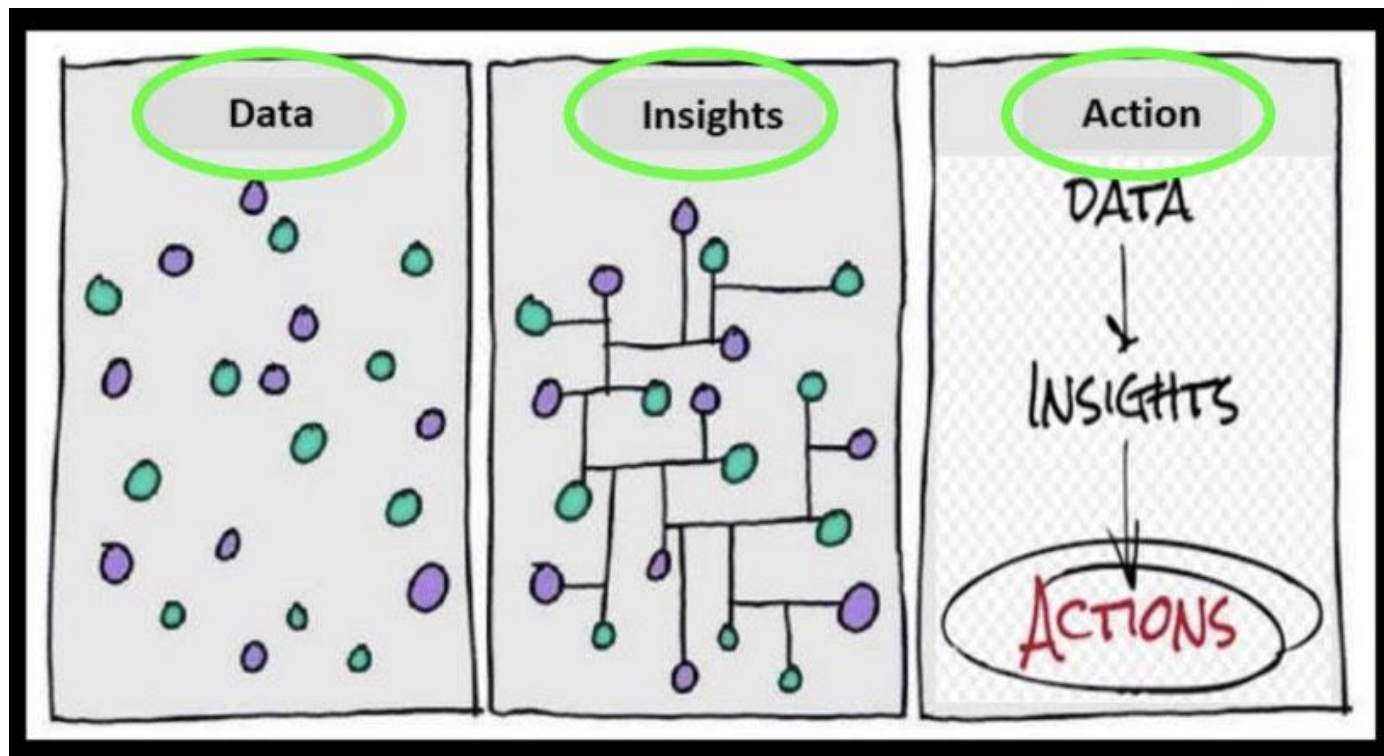
In a Nutshell

Find the pattern in the data



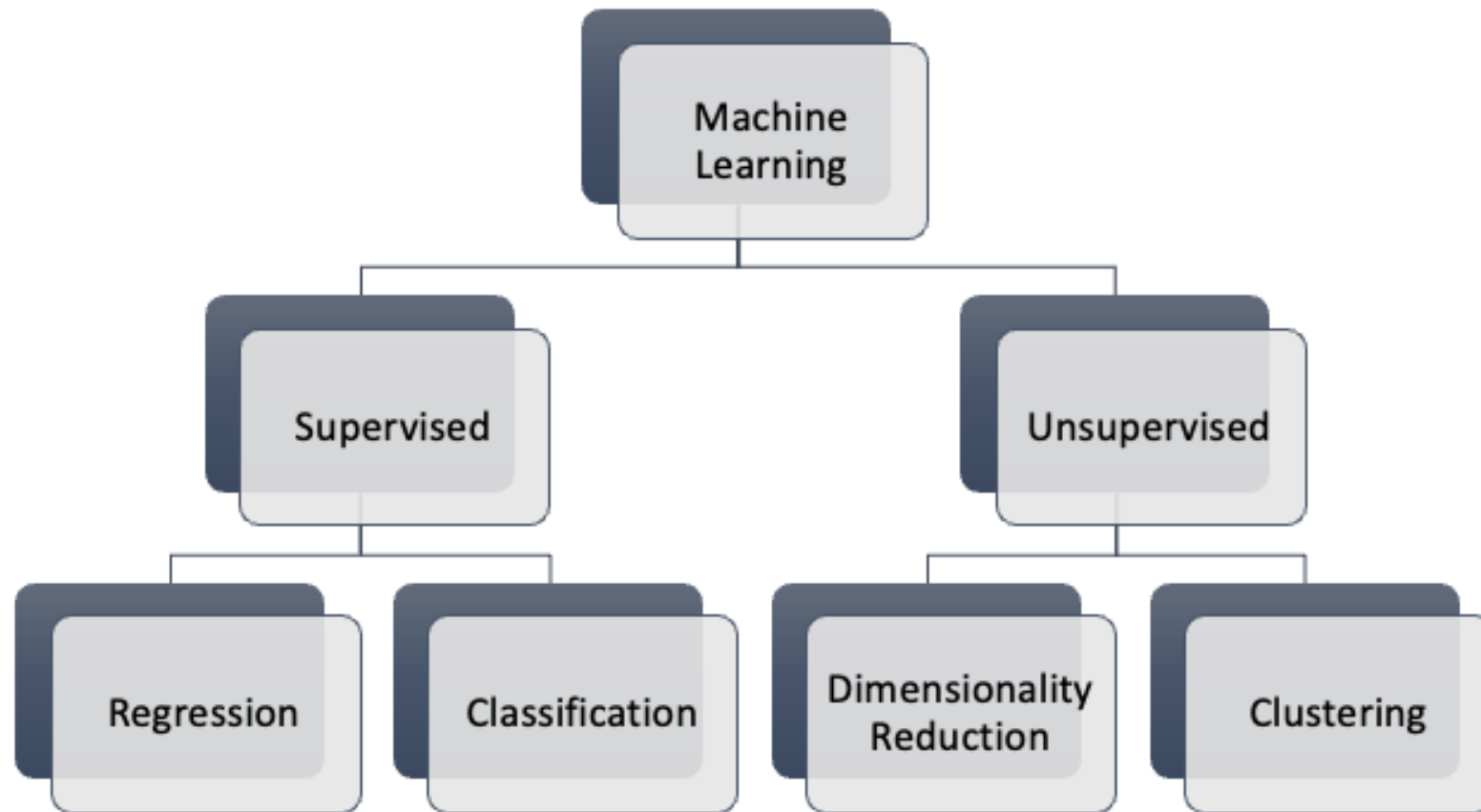


From Data to Insights to Actions





Types of Learning





Summary of ML Techniques

Algorithm	Computationally expensive?	Requires lots of data?	Interpretable?
Linear Regression	No	No	Yes
Logistic Regression	No	No	Yes
PCA	Yes	Yes	No
K-means	No	No	Yes
Neural Networks	Yes	Yes	No



Lessons Learned

- Navigate through a data science project using the seven-step data science process
 - Form a SMART problem statement, understanding what data science can and cannot do
 - Acquire useful data that can assist in solving the problem statement
 - Explore data and analyze preliminary findings to leverage initial insights from the data
 - Prepare data for use in machine learning pipelines
 - Develop models to represent relationships within the data
 - Render compelling visualizations to communicate data-driven narratives to your colleagues
 - Applying actionable insight to your problem statement
- Identify data opportunities within the organization to apply higher-level analytics, data science, and machine learning
 - Understand different machine learning algorithms and how to apply them
 - Recognize data science specialties, such as natural language processing and computer vision
- Identify tools that can assist in all parts of the data science process



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Questions?





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Dr. Gordon Aiello - Aiello_Gordon@bah.com

March 27 - AI Fundamentals Part 1

April 24 - AI Fundamentals Part 2



Thank You!