An Introduction To Machine Learning

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What is Machine Learning?

- A branch of artificial intelligence (AI)

 Focuses on the use of data and algorithms to imitate the way humans learn, gradually increasing accuracy

- Can be used to learn about the data you have, classify objects, or predict

- ML is basically solving optimization problems

Major Categories of Machine Learning

Supervised: Maps input variables (X) to an output (Y)

Unsupervised: You have inputs (X) but no output (Y)



Supervised Learning: Regression vs. Classification

Regression: Aims to predict a continuous quantity

Classification: Aims to predict the group a member belongs to









Ridge & Lasso

- Extension of Linear Regression
- Places a penalty on less important features

- Ridge Regression: Shrinks coefficients of the unimportant features
- Lasso Regression: Pushes the coefficients of unimportant features to "0"

$$L = \sum (y - \hat{y})^2 + \alpha \sum |m|$$

Sum of Squared Residuals

Classification Models

Logistic Regression

Similar to linear regression (quantitative variables in, quantitative variables out) w/ 2 key differences:

- You want to classify
- You have bound the range of output to between 0 and 1





Example: Predict whether a political candidate will win or lose

Outcome: Win/Lose (binary 0/1)

Inputs: Money spent, time spent campaigning, and poll ratings

Support Vector Machine

- Plots samples to points in space
- Separates classes with a line

-Works well with non-linear as well by changing the kernel



K-Nearest Neighbors

- Plots samples to a point in space
- Counts the neighbors closest to it to determine which class if belongs to

Example:

- For k = 3 Nearest Neighbors, Sample is classified as Class B
- For k = 6 Nearest Neighbors, Sample is classified as Class A



Decision Tree

- Generally, the most important features are those used in the splits

- Upgrades:
 - Random Forest: Builds many independent trees from subsets of data and combines them
 - Boosted Models: Builds a tree, learns what it did "wrong", builds a better one, repeat



Unsupervised Learning

K Means Clustering



Hierarchical Clustering

Components of dendrogram and corresponding data shown on a scatter plot



Hierarchical clustering dendrogram (Ward distance)

Scatter plot of same data with points colored by hierarchical clustering

Principal Component Analysis

Goal: Reduce dimensionality while still keeping most of the information of the original data set

- A Principal Component is a linear combination of all or most of the initial features
- A Principal Component is much less interpretable than original features



Deep Learning

Output: solute-transport parameters

What is Deep Learning

- Can perform supervised or unsupervised learning
- Formed of interconnected neurons grouped into 3 layers:
 - Input Layer: Receives input data
 - Hidden Layer: Performs mathematical computations on inputs
 - "Deep" refers to having more than one hidden layer
 - Output Layer: Returns the result
 - Each layer transforms the data, determining its features



Commonly Used Neural Network Types



Recurrent Neural Networks





Model Building & Performance

The Machine Learning Process



Training and Testing Sets

Training Set: Used to develop model

Test Set: Used to test the models accuracy





Cross Validation

- Allows us to train and test/validate on all our data
- Gets more metrics: 92.0, **44.0**, 91.5, and 92.5
- Aids in parameter tuning



Regression Model Accuracy

- 1) Mean Squared Error (MSE) punishes models with larger errors
 - If you are accustomed to seeing an R² value, this is simply the standardized version of MSE
- Root Mean Squared Error (RMSE) more understandable (dollars vs dollars squared)
- Mean Absolute Error (MAE) Easy to understand; units are interpretable and error is linear
- 3) Adjusted R², AIC, BIC, Mallows Cp
 - a) More robust
 - Adding features will always decrease RMSE and increase R²
 - b) All unbiased estimates of the MSE

Classification Model Accuracy

Precision: Out of all the positives predicted, how many are actually positive

Recall/Sensitivity: How good a test is at actually detecting positive cases

Specificity: Out of all the people that don't have the disease, how many got negative results

		Ground truth		
		+	-	
Predicted	+	True positive (TP)	False positive (FP)	Precision = TP / (TP + FP)
	-	False negative (FN)	True negative (TN)	
		Recall = TP / (TP + FN)		Accuracy = (TP + TN) / (TP + FP + TN + FN)

What if your data is very unbalanced?

AUC: Area Under Receiver Operating Curve (ROC)

TPR (sensitivity) =
$$\frac{TP}{TP + FN}$$

FPR (1-specificity) = $\frac{FP}{TN + FP}$



The Bias/Variance Tradeoff

Variance: the variability of model prediction, i.e. how much the model will change if we change the training data set

High Variance = Very complex model

Bias: the difference between the average prediction of our model and the correct value we are trying to predict

High bias = oversimplified model



Bias Variance Plot



Image from http://scott.fortmann-roe.com/docs/BiasVariance.html

The End :)