Introduction to Supervised learning using scikit-learn

MAIN 2022 | July 2022

By

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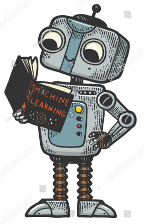

Objectives

- Define machine-learning nomenclature
- Describe basics of the “learning” process
- Explain model design choices and performance trade-offs
- Introduce model selection and validation frameworks
- Explain model performance metrics

Pop Quiz

Say, currently we have a population with 1% covid prevalence. We train a simple machine-learning model to identify COVID patients using their biometry.

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?

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

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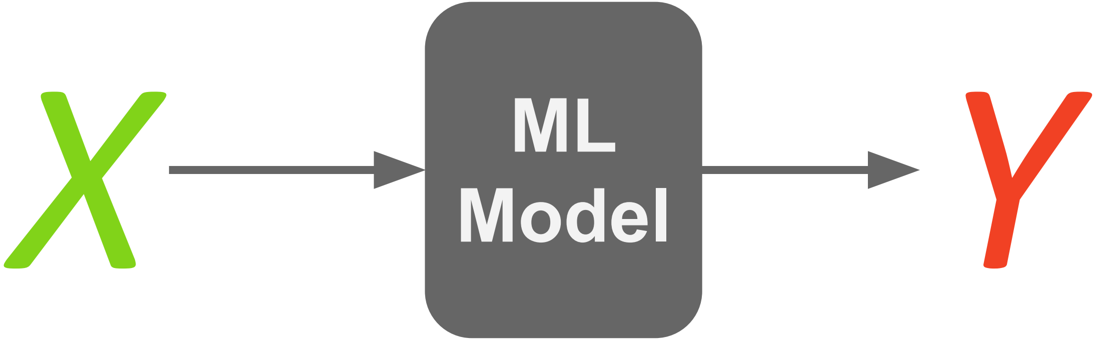
Later we train a fancy deep learning model to identify COVID patients using their chest CT! This model has accuracy of 99%! We calculate

- 80% sensitivity
- 99% specificity

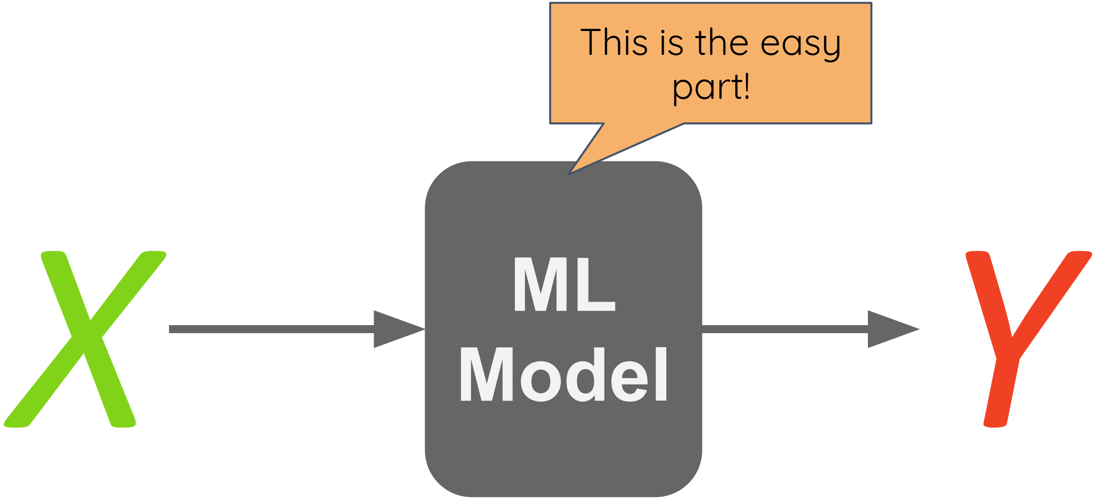
Which model is better?

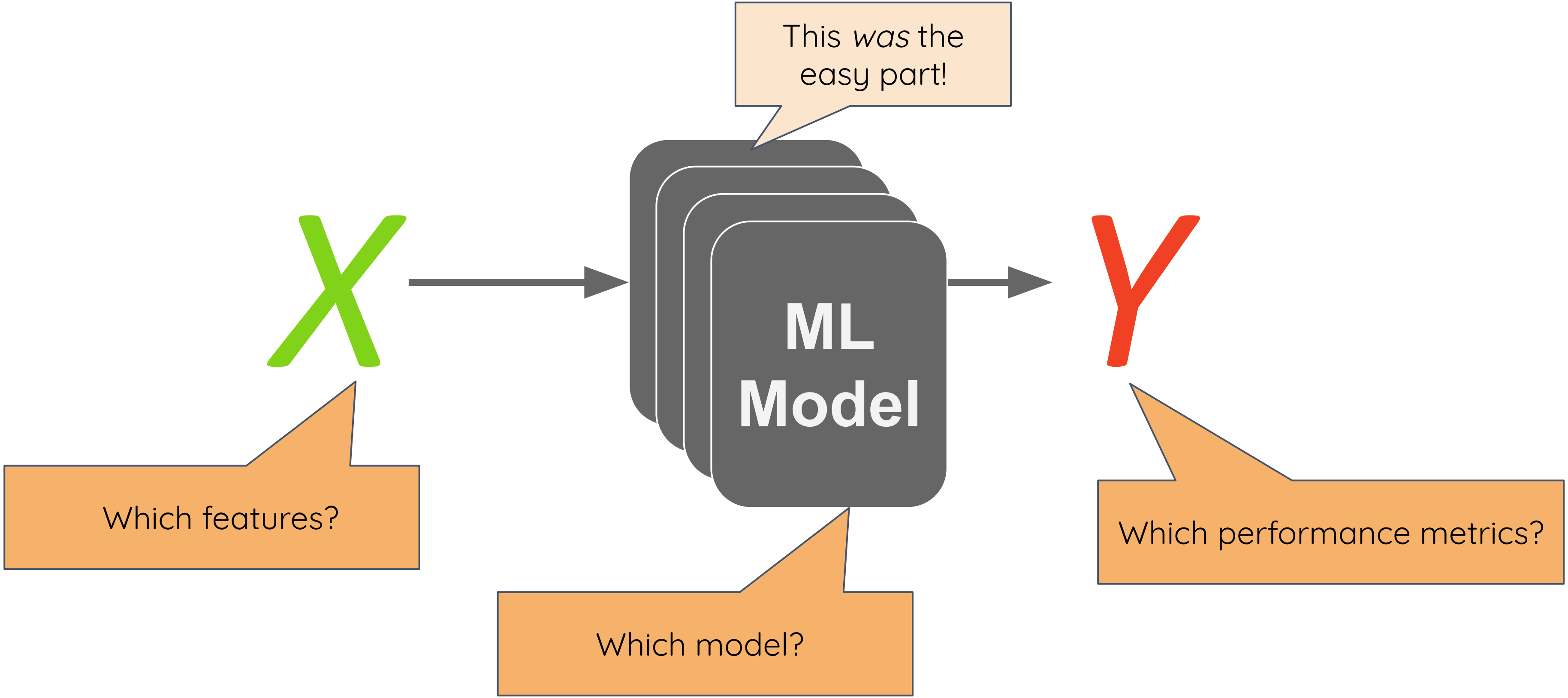
A) Simple B) Fancy

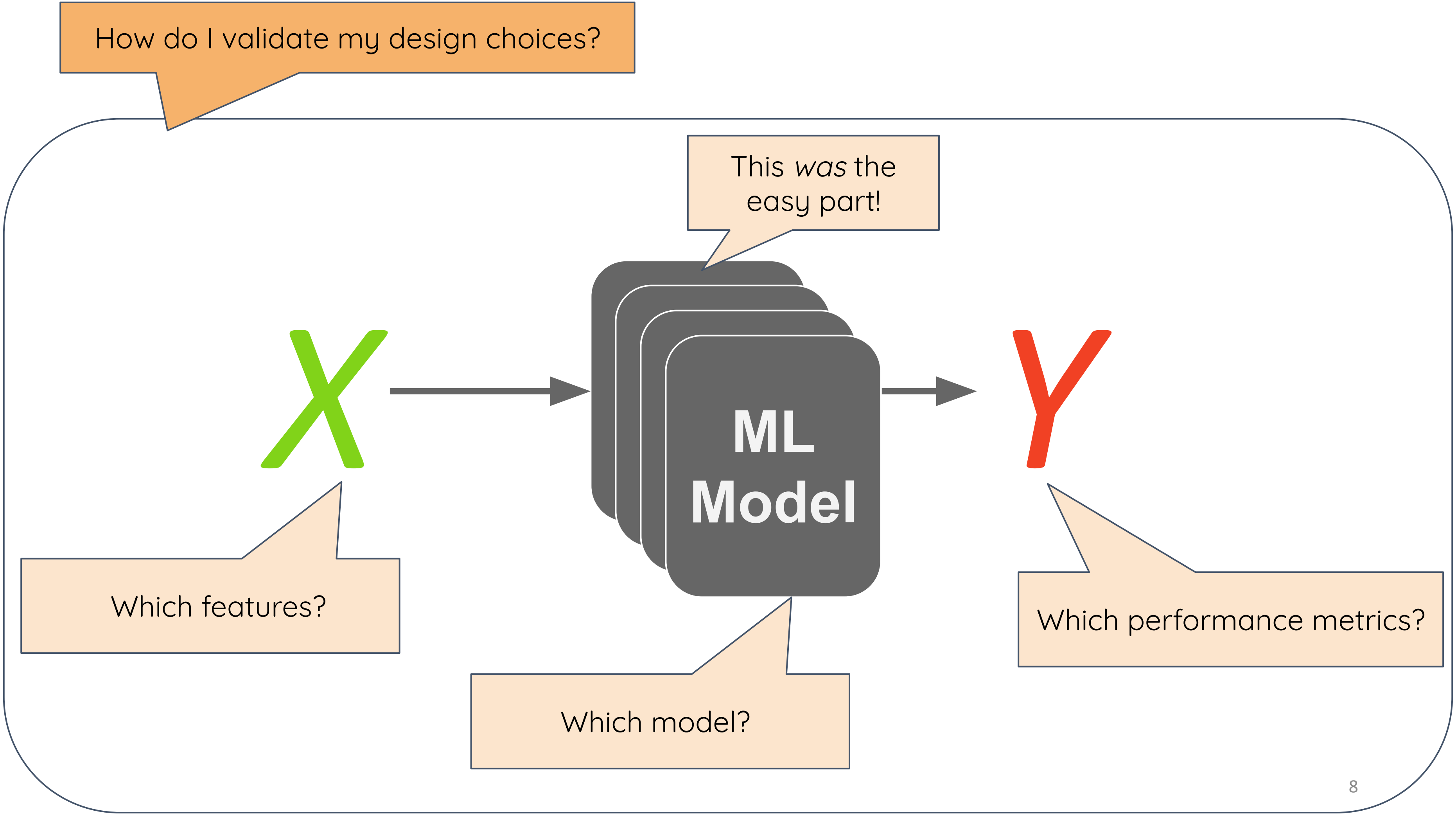
Training a machine-learning model



Training a machine-learning model




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


How do I validate my design choices?
This *was* the easy part!
X
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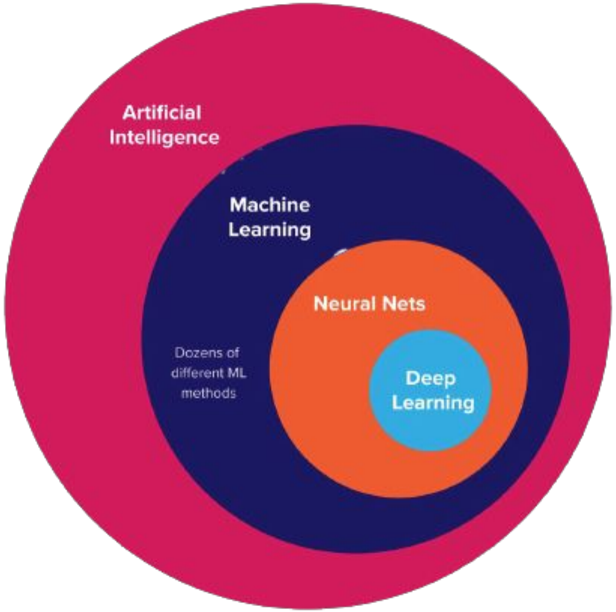
Machine-learning - what, why, and when?

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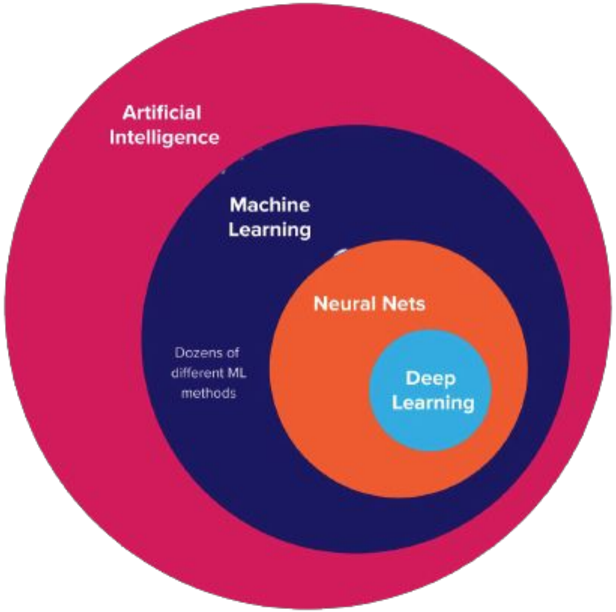
- Why is it useful - especially in life sciences?
  - Biology, Medicine, Environmental sciences comprise phenomenons (e.g. a disease) with large number of variables.
  - We want to model complex relationships within these variables and make accurate predictions.



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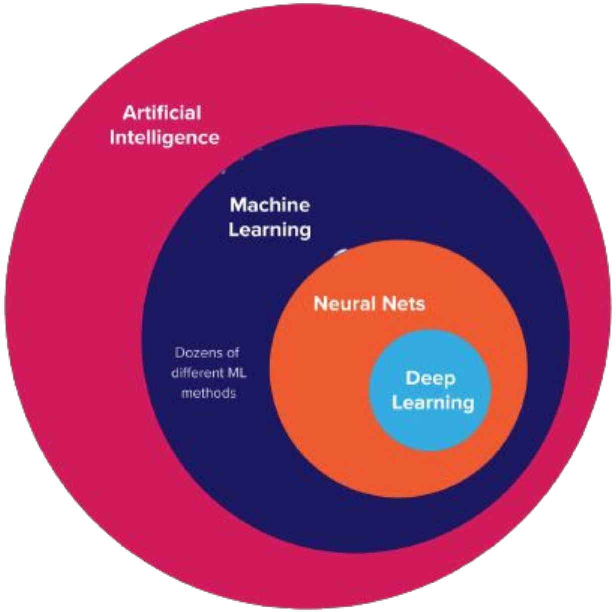
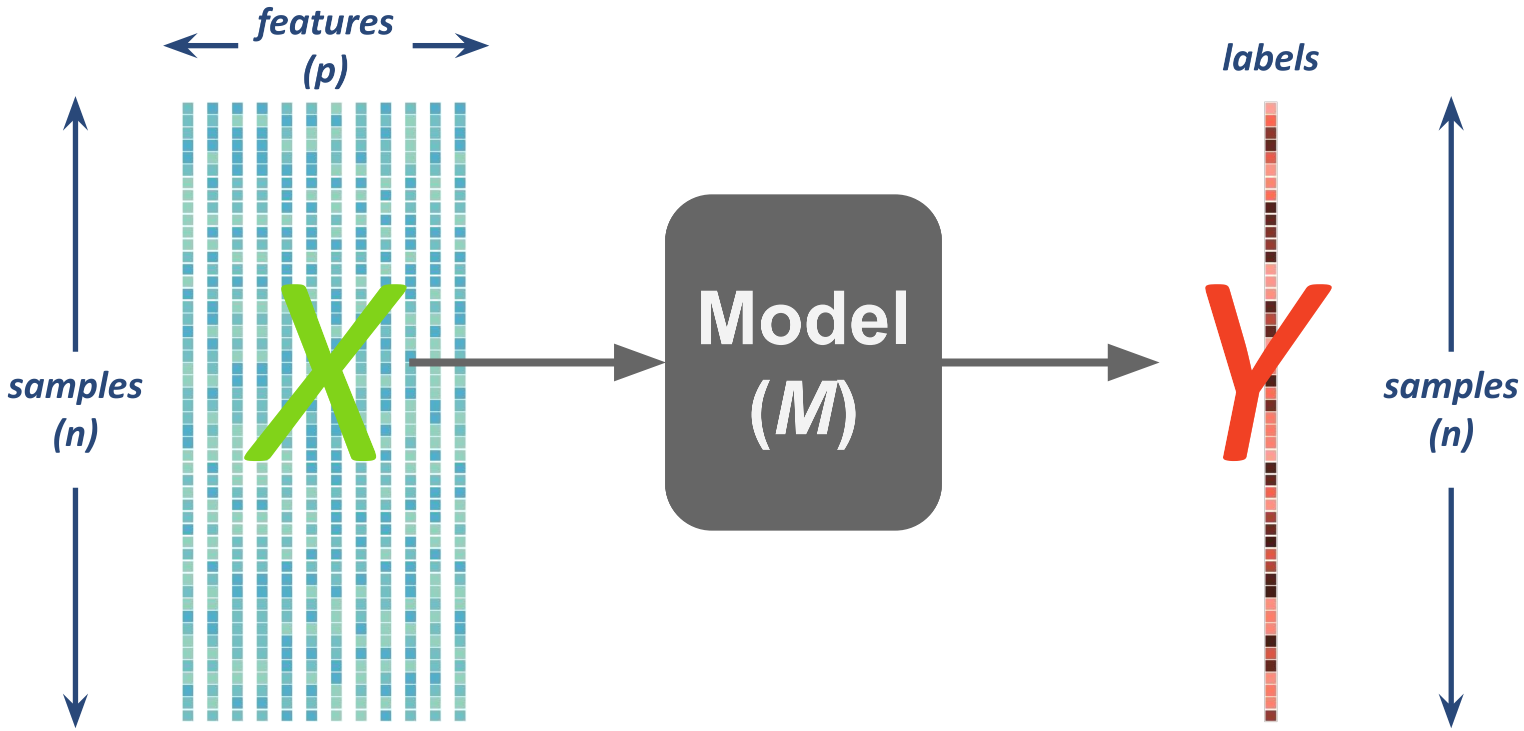
- When do I use it?
    - You are interested in 1) prediction tasks or 2) low-dimensional representation.
    - You have sufficient data.



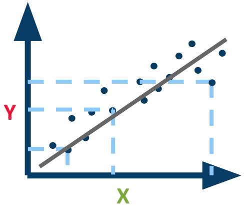
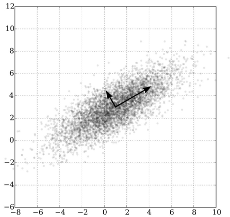
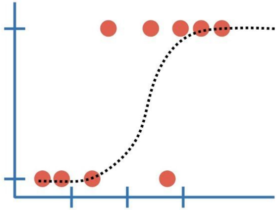
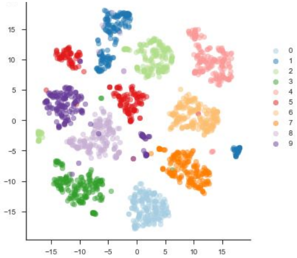
Terminology



Input
Examples: 

Output Examples: Clinical
measures

Types of ML Algorithms

Outcome	Supervised Learning	Unsupervised Learning
Continuous	Regression 	Dimensionality reduction 
Categorical	Classification 	Clustering 

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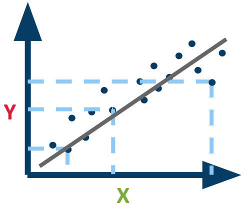
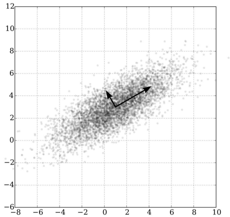
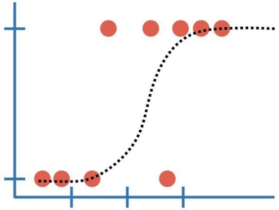
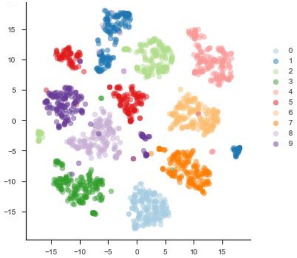
Continuous	Regression 	Dimensionality reduction 
Categorical	Classification 	Clustering 

Supervised Learning: Models

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

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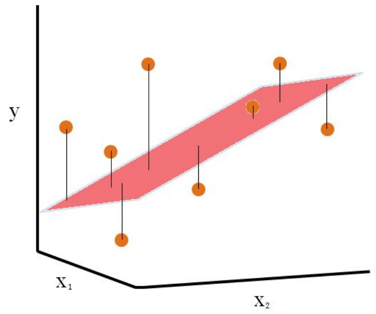

Linear Regression

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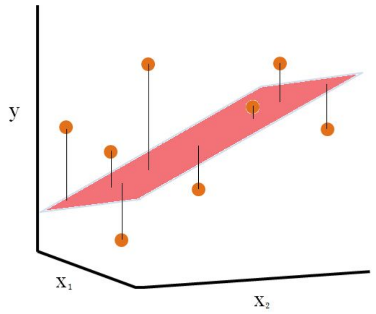
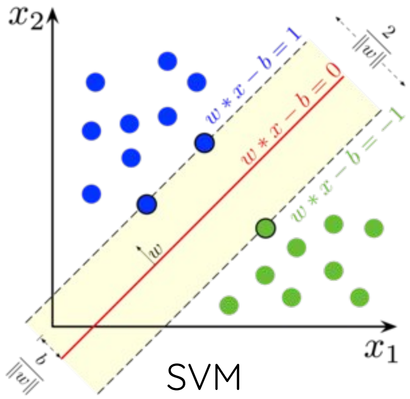


Linear Regression



SVM

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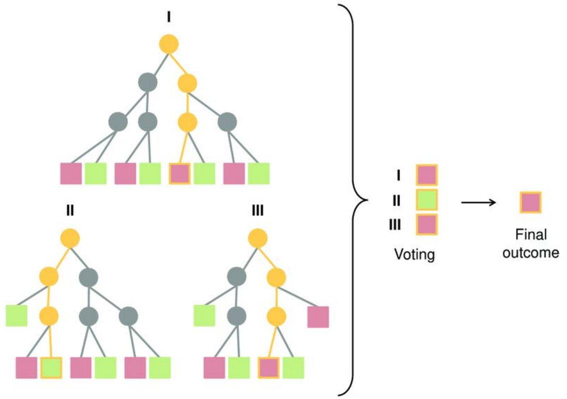
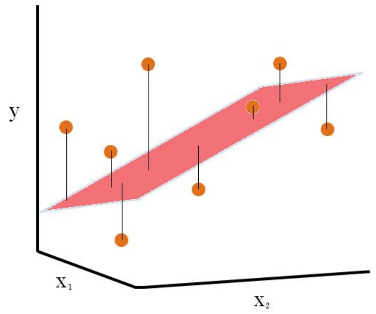


Tree-ensembles



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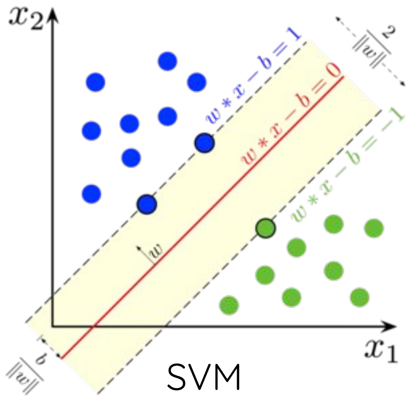

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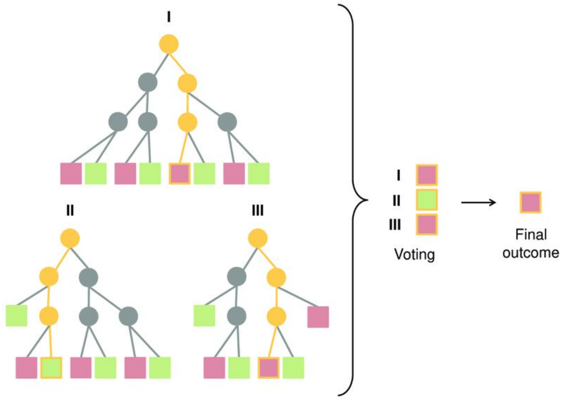
  - Artificial Neural networks



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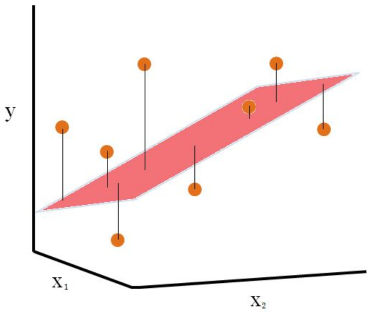

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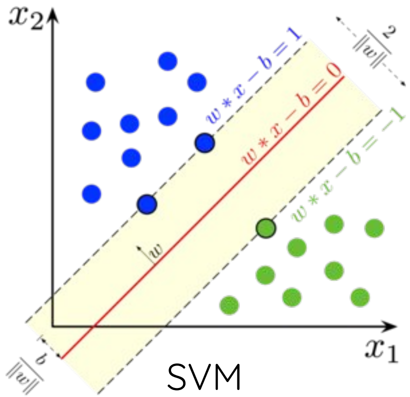

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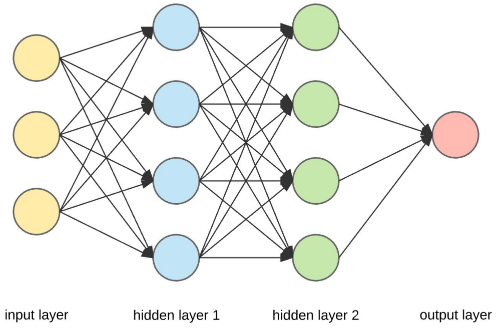
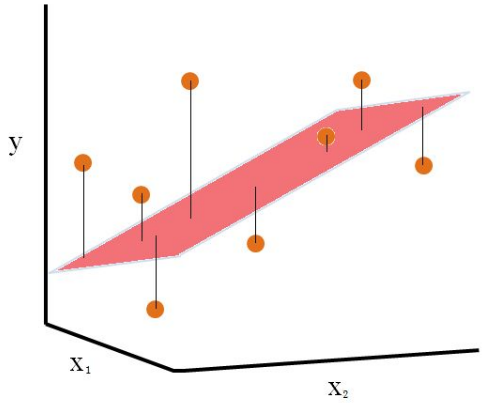
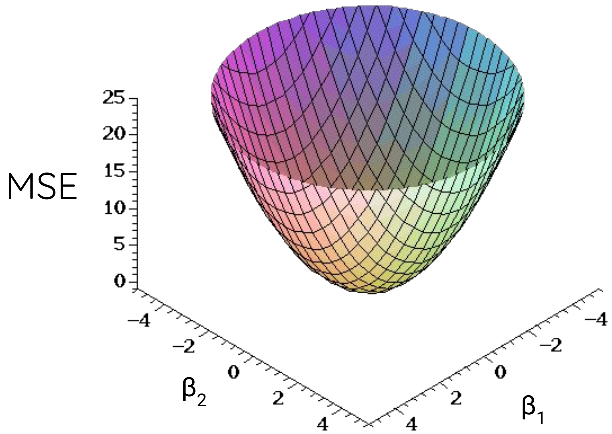


ANN

Model Fitting

- How do we learn the model weights?
    - Example: Linear regression
    - Model: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$
    - Loss function: $MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$
    - Optimization: Gradient descent



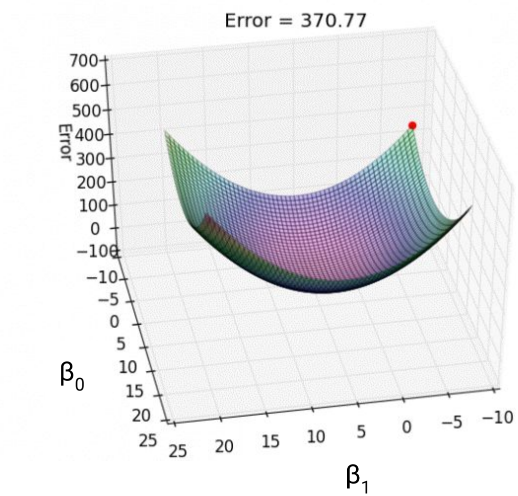


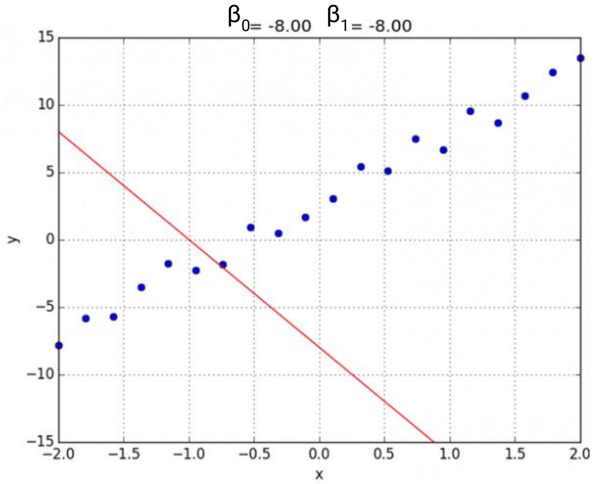
Model Fitting

- 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

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

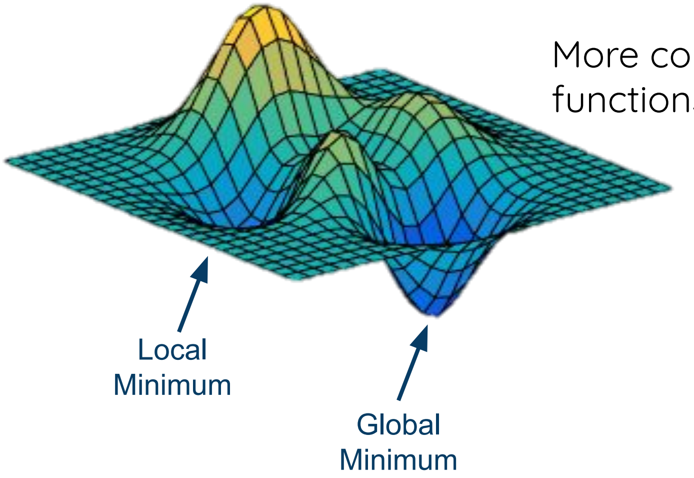
$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$





Model Fitting

- Gradient descent for complex models with non-convex loss functions
  - Start with random weights (β_0 and β_1)
  - Compute loss
  - Update weights based on the gradient



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

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  - We have strong prior beliefs about what is a **plausible** model
    - e.g. I believe this symptom can be predicted with handful of genes.
  - Practical reasons
    - Prevent overfitting (n_features >> n_samples)

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

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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
  - L2 i.e. Ridge

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***

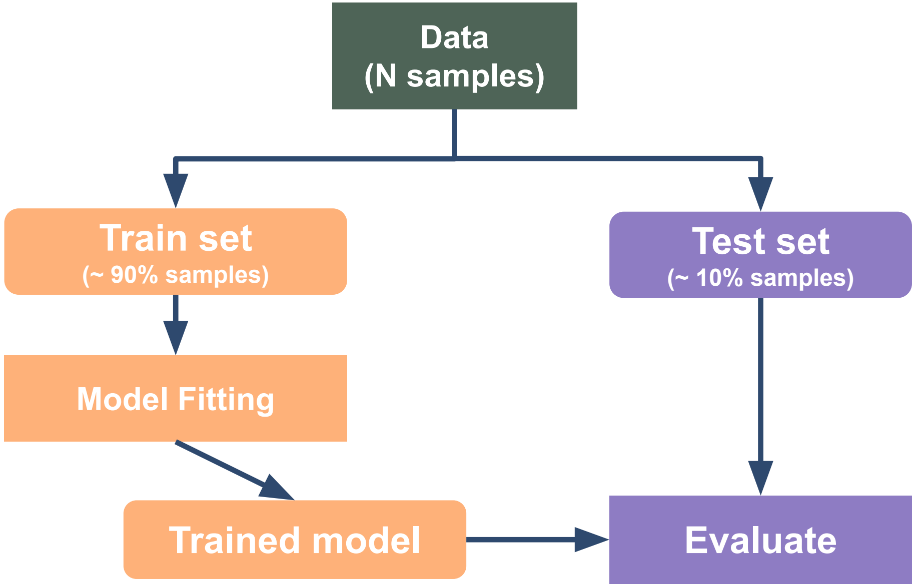
$$MSE = \sum_{i=1}^{n}(y_i - \underbrace{[\,\beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j\,]}_{\hat{y}_i})^2 + \underbrace{\lambda \sum_{j=1}^{p} \beta_j^2}_{L_2}$$

Model Fitting: Scikit-learn syntax

```
# import
from sklearn import linear_model, svm

# data
X = [[0, 0], [1, 1]]
y = [0, 1]

# pick a model
model = linear_model.Lasso(alpha=0.1)   # model = svm.SVC()

# fit the model with data
model.fit(X, y)

# 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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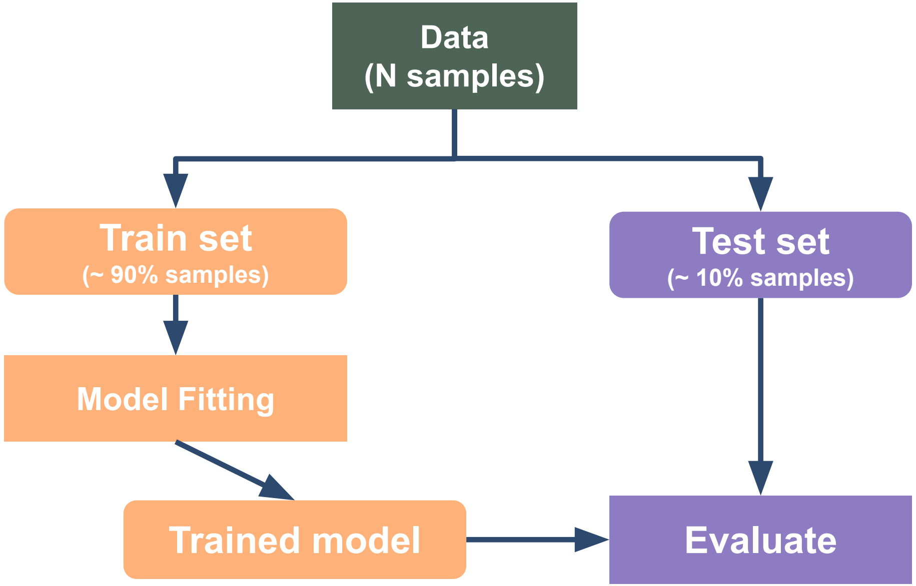
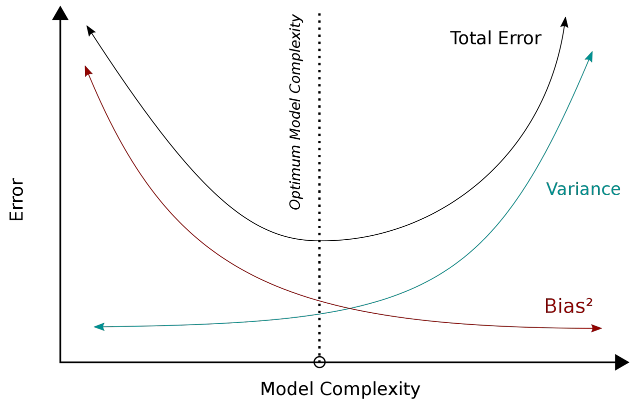
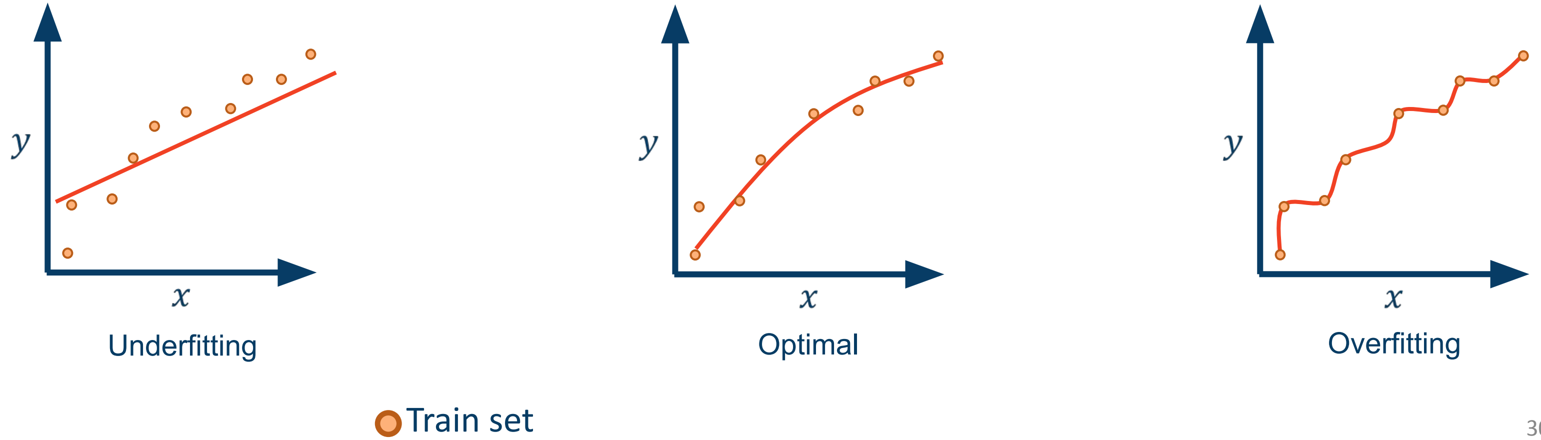


Model Evaluation

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





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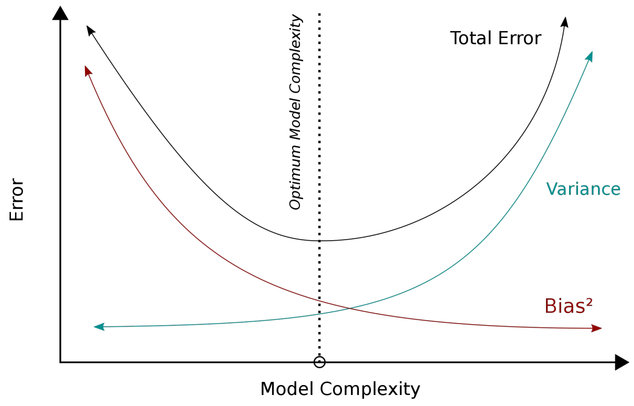

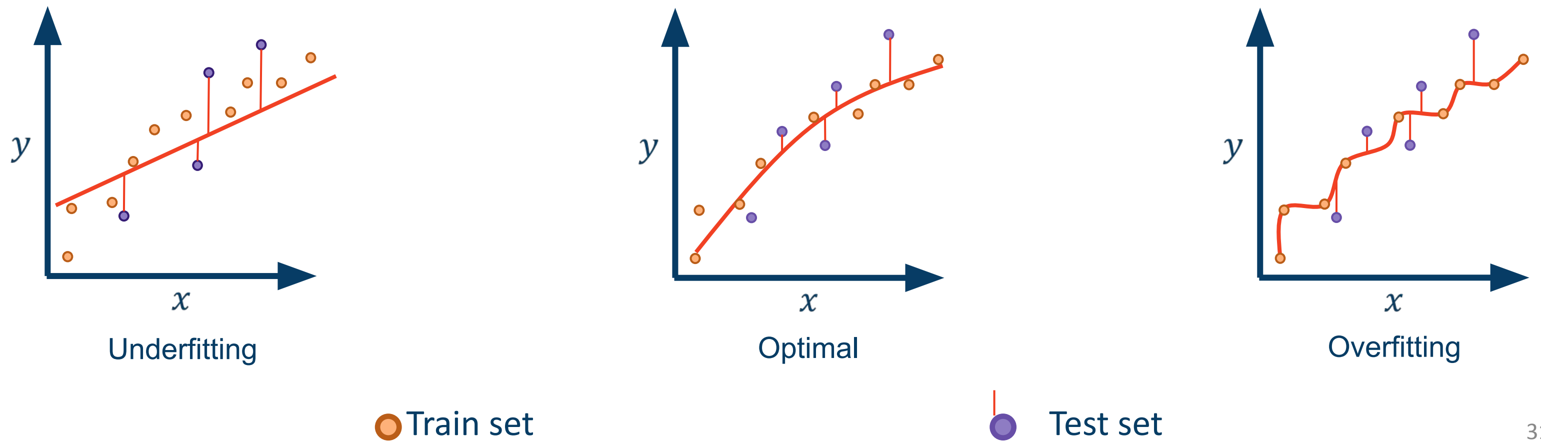

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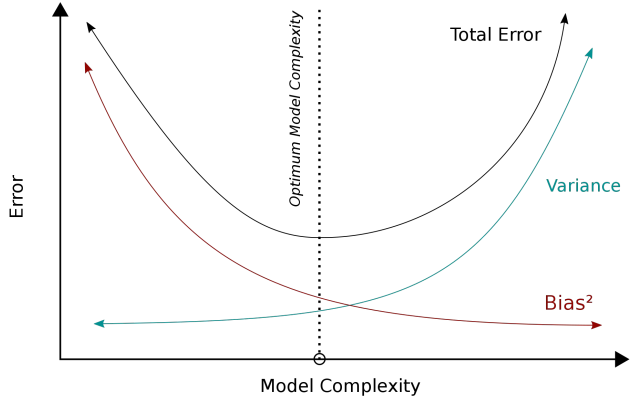

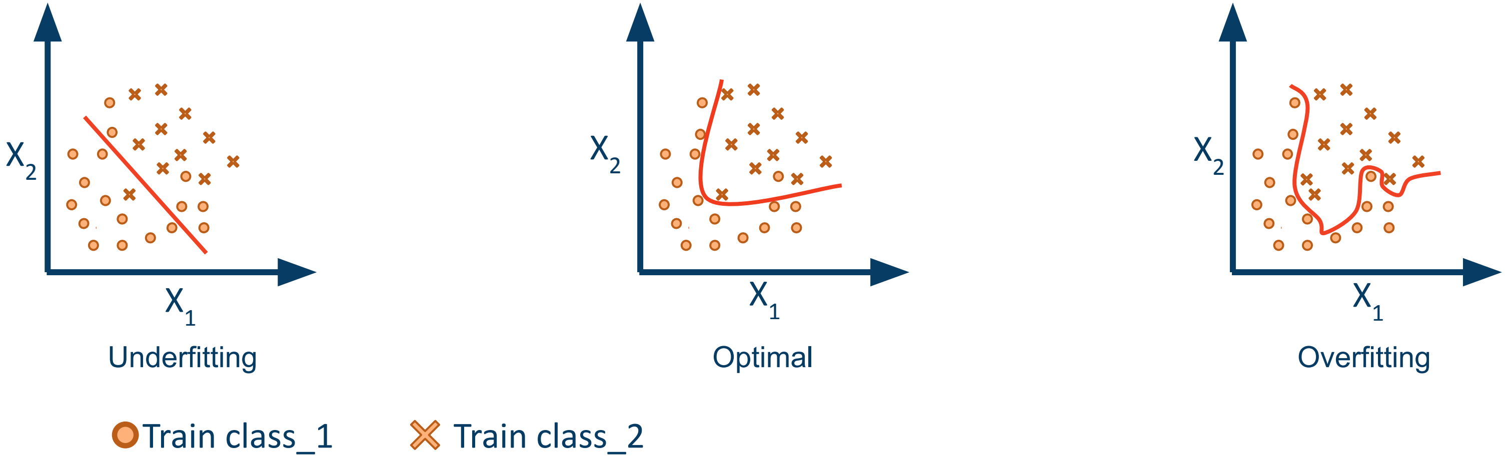

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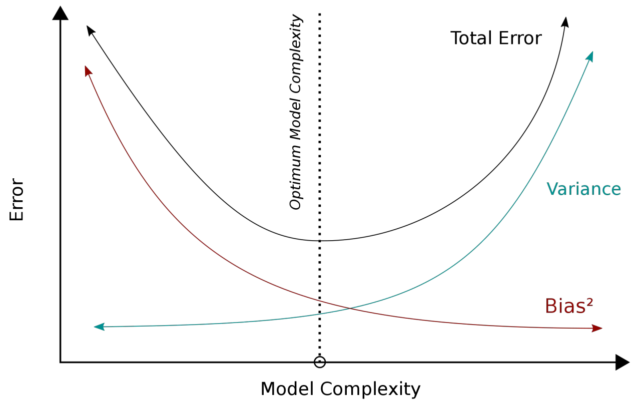

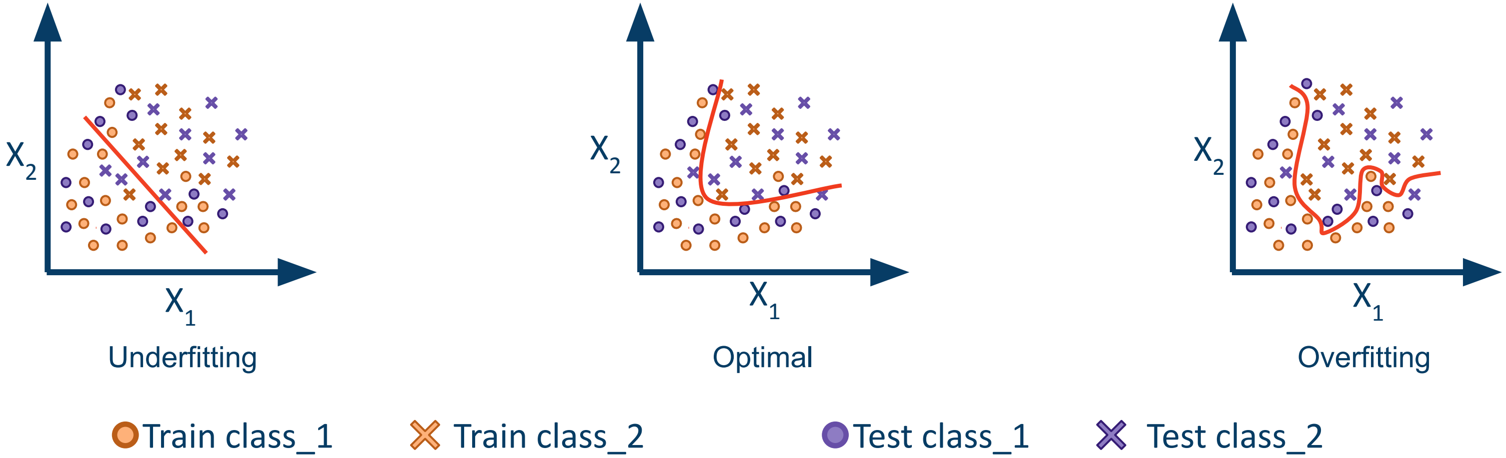

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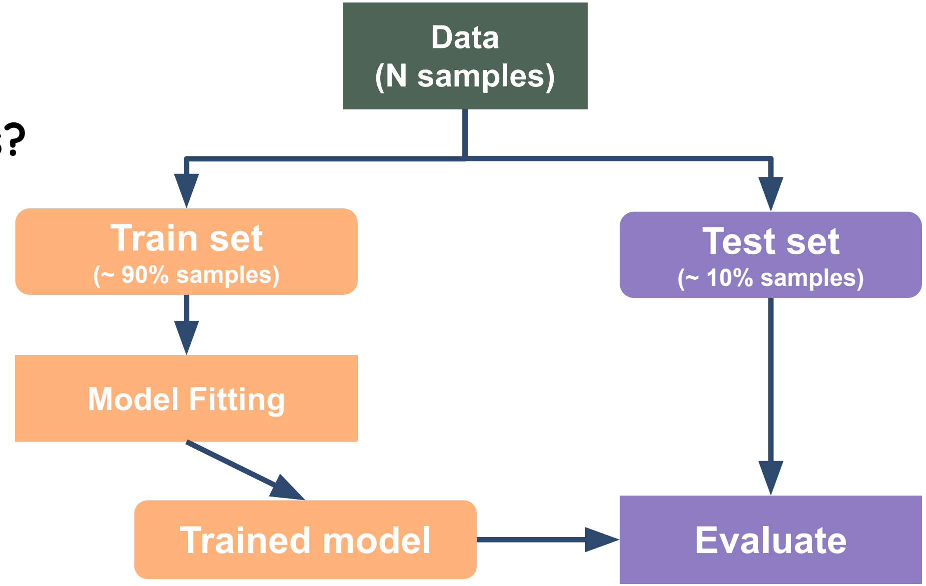
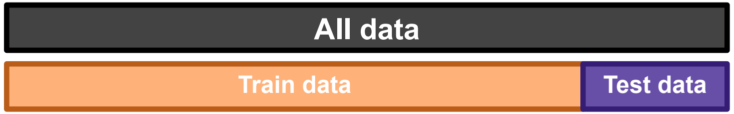


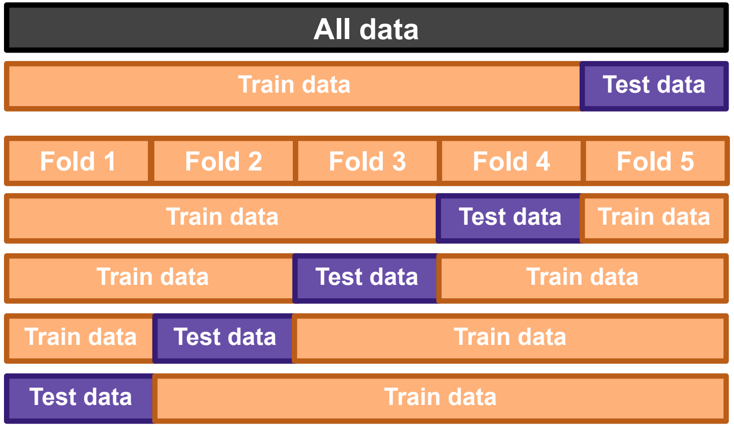
Model Evaluation: Cross-Validation (Outer loop)

- 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
  - Test set (a.k.a held-out sample): Evaluate model performance
  - Repeat for different Train-Test splits
    - k-fold, shuffle-split
  - Report performance statistics over all test folds



CV outer loop

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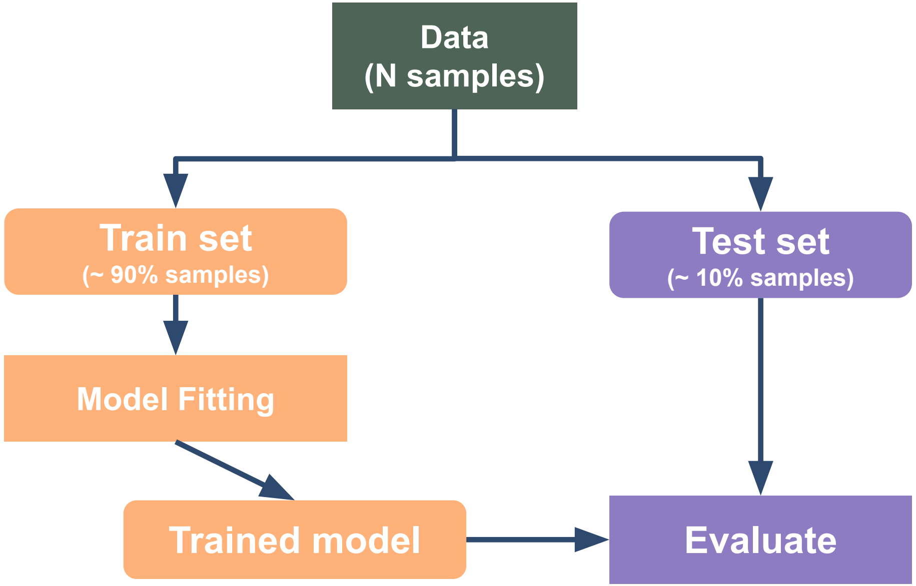
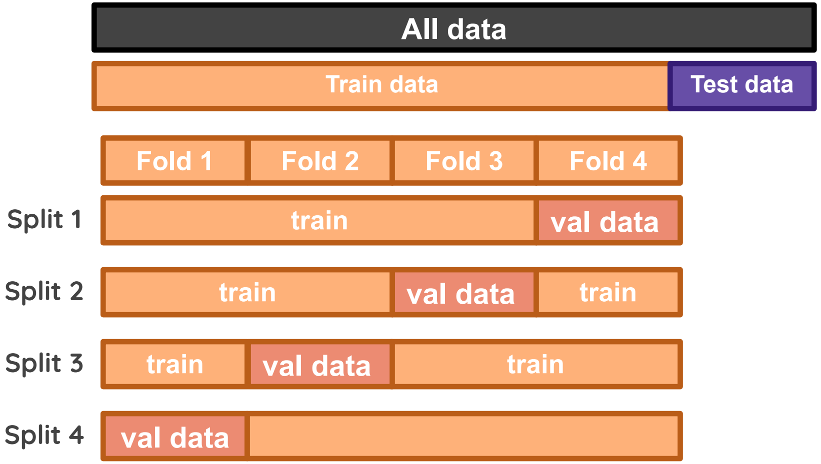


Model Evaluation: Cross-Validation (Inner loop)

- 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

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

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- 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.

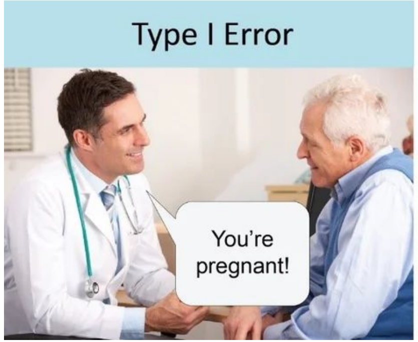
Performance Scores

- 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

- 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?

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 (i.e. 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

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 their chest CT! This model has accuracy of 99%! We calculate

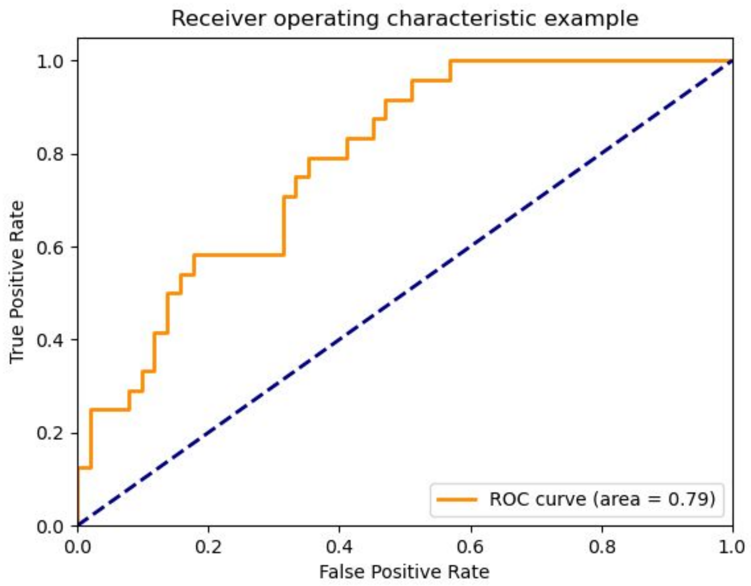
- 80% sensitivity
- 99% specificity

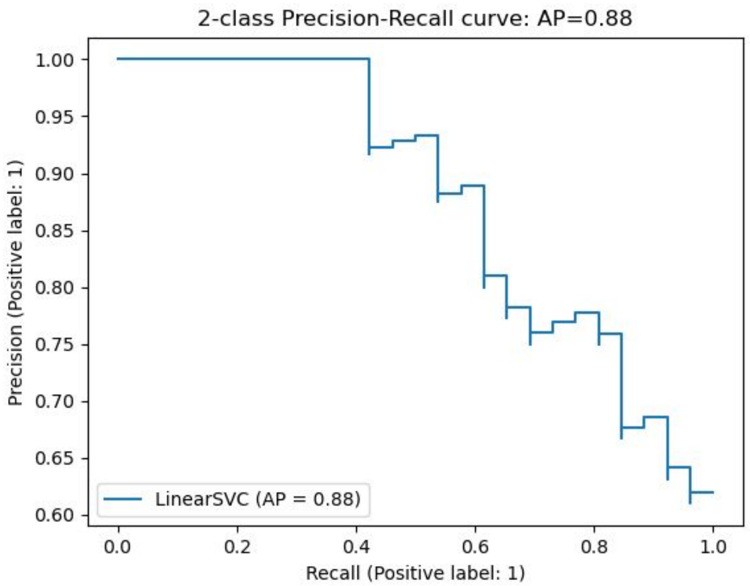
Which model is better? (We want to avoid FN to reduce the spread → we want high-sensitivity)

A) Simple B) Fancy

Performance Curves

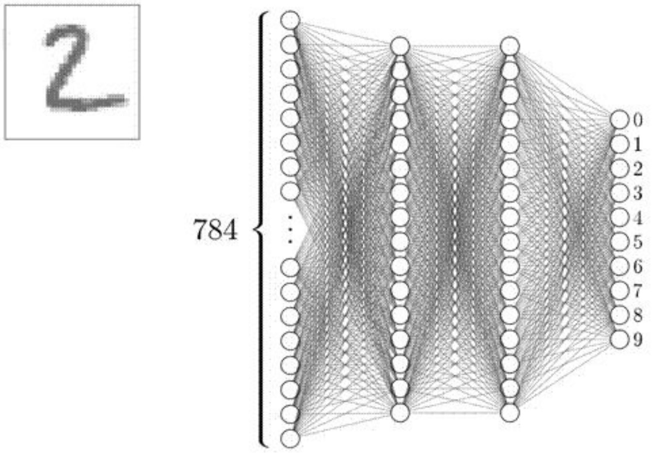
- Receiver Operating Characteristic (ROC) → Want high area-under-the-curve (AUC)
- Precision-Recall → Want high AUC or high Average precision (AP)





Deep-learning

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



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

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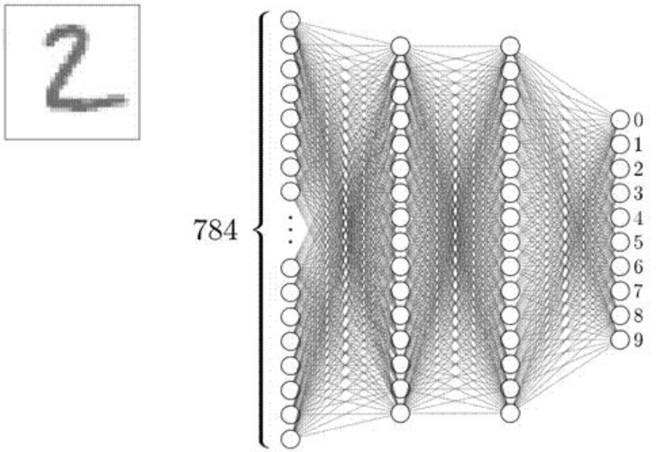

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- What are the challenges?
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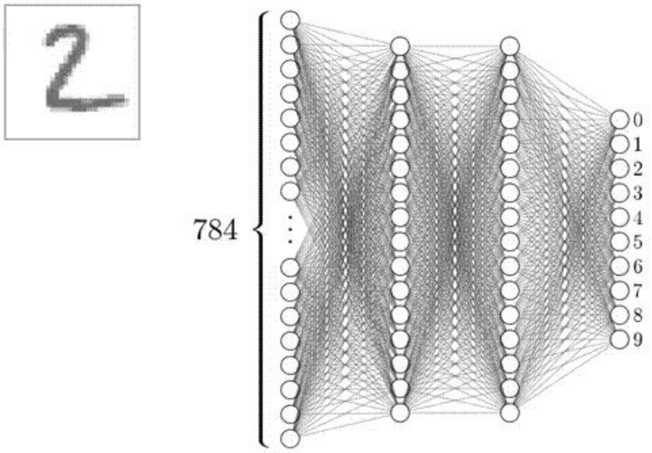
- When do I use it?
  - If you have highly-structured input, eg. medical images.
  - You have a lot of data and computational resources.



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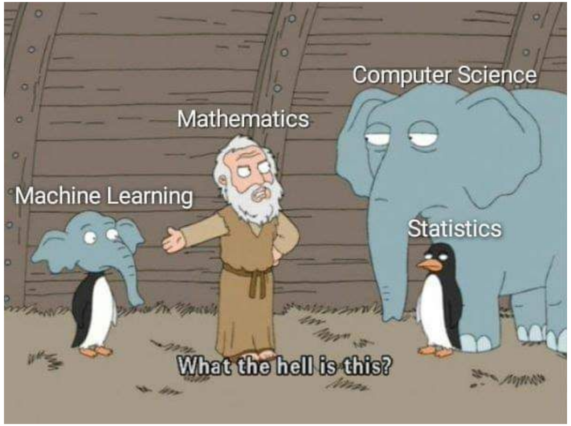
Pitfalls and Challenges

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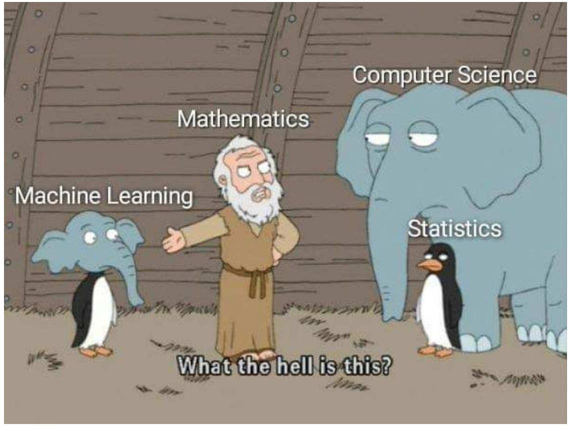
- Unnecessary complexity
  - Do I really need a giant deep-net or a simple linear model would do?



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?

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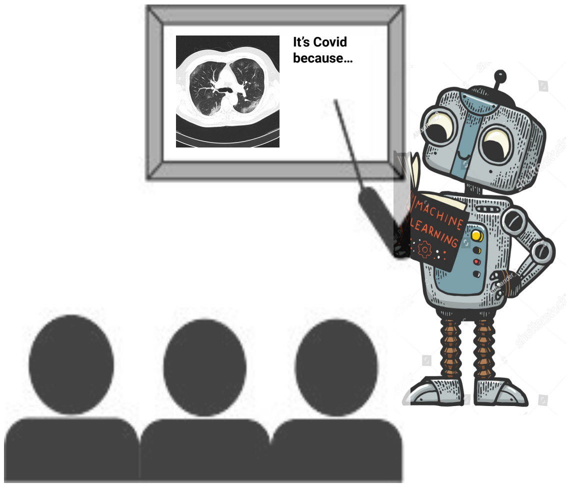
- Model
  - Do my performance metrics capture the practical use-case of interest?
  - What is the null / dummy model performance?
    - Classification: Predict majority class all the time
    - Regression: Predict the median value all the time
  - Am I interpreting model parameters (i.e. weights) correctly?

Takeaways

- Supervised models are useful for **predictions**
  - eg. image segmentation, prognosis, drug development
- Our job is to ensure **generalizability** of these models
  - Multitude of validations
  - Understanding model biases and limitations
- Food for thought: ***engineering tools*** vs *scientific discovery*
  - Interpretability and explainability
  - Causality, reliability, fairness



Explainable AI