Introduction to machine learning and `scikit-learn`

Part I: Supervised learning

QLSC 612 | 29 May 2025

By

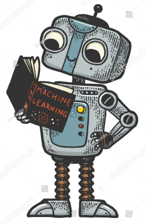
Michelle Wang & Mohammad Torabi

(reusing some of Nikhil Bhagwat's slides)

McGill UNIVERSITY

ORIGAMI Lab

neuro Montreal Neurological Institute-Hospital



Objectives

-

What is machine learning?

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Quick Internet search*: It is a branch of artificial intelligence (AI) and computer science that focuses on the using data and algorithms to enable AI to imitate the way that humans learn.*

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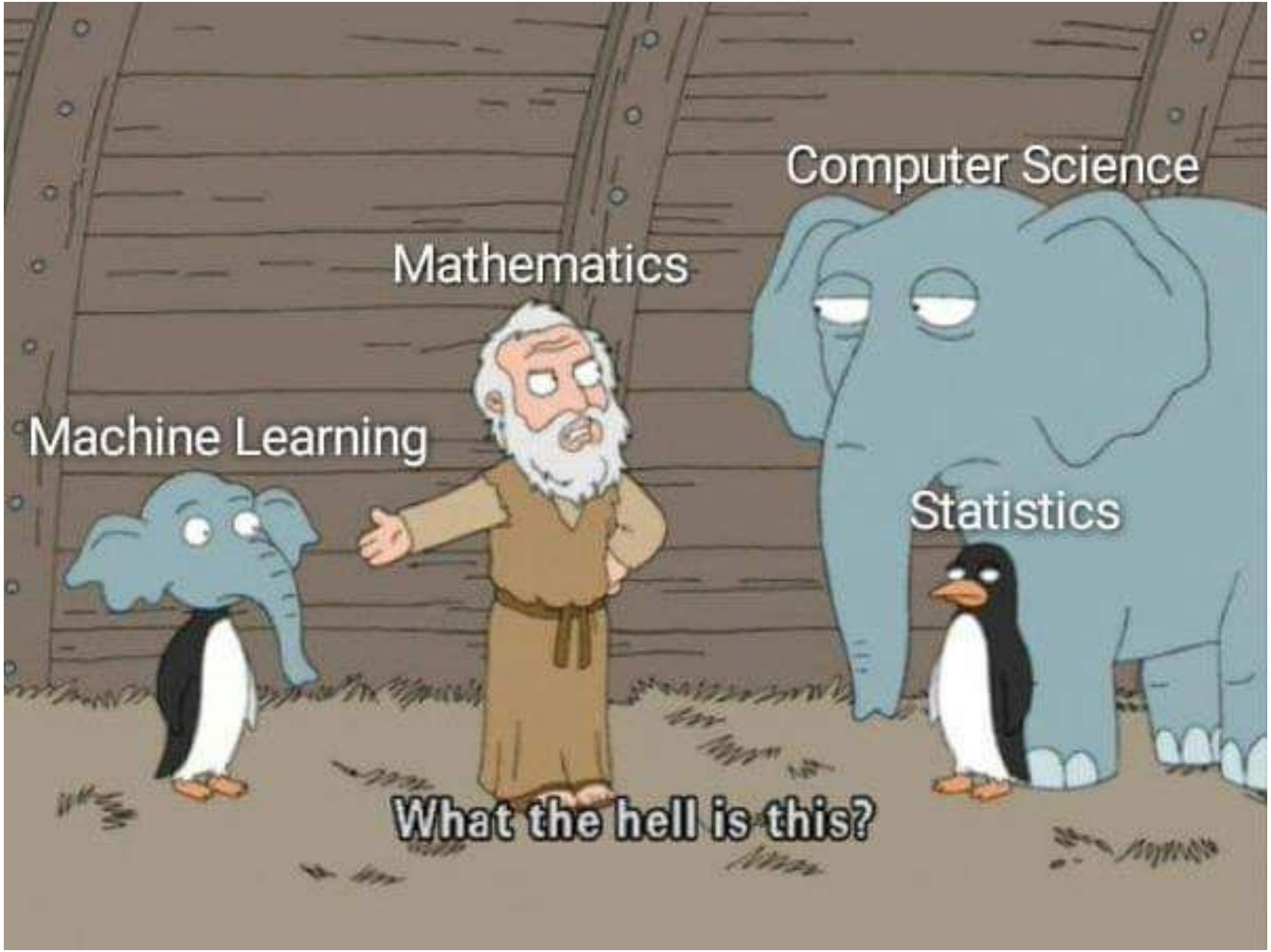
Philosophy professor: *You do not control what you make but you control the process of its creation.*

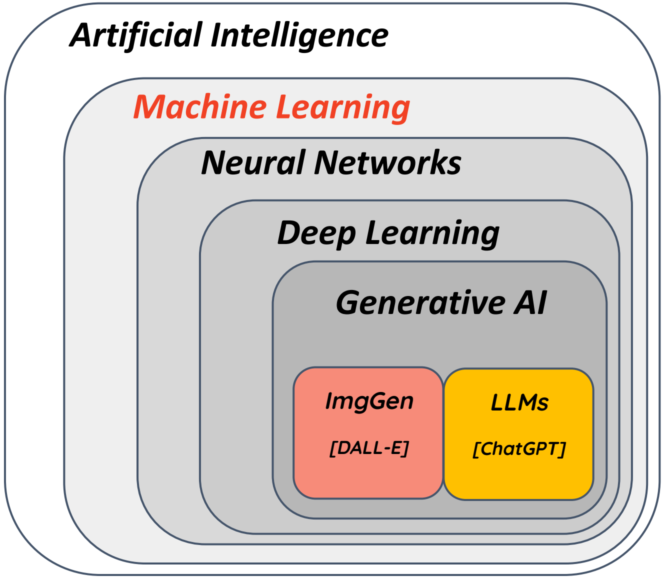
ChatGPT: It is is a type of AI that allows software applications to become more accurate at predicting outcomes without being explicitly programmed. It is based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention.

In practice…


Computer Science
Mathematics
Machine Learning
Statistics
What the hell is this?

Machine-learning - what, why, and when?

- What is Machine learning (ML)?
    - ML is the study of computer algorithms that improve automatically through “experience” and by the use of data.



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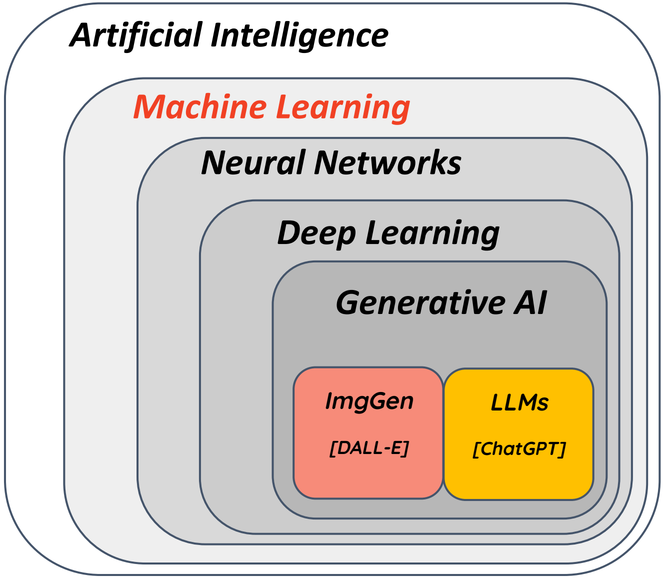
- Why is it useful - especially in life sciences?
  - Biology, medicine, environmental sciences comprise phenomenons (e.g. a disease) with large number of variables.
  - We want to model complex relationships within these variables and **make accurate predictions**.



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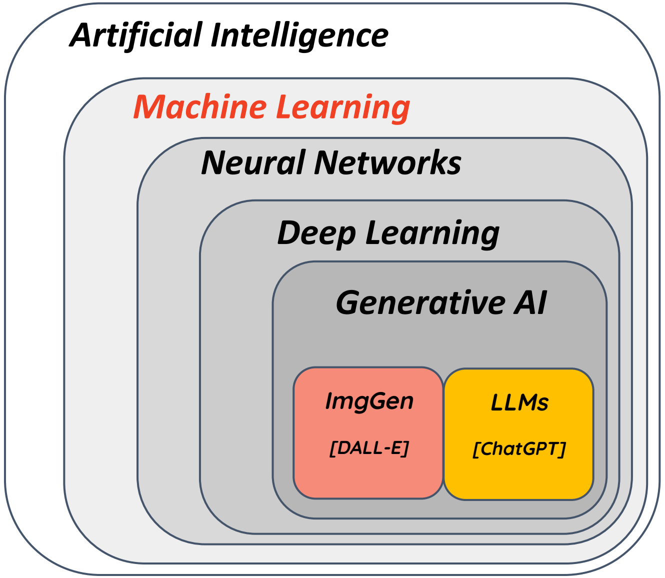
- When do I use it?
    - You are interested in 1) prediction tasks or 2) low-dimensional representation.
    - **You have sufficient data.**



Types of ML Algorithms

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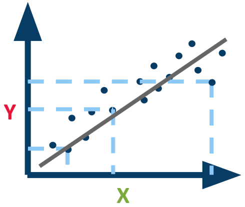
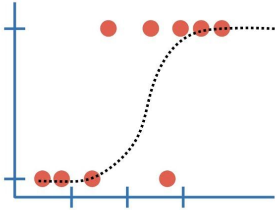
Outcome	Supervised Learning	
Continuous	Regression 	
Categorical	Classification 	

Types of ML Algorithms

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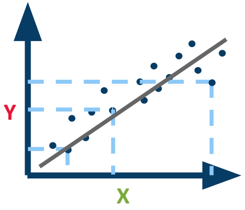
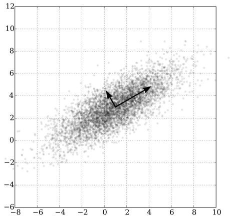
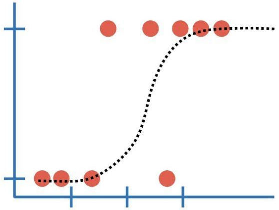
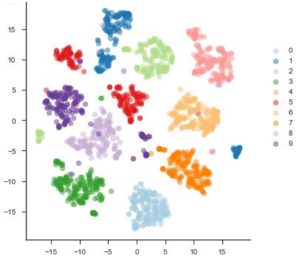
Continuous	Regression 	Principal Component 
Categorical	Classification 	Clustering 

** … and Reinforcement Learning*

Types of ML Algorithms

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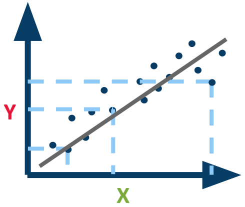
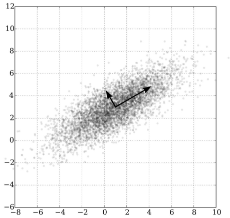
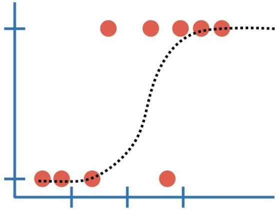
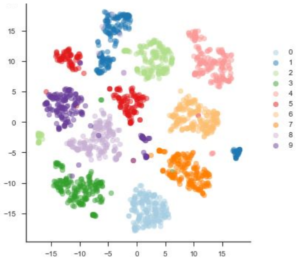
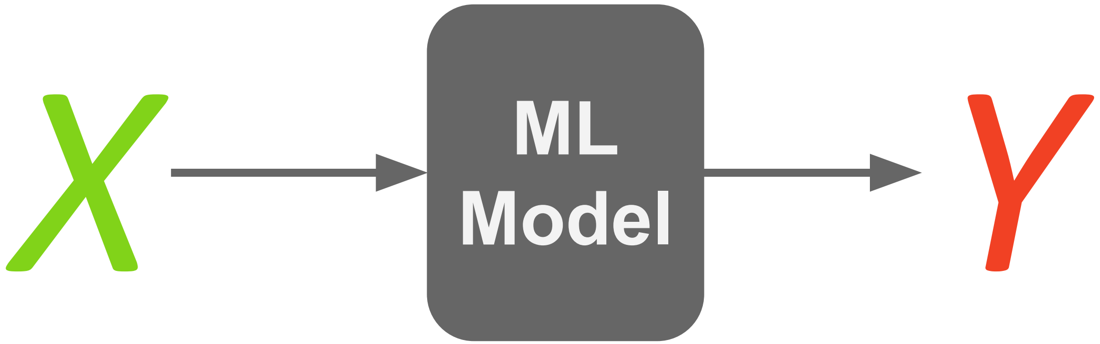
Continuous	Regression 	Principal Component 
Categorical	Classification 	Clustering 

Training a machine-learning model



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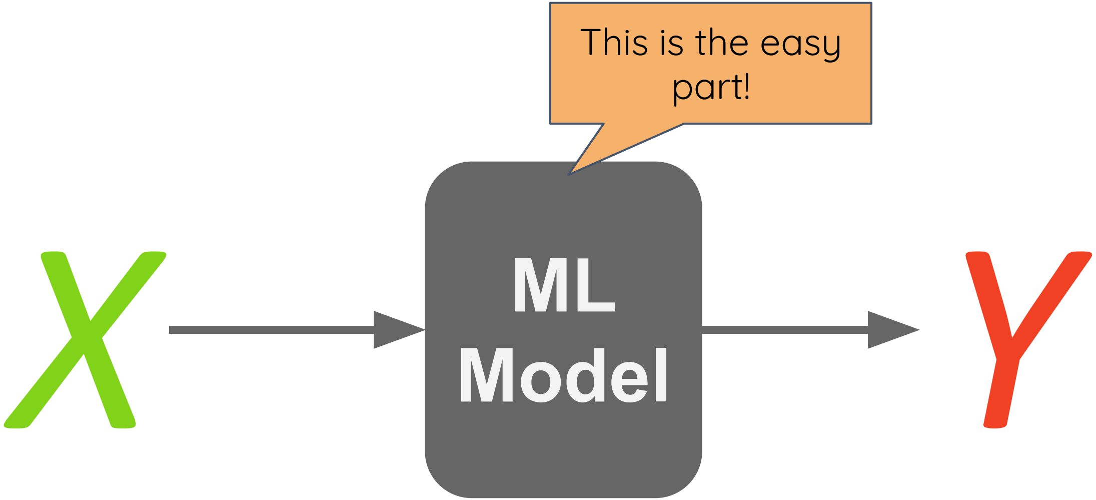
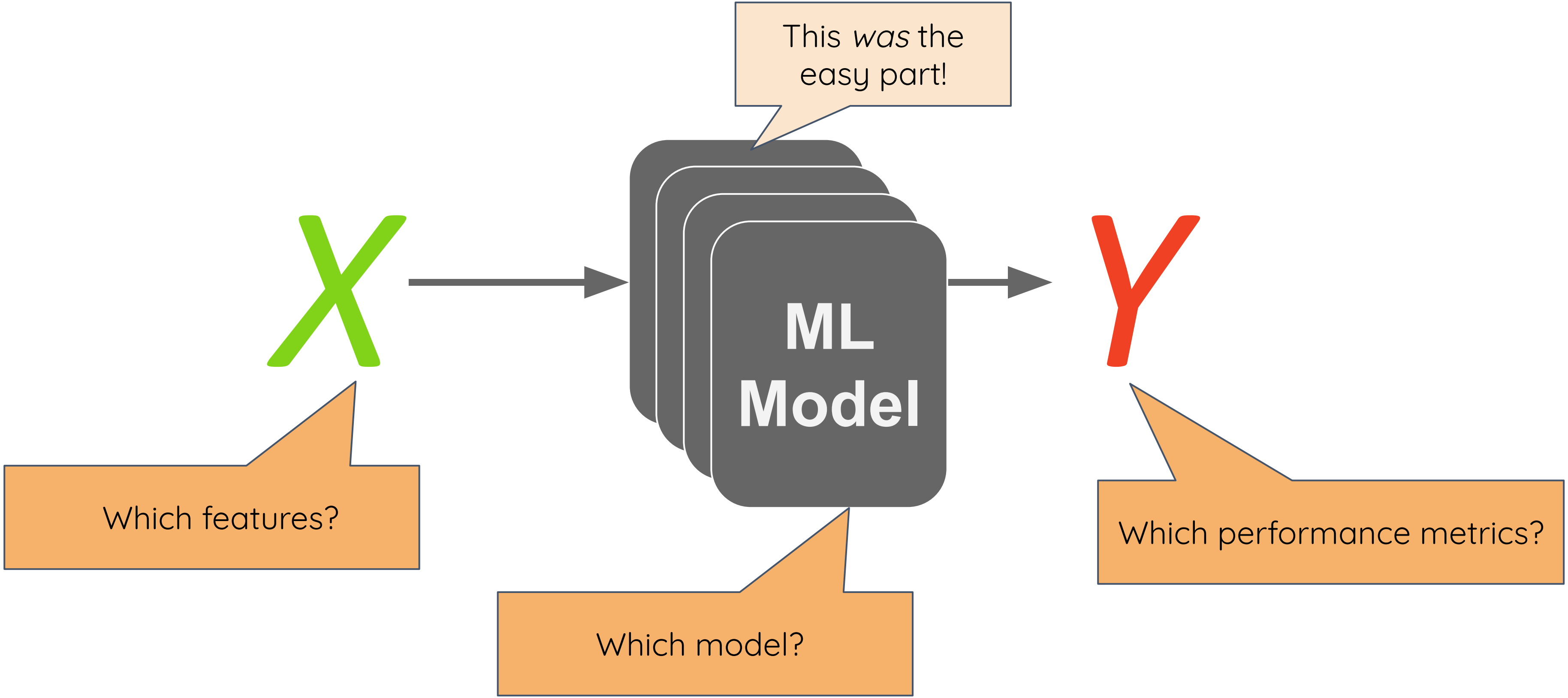
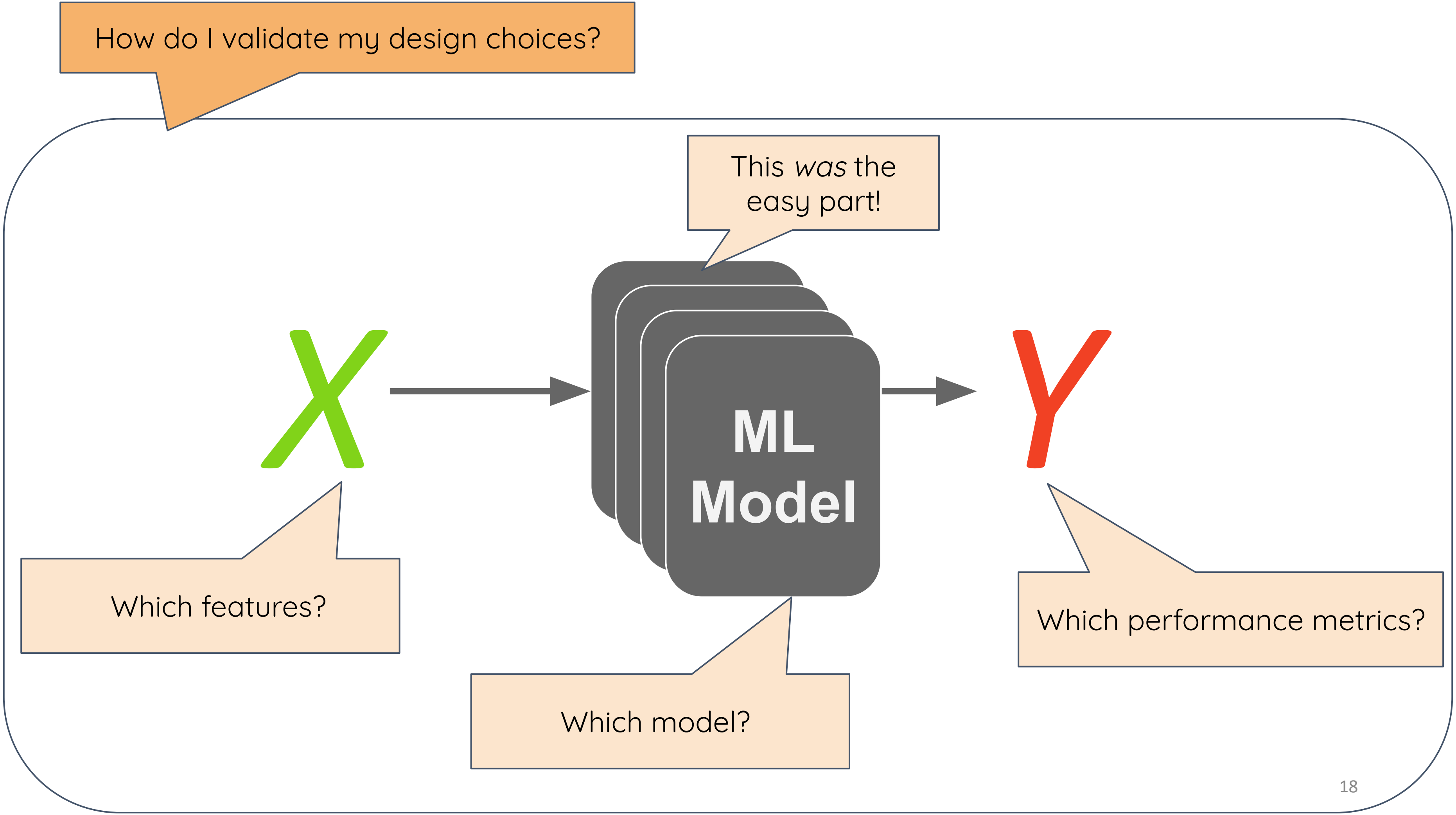



This *was* the easy part!
X
ML Model
Y
Which features?
Which model?
Which performance metrics?


How do I validate my design choices?
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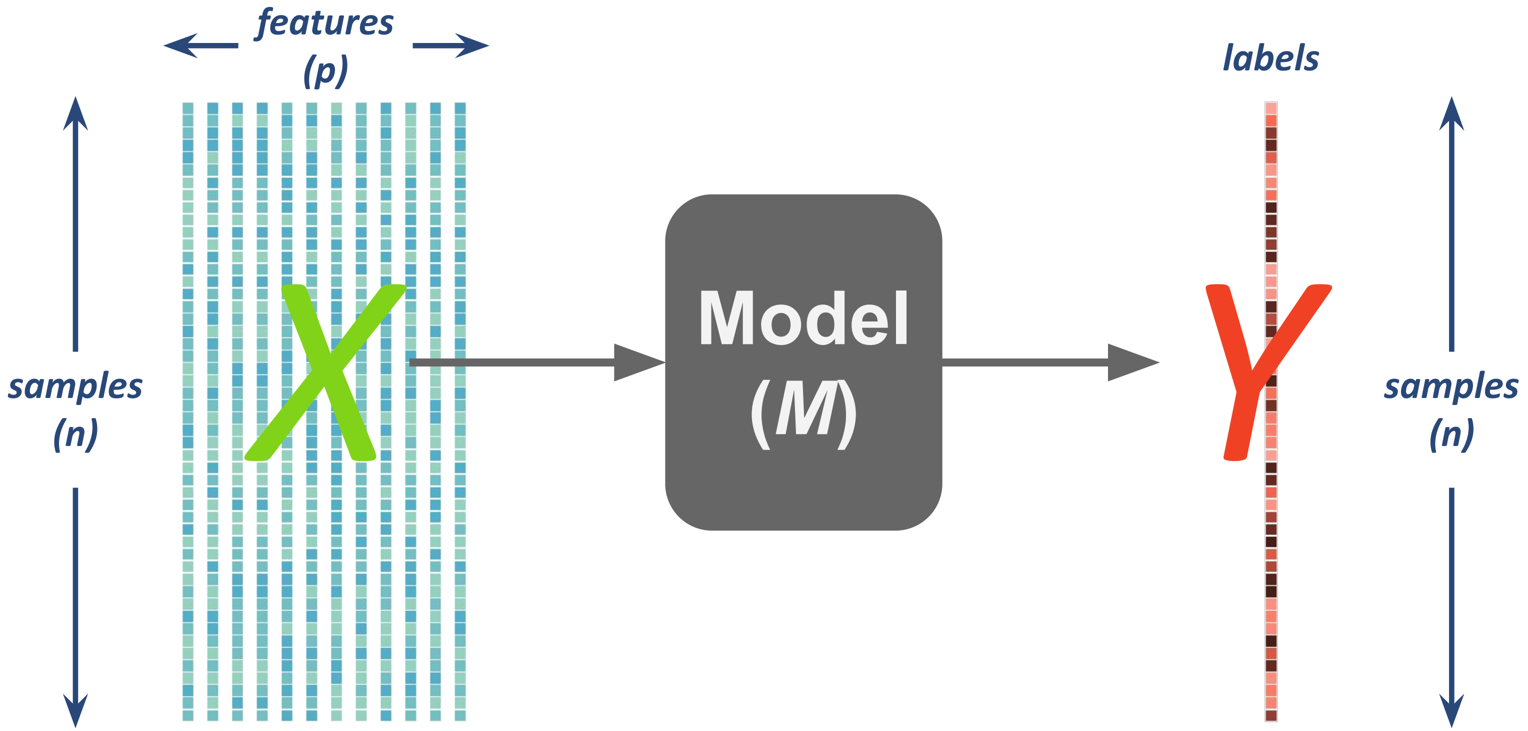
Terminology



Input Examples:

Output Examples: Clinical measures

Supervised Learning: Models

- Goal: *Learn* parameters (or weights) of a model (M) that maps X to y

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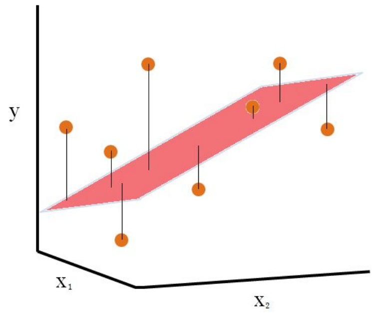
- Example models:
  - Linear / Logistic regression



Linear Regression

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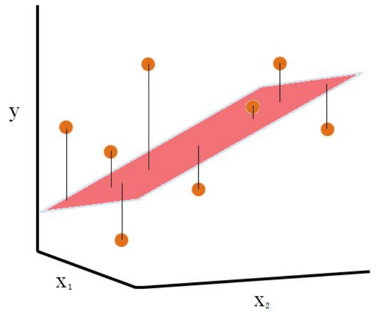
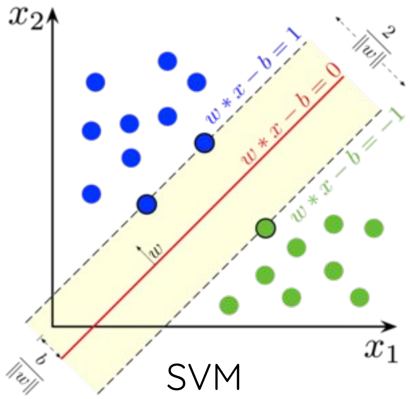


Linear Regression



SVM

Supervised Learning: Models

- Goal: *Learn* parameters (or weights) of a model (M) that maps X to y
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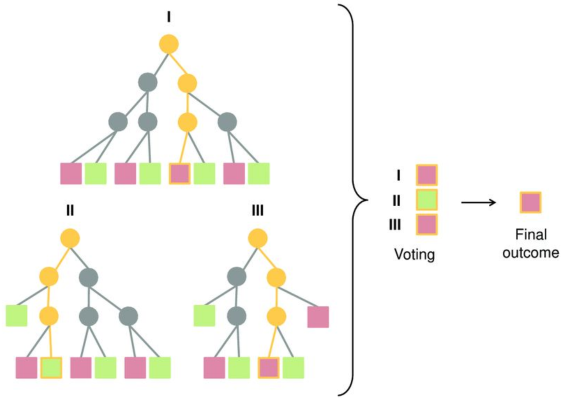
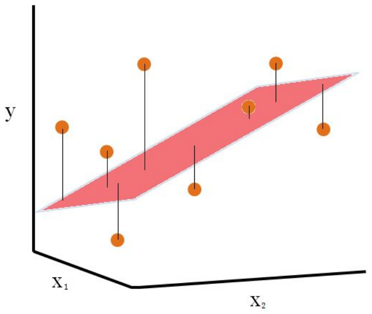
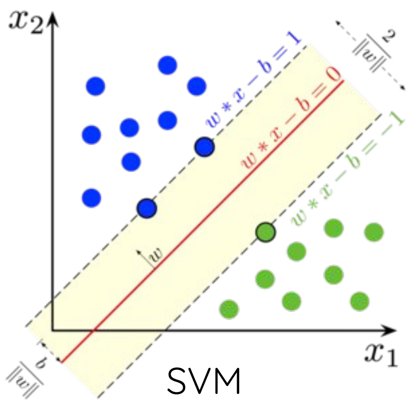
  - Tree-ensembles: random forests, gradient boosting



Tree-ensembles



Linear Regression



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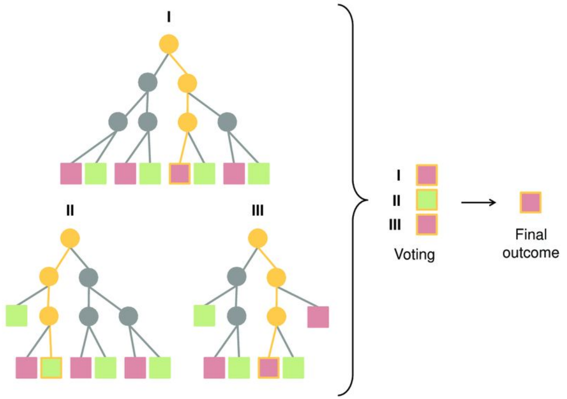
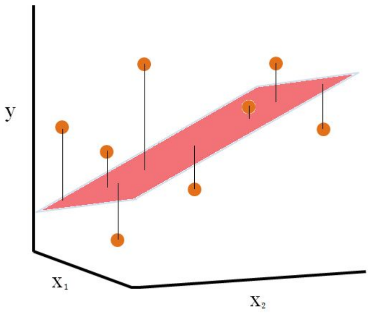
    - Tree-ensembles: random forests, gradient boosting
    - Artificial Neural networks



Tree-ensembles



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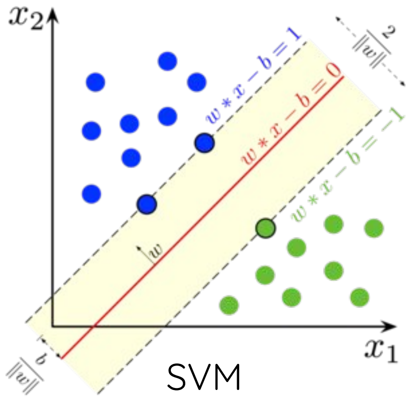

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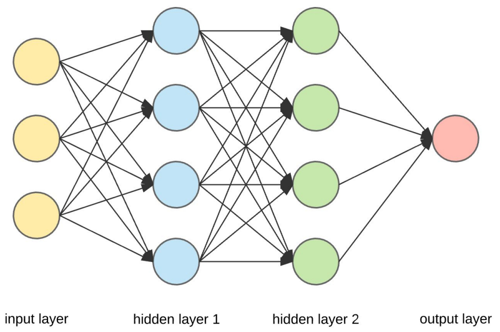


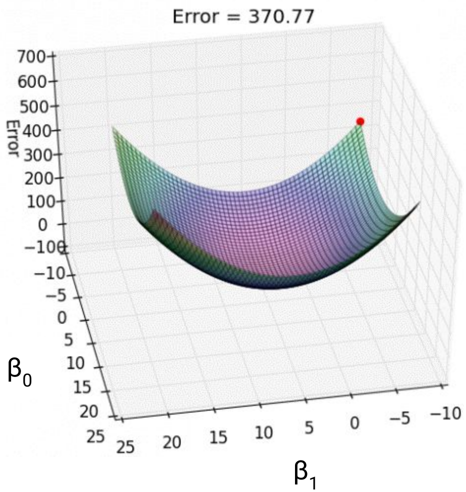
ANN

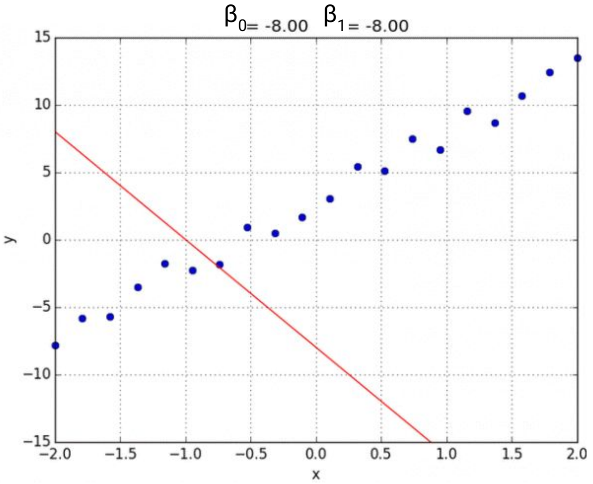
Model Fitting

- Gradient descent with a **single** input variable and **n** samples
  - Start with random weights (β_0 and β_1)
  - Compute loss (i.e. MSE)
  - Update weights based on the gradient

$$\hat{y}_i = \beta_0 + \beta_1 x_i$$

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





Model Fitting

- Gradient descent for complex models with non-convex loss functions
  - Start with random weights (β_0 and β_1)
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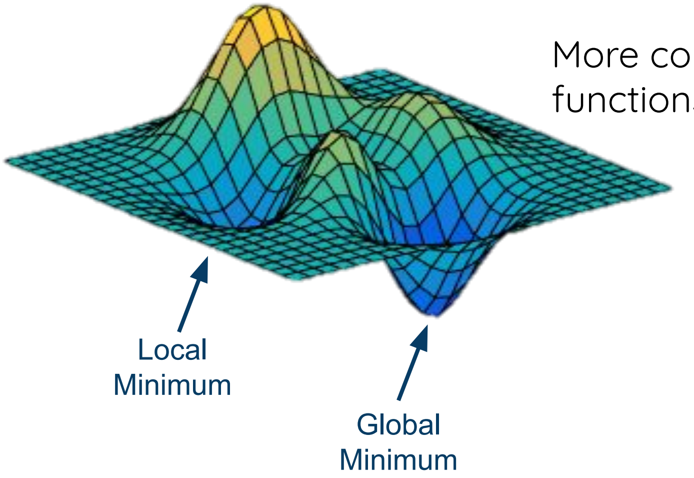

More complex models / loss functions (e.g. ANNs)

Model Fitting

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    - e.g. I believe a disease symptom can be predicted with few genes.
  - Practical reasons
    - Prevent overfitting (n_features >> n_samples)

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_{p-1} x_{p-1} + \beta_p x_p$$

Model Fitting

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- **Yes! → Model regularization**

Model Fitting: Regularization

- How do we do it?
  - Modify the loss function
  - Constrain the learning process

- Examples:
  - L1 i.e. Lasso
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1) L1/Lasso: constrains parameters to be ***sparse***

$$MSE = \sum_{i=1}^{n} (y_i - \underbrace{[\, \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j \,]}_{\hat{y}_i})^2 + \underbrace{\lambda \sum_{j=1}^{p} |\beta_j|}_{L_1}$$

2) L2/Ridge: constrains parameters to be ***small***

$$MSE = \sum_{i=1}^{n} (y_i - \underbrace{[\, \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j \,]}_{\hat{y}_i})^2 + \underbrace{\lambda \sum_{j=1}^{p} \beta_j^2}_{L_2}$$

Model Fitting: Scikit-learn syntax

```
# import
from sklearn import linear_model, svm

# data
X = [[0, 0], [1, 1]]
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# predict on new data
y_pred = model.predict([[1, 0]])
```
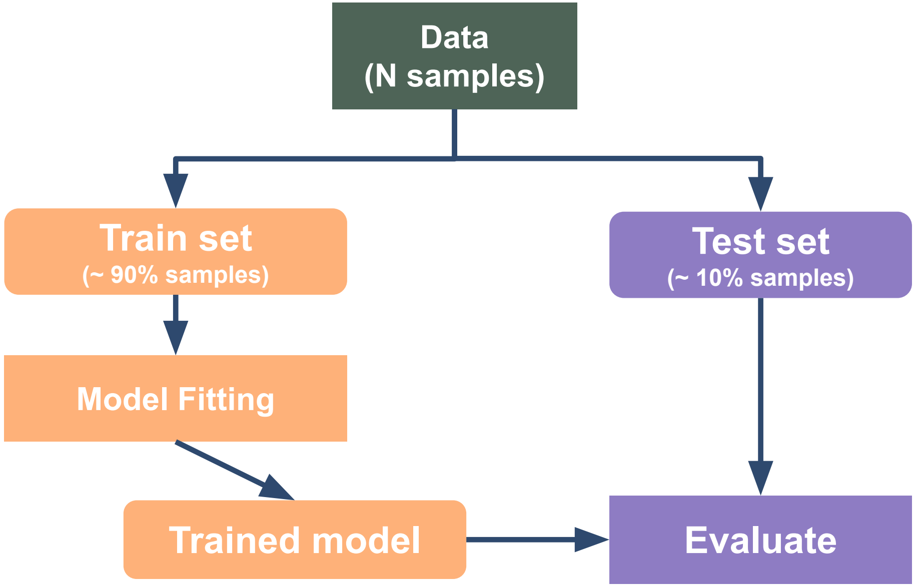

Model Evaluation

- Is the model generalizable?
- How do we sample train and test sets?
- How do we select a model?



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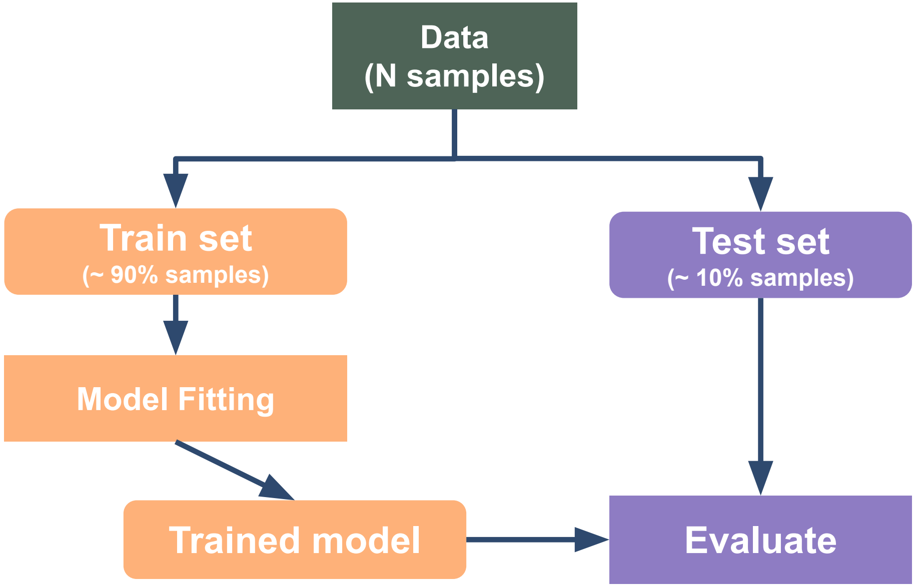
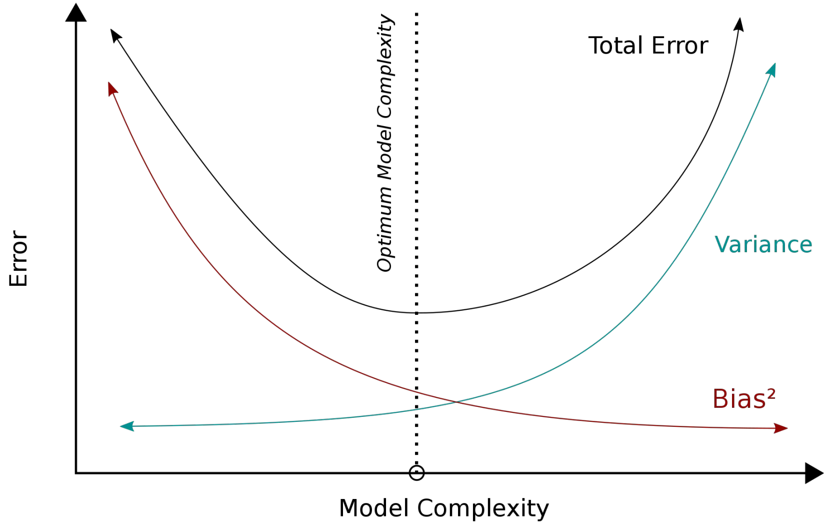
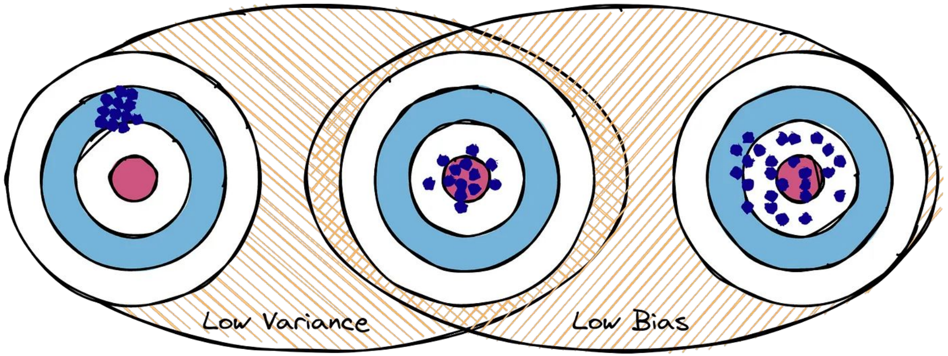


Model Evaluation

- Train performance ≠ Test performance
  - Model: Underfitting vs Overfitting
  - Errors: Bias - Variance tradeoff





Model Evaluation

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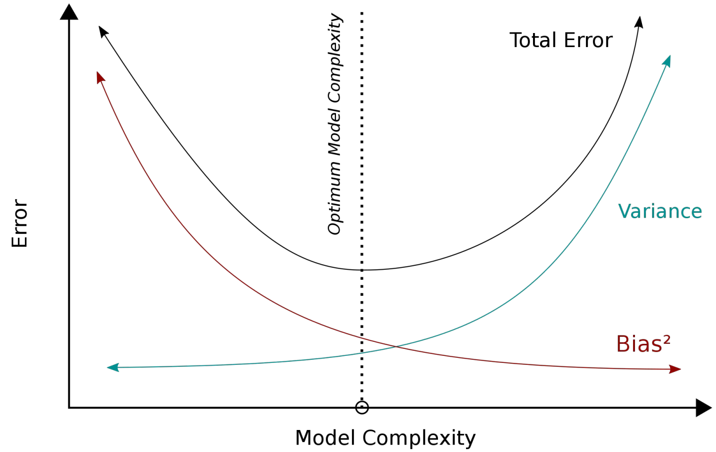

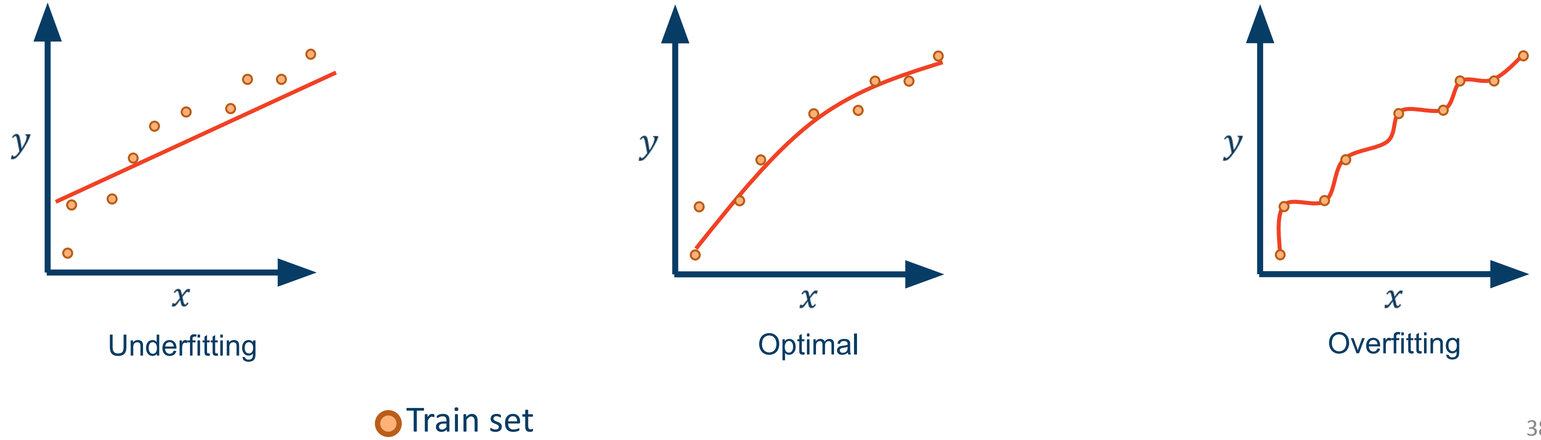

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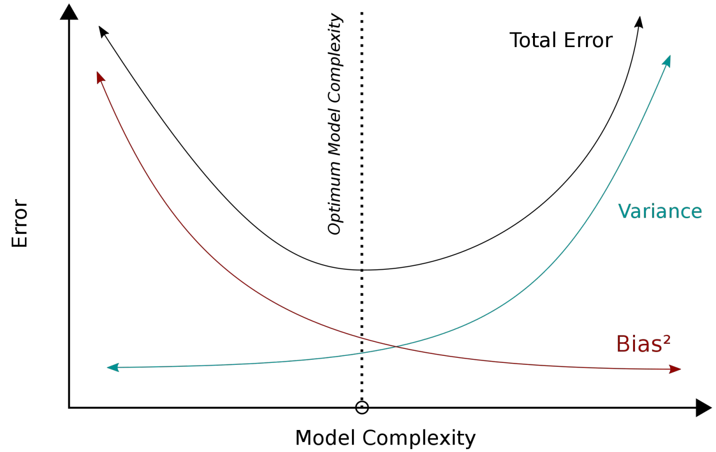

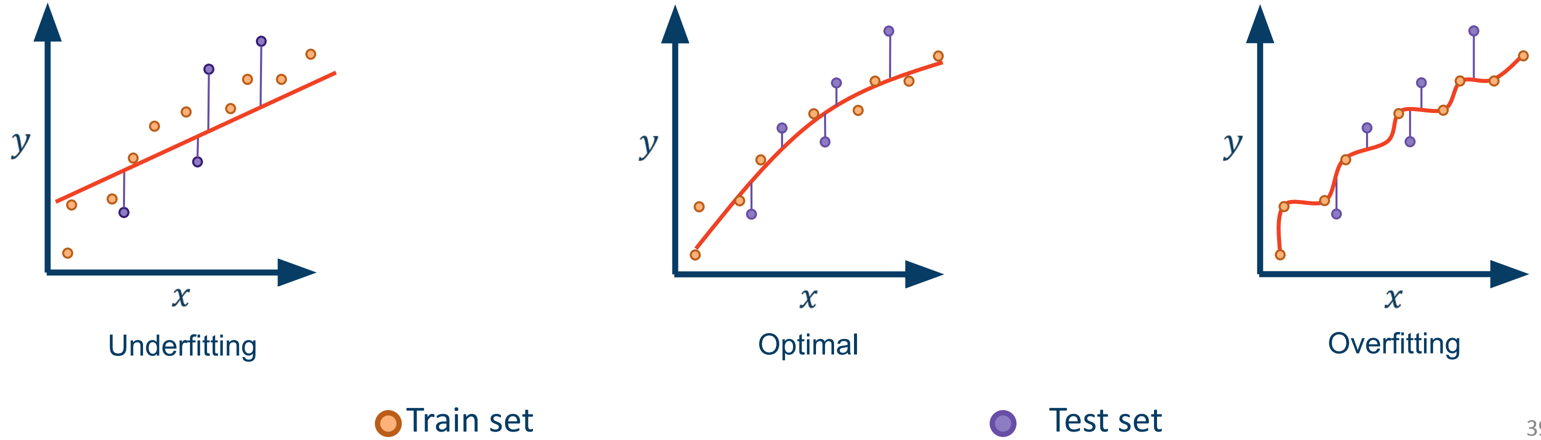

Model Evaluation

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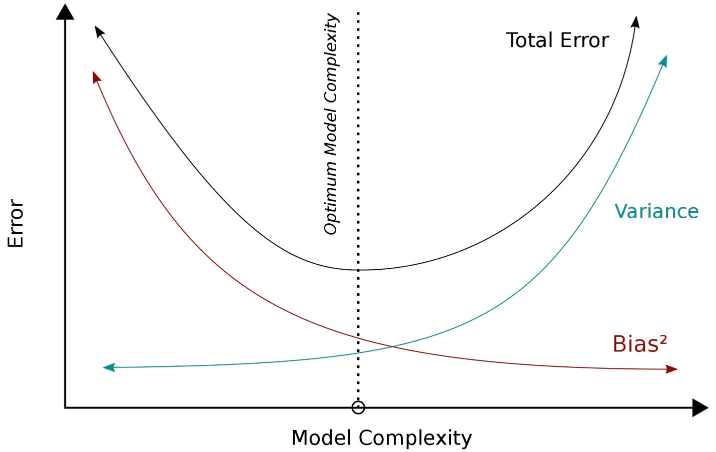
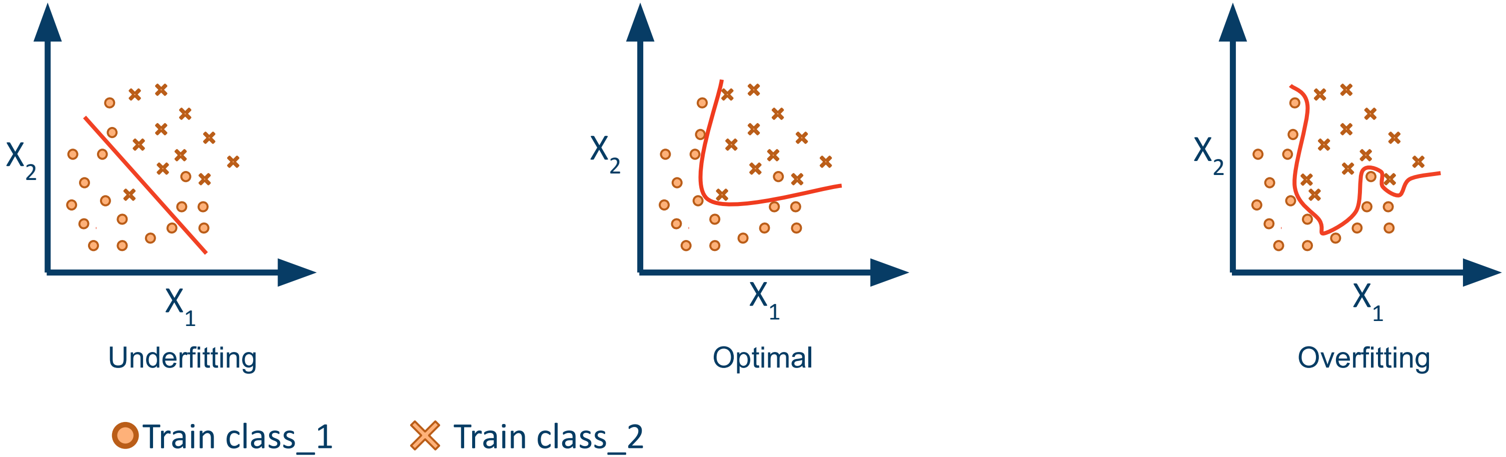
  - Classification example (i.e. separate **"o"** vs **"x"**)





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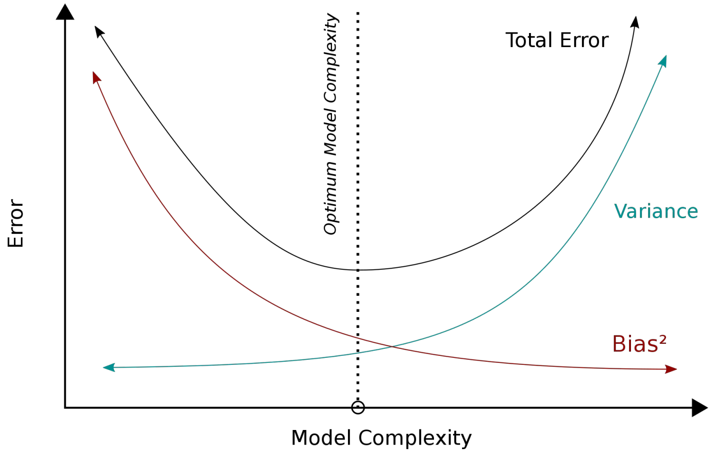

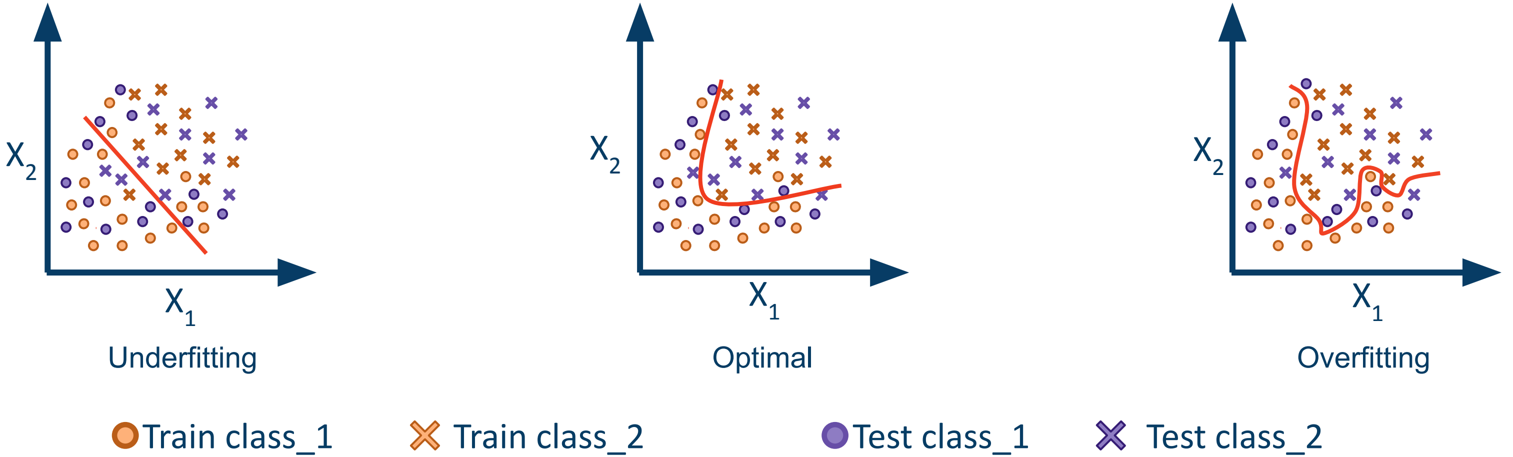

Exercise 1!

Model Evaluation

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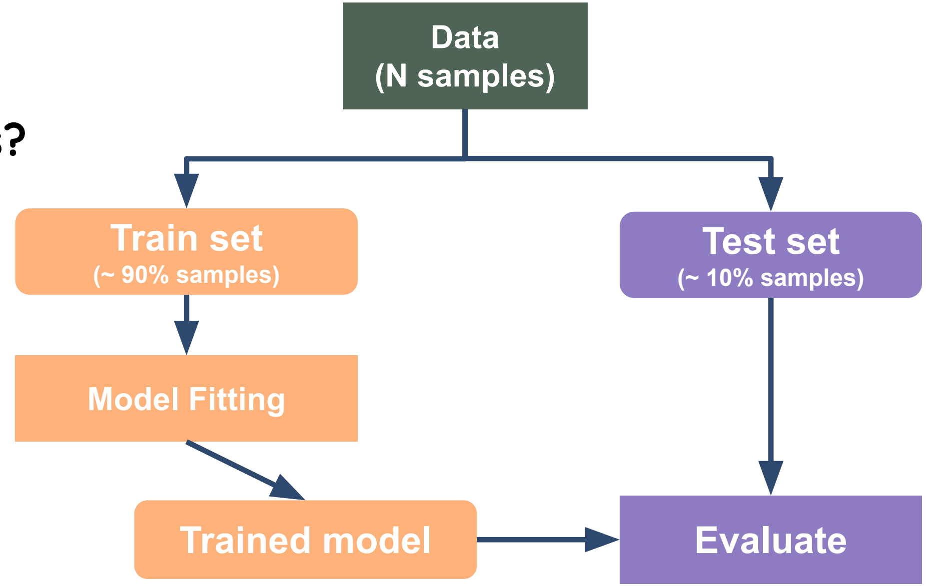
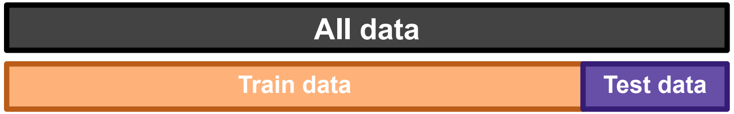
- **How do we sample train and test sets?**
- How do we select a model?



Model Evaluation: Cross-Validation (Outer loop)

- How do we sample train and test sets?
  - Train set: learn model parameters
  - Test set (a.k.a held-out sample): Evaluate model performance



Model Evaluation: Cross-Validation (Outer loop)

- How do we sample train and test sets?
  - Train set: learn model parameters
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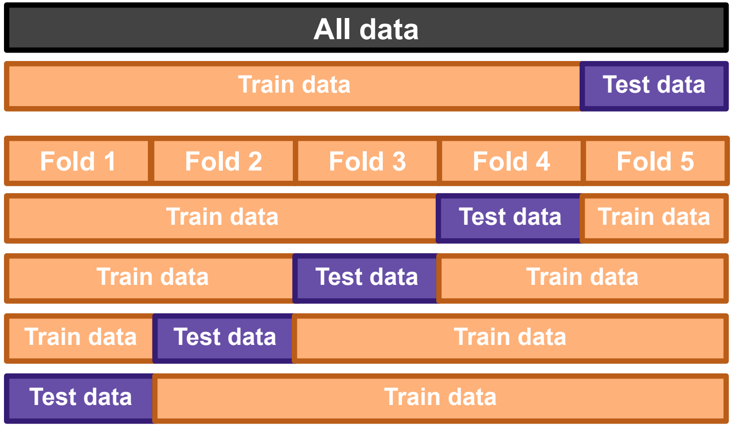
  - Repeat for different Train-Test splits
    - k-fold, shuffle-split
  - Report performance statistics over all test folds



CV outer loop

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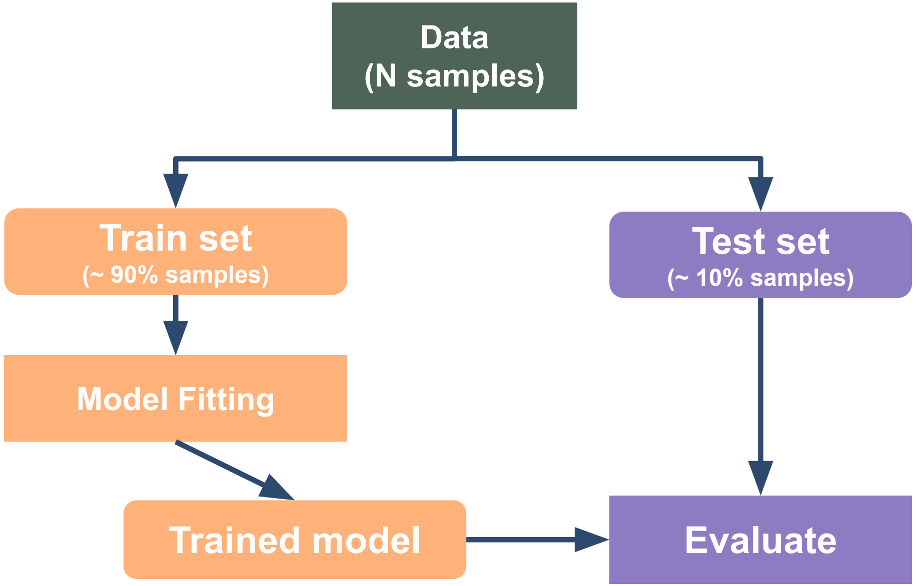
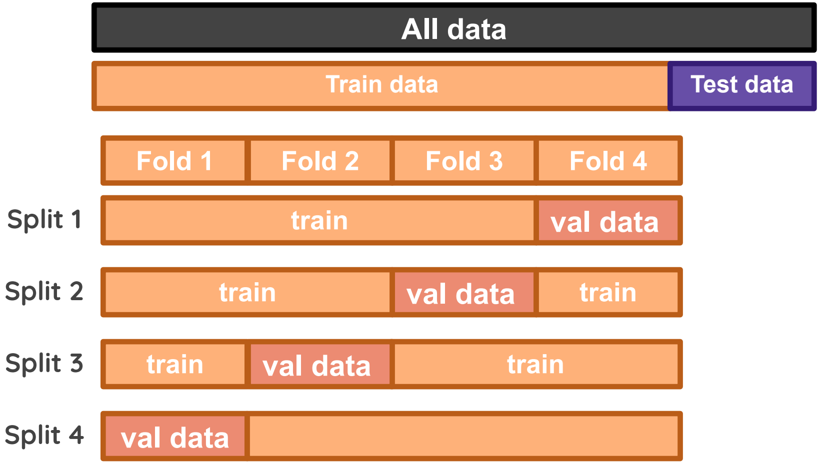


Model Evaluation: Cross-Validation (Inner loop)

- How do we select a model?
  - Tune *hyper-parameters* of a model
  - Compare several different model architectures
  - Select / transform raw features

- This repeats for all train-test splits in the outer loop



CV inner loop

Model Evaluation: Hyper-parameters

- Hyper-parameter ≠ parameter (or weights)
  - Parameters are **learned**; hyper-parameters are **chosen**!

Model Evaluation: Hyper-parameters

- Hyper-parameter ≠ parameter (or weights)
  - Parameters are **learned**; hyper-parameters are **chosen**!

- Examples:
  - Degree of model (eg. linear vs quadratic)
  - Kernels
  - Number of trees
  - Number of layers, filters, batch-size, learning-rate in ANNs

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  - Kernels
  - Number of trees
  - Number of layers, filters, batch-size, learning-rate in ANNs

- How do we choose them?
  - Prior beliefs → eg. cortical thickness and age have quadratic relationship.
  - Arbitrarily → we gotta start with something!
  - Trial and error → do a computationally feasible grid-search.

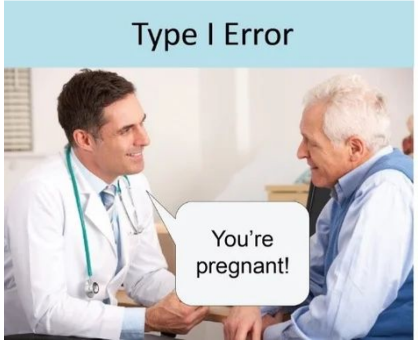
Performance Scores

- Loss functions → computationally well-suited metrics
  - May / need not completely capture performance metrics of interest

- Scores → practically useful metrics
  - Binary classification

Confusion Matrix		**Ground Truth**	
		POSITIVE	**NEGATIVE**
Prediction	**POSITIVE**	TP	FP
	NEGATIVE	FN	TN

False Positive



False Negative

Performance Scores

- ML model that detects Covid from chest CTs. Current Covid prevalence ~ 1%.
  - FP: model predicts *Covid* when person is *healthy*
  - FN: model predicts *healthy* when person has *Covid*
- What happens if we build model that predicts everyone as healthy?
  - i.e. zero FPs!

Performance Scores

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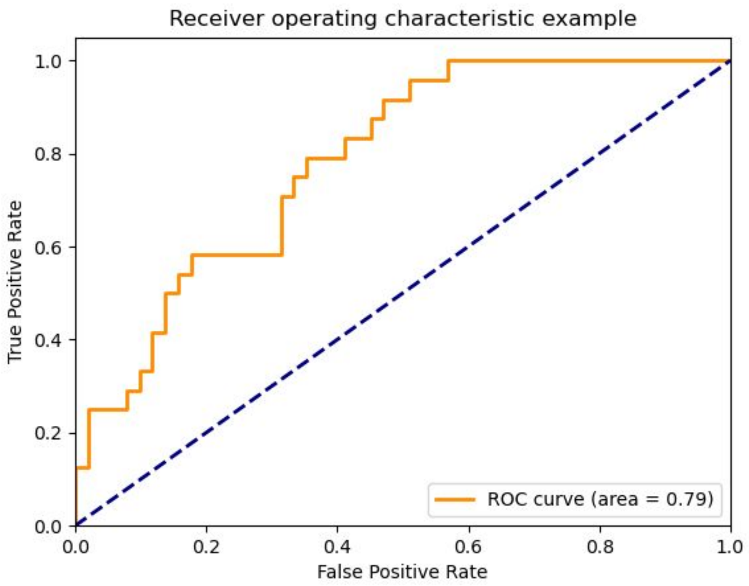
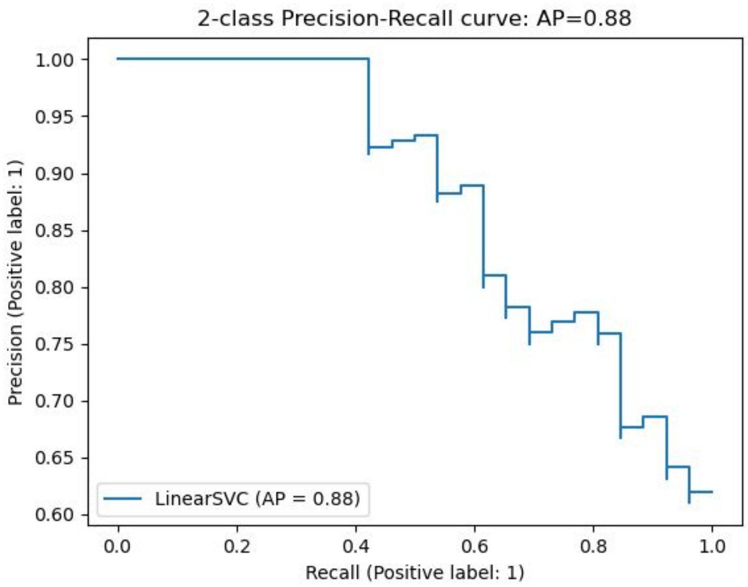
- What happens if we build model that predicts everyone as healthy?

Score	Formula	Null	What does it tell us?	When do I use it?
Accuracy	(TP+TN) / (TP+FP+FN+TN)	0.99	How many people did we correctly predict out of all the people scanned?	FNs & FPs have similar costs
Precision (aka PPV)	TP/(TP+FP)	NaN	How many of those who we predicted as "covid" do actually have "covid"?	If you want to be more confident of your TPs
Recall (aka Sensitivity)	TP/(TP+FN)	0	Of all the people who have covid, how many of those did we correctly predict?	If you prefer FPs over FNs.
Specificity	TN/(TN+FP)	1	Of all the people who are healthy, how many of those did we correctly predict?	If you prefer FNs over FPs.
F1	2*(Recall * Precision) / (Recall + Precision)	NaN	Harmonic mean(average) of the precision and recall.	When you have an uneven class distribution

Performance Curves

- Receiver Operating Characteristic (ROC) → Want high area-under-the-curve (AUC)
- Precision-Recall → Want high AUC or high Average precision (AP)





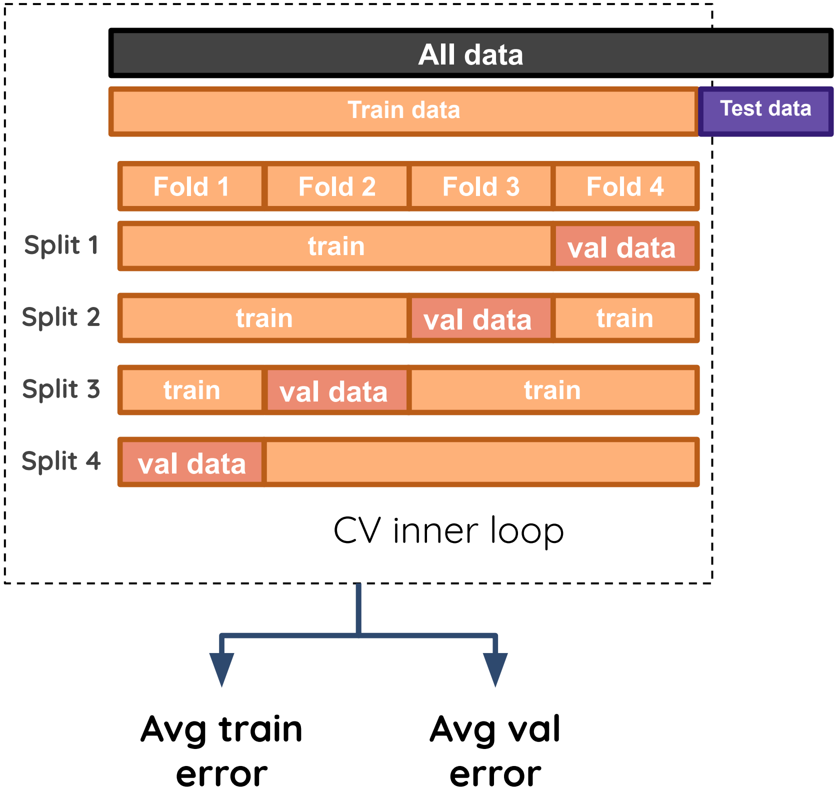
Practical intuition

Task: Segmentation, diagnosis etc

- Human error ~ 2%
- Train error ~ 10%
- Val error ~ 20%

Bias / underfit

Variance / overfit



What do we do?

- Underfitting → Bigger/different model
- Overfitting → More data / regularization

Practical intuition

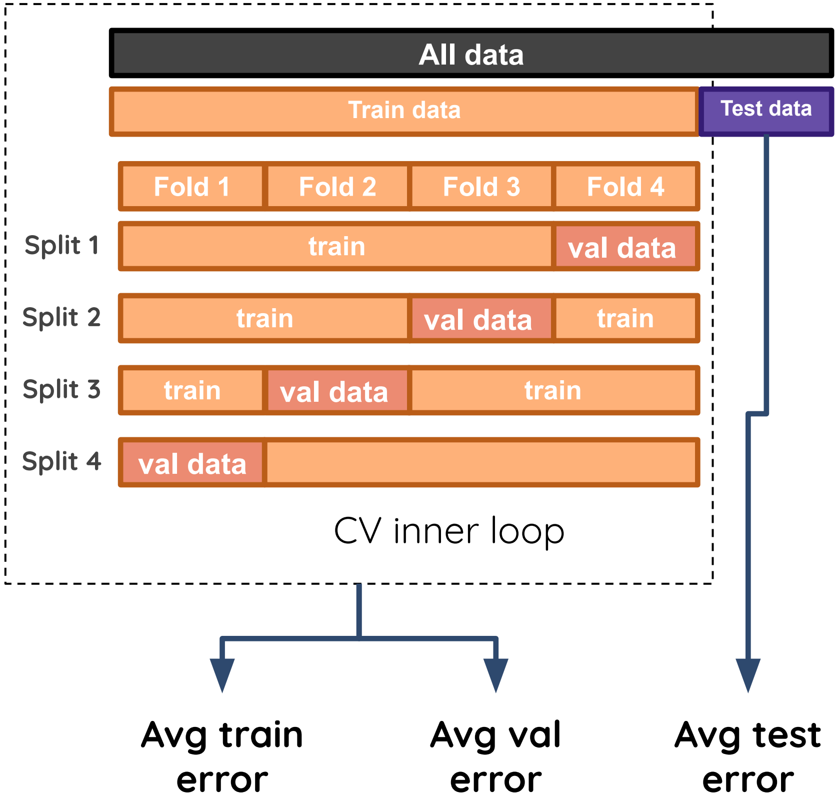
Task: Segmentation, diagnosis etc

- Human error ~ 2%
- Train error ~ 5%
- Val error ~ 5%
- Test error ~ 20%

dataset shift (overfit)

What do we do?

- Feature shift → get / generate more data
- Concept drift → fix / refine labels



Pop Quiz Answers

We train a simple machine-learning model to identify COVID patients using their biometry, in a population with 1% covid prevalence. Our model is 91% accurate! Then we also calculate,

- 90% sensitivity (i.e. probability that prediction is positive if patient has COVID)
- 91% specificity (i.e. probability that prediction is negative if patient doesn't have COVID)

What are my chances that I have COVID if my test is positive?

(Imagine a sample of 1000 individuals → 10 COVID patients → 9 TP & 89 FP)

A) 9 in 10 B) 1 in 2 **C) 1 in 10** D) 1 in 100

Later we train a fancy deep Learning model to identify COVID patients using chest CT and brain MRI! This model has accuracy of 99%! We calculate

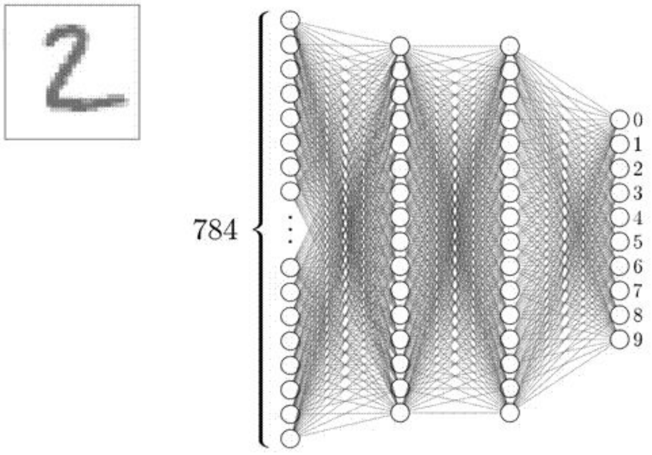
- 80% sensitivity
- 99% specificity

Which model is better? (We want to avoid FN to reduce the spread → we want high-sensitivity)

A) Simple B) Fancy

Deep-learning

- Why the buzz?
  - Works amazing on spatio-temporal input
  - Highly flexible → universal function approximator



ANN for handwritten-digit images
(gif source: 3b1b)

Deep-learning

- Why the buzz?
  - Works amazing on spatio-temporal input
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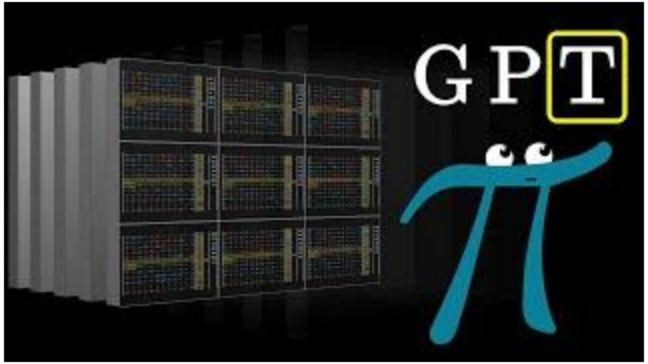
- What are the challenges?
  - Large number of parameters (175B!) → data hungry
  - Large number of hyper-parameters → difficult to train



LLM Transformers
(gif source: 3b1b)

Deep-learning

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- What are the challenges?
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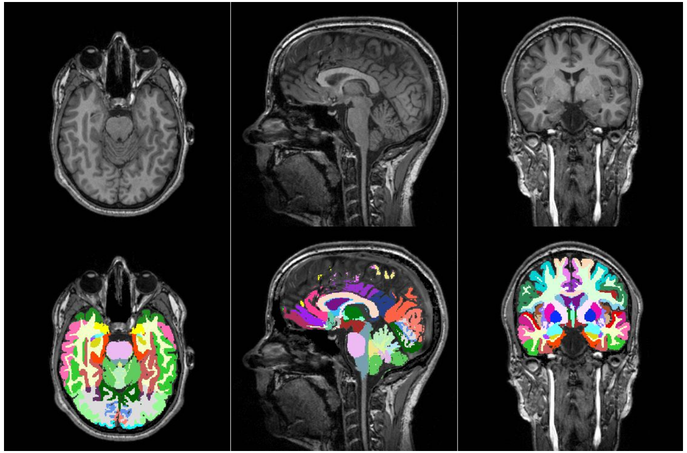
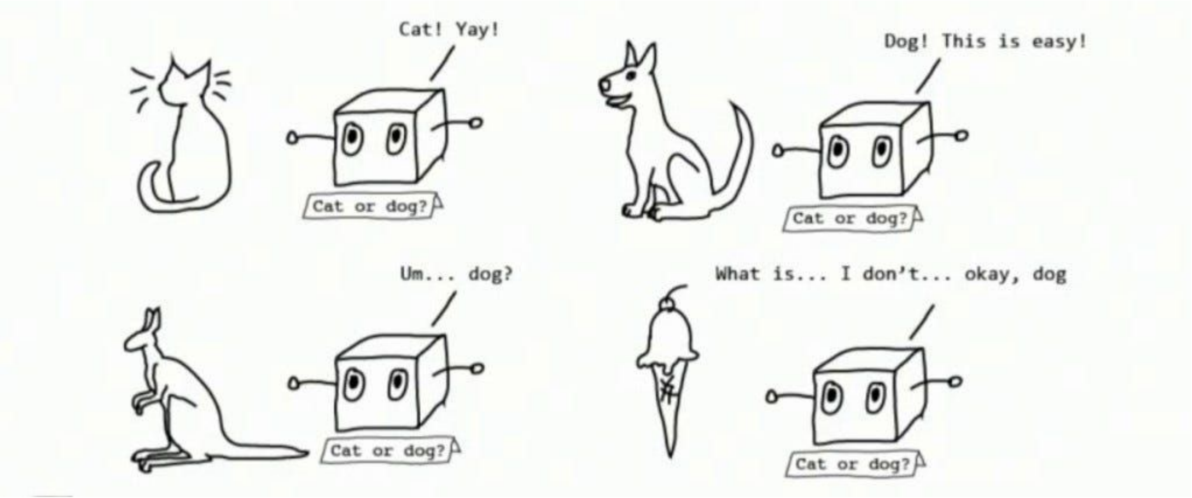
- When do I use it?
  - If you have highly-structured input, eg. medical images.
  - You have a lot of data and computational resources.



Source:
https://github.com/fepegar/torchio

Pitfalls and Challenges

- Models do not generalize even after good CV performance
  - Implicit double-dipping
  - Dataset biases (eg. North-American demographics)
  - Noisy labels (eg. diagnosis definitions)
  - Data distribution shifts (eg. assay, scanner upgrades)



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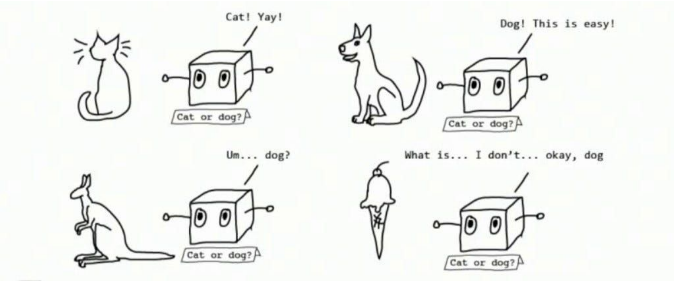


- Unnecessary complexity
  - Do I really need a giant deep-net or a simple linear model would do?

ML Novice Checklist

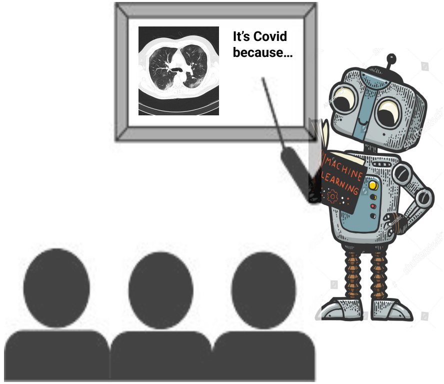
- Data
  - What is my n_features and n_samples?
  - Am I encoding categorical data correctly?
  - Am I using information (e.g. mean) from test set to preprocess (eg. zscore) the data?

ML Novice Checklist

- Data
  - What is my n_features and n_samples?
  - Am I encoding categorical data correctly?
  - Am I using information (e.g. mean) from test set to preprocess (eg. zscore) the data?
- Model
  - Do my performance metrics capture the practical use-case of interest?
  - What is the null / dummy model performance?
    - Classification: Predict majority class all the time
    - Regression: Predict the median value all the time
  - Am I interpreting model parameters (i.e. weights) correctly?

Takeaways

- Supervised ML is useful for **predictions** but **not really for explanations**
  - eg. image segmentation, prognosis, drug development
- Our job is to ensure **generalizability** of these models
  - Multitude of validations
  - Understanding model biases and limitations
- ***Engineering tools*** vs *Scientific discovery*
  - Interpretability and explainability



Explainable AI

Food for thought

- Ethical dilemmas
- Socialietal implications
- What's real?

Ceci n'est pas un pape

Exercise 2!

Extra slides

Useful resources

- https://inria.github.io/scikit-learn-mooc/ml_concepts/slides.html
- https://www.3blue1brown.com/topics/linear-algebra
- 3b1b Gradient Descent:
  https://www.youtube.com/watch?v=IHZwWFHWa-w