Computational Social Science

Supervised Machine Learning

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Plan

1. Course updates
2. Introduction to machine learning
3. Model evaluation
4. Classification algorithms

Course updates

Homework

- Homework 3 due Thursday at 5pm
  - Link on Canvas
  - Clone repository via Github
  - Submit on Github & Canvas

Course updates

Projects

- Feedback shared on Canvas last week
  - Start working on data collection as soon as possible
- Prototype due 11/20, submission via Canvas
  - A minimal working version of the app
- In-class project workshops
  - 11/10 (virtual), 11/20, and 12/4

Roadmap

Topics in machine learning

1. Introduction to supervised machine learning
2. Supervised text classification
3. Large language models
4. Computer vision
5. Generative artificial intelligence

Introduction to machine learning

What is machine learning?

- Machine learning is a method to "automate discovery from data" (Molina and Garip 2019)
- An approach that draws upon statistical methodology and computer science
- Often referred to as "artificial intelligence," particularly over the past two years

Introduction to machine learning

Two cultures of statistical modeling

- Consider the following linear model:

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x + u$$

- $\hat{Y}$ (pronounced, "Y-hat") is a predicted outcome (e.g probability of college attendance)
- $\hat{\beta}_0$ and $\hat{\beta}_1$ are *coefficients*.
  - $\hat{\beta}_0$ is the *intercept*.
  - $\hat{\beta}_1$ captures the effect of a predictor variable x on the outcome.
- u is the error-term and accounts for unexplained variation in the outcome.

Introduction to machine learning

Two cultures of statistical modeling

- Social scientists are typically interested in the $\hat{\beta}$ given Y, i.e. the estimated effect of the variable x
- Computer scientists are more interested in how well the model predicts $\hat{Y}$, paying less attention to the estimated coefficients.
- Given these different cultures. What can social scientists learn by constructing models optimized to predict Y?

Prediction vs. explanation

- Predictive models are specified differently to explanatory ones
  - In a regression context, we might use theory to guide the selection of a handful of *variables* to appropriately estimate $\hat{\beta}$.
  - In a predictive context, we want to find the function $f(X)$, such that $Y = f(X)$. This often involves many more variables and a more complex functional form.
    - Variables in the ML context are referred to as *features*.

Introduction to machine learning

Supervised and unsupervised learning

- *Supervised machine learning*
  - We observe an output Y for each input X.
  - The goal is to learn a function to predict Y given X, $Y = f(X)$
  - Often SML is used for *classification* problems, where the objective is to classify the observed data into discrete classes
    - The learning is "supervised" because we have this information
- *Unsupervised machine learning*
  - We only observe X, but there no "correct" answer Y
  - The goal is typically to partition X into a set of classes, but the classes are not known in advance
    - Topic modeling is an example of an unsupervised learning algorithm

Introduction to machine learning

Why predict?

- Policy interventions
  - e.g. Which households would benefit most from lead abatement?
- Document classification
  - e.g. Which tweets should be flagged as hate speech?
- Record linkage and data imputation
  - e.g. Which records in a database correspond to the same person?
- Causal inference
  - e.g. How does the effect of a policy vary across groups?

Introduction to machine learning

Data splitting and model training

- In supervised machine learning, we generally split our data into two groups, *training* and *testing*
- The *training* data is used to train a model or to estimate $Y = f(X)$.
  - The model uses data matrix X to predict a *known* Y.
- The *testing* data is used to chose and evaluate a model. This is also referred to as *held-out* or *out-of-sample* data.
  - We take our trained model and predict $\hat{Y}$ for the test examples.
  - We then compare $\hat{Y}$ to Y to assess predictive accuracy.

Introduction to machine learning

Vignette: Explanatory paradigm

- Let's say we want to predict a college-attendance given information about their early childhood.
- Someone working in the explanatory framework would be to construct some regression model to predict

$$Y_{college} = \hat{\beta}_0 + \hat{\beta_{1:K}} X_{1:K} + \epsilon$$

  using K predictor variables, each carefully selected based on social scientific theory.
- Assuming the model is appropriately specified, we might want to make the following kinds of inferences:
  - e.g "Mother's level of education is a positive predictor of college attendance. A one-year increase in mother's education is associated with a 3% increase in the probability of college attendance ($p < 0.05$)."

Introduction to machine learning

Vignette: Predictive paradigm

- Now consider a predictive version of this model. Here the goal is to develop the best possible prediction of $Y_{college}$.
- We estimate a model using our training data,

$$Y_{college_{train}} = \hat{\beta}_0 + \hat{\beta_{1:M}} X_{1:M} + \epsilon$$

  - Unlike the previous model, we will include a large set of M predictor variables, where $M >> K$.
- We then use this model to predict $\hat{Y}_{college_{test}}$ and compare the predictions to the known values, $Y_{college_{test}}$.
- Finally, we make a statement about the accuracy of our model.
  - e.g. "The model predicted out-of-sample college attendance with 85% accuracy."

Introduction to machine learning

Explanatory models $\neq$ predictive models

- Economists Mullainathan and Spiess (2017) evaluate the relationship between predictive and explanatory models. In an ideal world, we might want to have a model optimized for predicting Y hats and Beta hat's.
- Explanatory models often have low-predictive power. But can predictive models be produce useful explanations?

See Mullainathan, Sendhil, and Jann Spiess. 2017. "Machine Learning: An Applied Econometric Approach." Journal of Economic Perspectives 31 (2): 87–106.

Introduction to machine learning

Explanatory models $\neq$ predictive models

- "The very appeal of these algorithms is that they can fit many different functions. But this creates an Achilles' heel: more functions mean a greater chance that two functions with very different coefficients can produce similar prediction quality" (Mullainathan and Spiess 2017: 97–98).
- In short, there might be many different subsets of a dataset that produce equally good predictions. This makes it hard to develop a coherent explanation based on a predictive model.

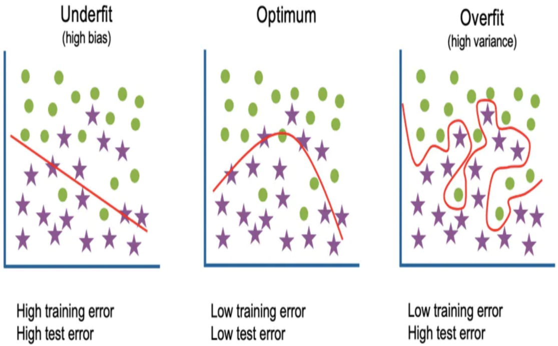
Model evaluation

Underfitting and overfitting

- *Underfitting* occurs when a model poorly fits the data.
  - e.g. A linear model may not capture non-linear relationships between variables.
- *Overfitting* occurs when a model fits random noise in the training data.
  - If a model has overfit then it does not generalize well to unseen data.
  - This tends to be a more serious problem in machine-learning than underfitting since we often have richly parameterized models

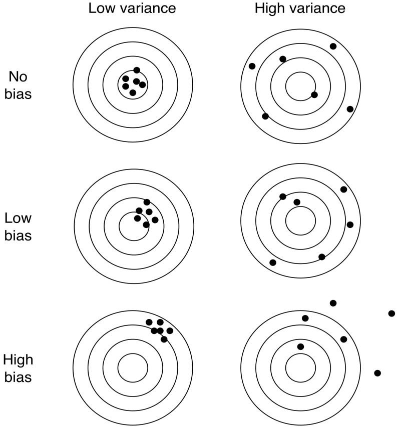
Model evaluation

Underfitting and overfitting



Model evaluation

Bias-variance trade-offs



Salganik 2017. See this website for a visualization of the bias-variance trade-off.

Model evaluation

Out-of-sample validation

- *Out-of-sample validation* is used to directly measure over/underfitting, something generally ignored in explanatory approaches to statistics (Watts 2014).
  - An underfit model will perform poorly both in and out-of-sample
  - An overfit model will perform well in-sample but poorly on unseen data
- The main challenge is to estimate a model that will generalize well to unseen data without learning too much about idiosyncratic variance in the training data

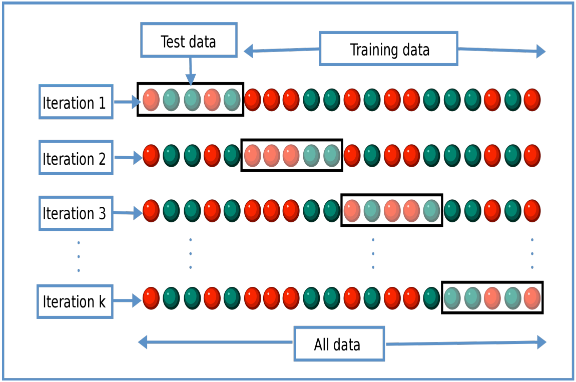
Model evaluation

Cross-validation

- Train-test splits reduce the amount of data available to us, increasing risk of underfitting and potentially making results sensitive to the particular split.
- *Cross-validation* is an approach to split the data into small test-train subsets.
- A popular approach is *k-fold* cross-validation where we split the data into k subsets.
  - We successively train a model of each $k-1$ folds and test it on the k^{th} fold.
  - The results are then averaged across all k folds.

Model evaluation

Cross-validation



Source: Wikipedia.

Model evaluation

Cross-validation

- The extreme is called *leave-one-out* (LOO) cross-validation.'
  - Given N observations, we train N models, each time using $N-1$ data points.
  - This is rarely used on large datasets because it is very computationally expensive, although variations are common in Bayesian statistics.

Model evaluation

Regularization

- Machine learning techniques are often prone to overfitting because the models are complex with many parameters
- *Regularization* is another approach we can use to prevent overfitting.
  - We constrain the parameter space by removing some complexity to try to prevent the model fitting "noise" in the data
- Most machine learning algorithms have regularization procedures

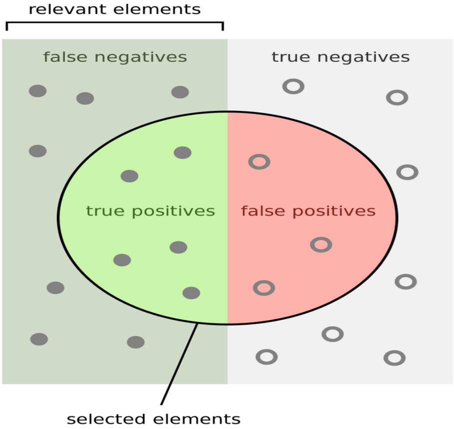
Model evaluation

Metrics: Binary classification

- The following metrics apply to binary classification problems, although many can be generalized to multi-class or continuous outcomes.
- A binary classifier learns a function $f(X)$ to predict Y, where $Y = 1$ or $Y = 0$.
  - Many algorithms return a predicted probability $P(Y|X)$, but some only return a discrete value (1 or 0).

Model evaluation

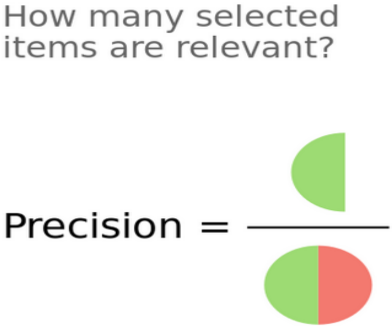
Metrics: TP, FP, TN, FN



Source: Wikipedia.

Model evaluation

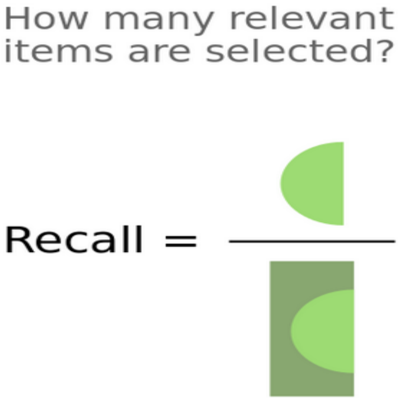
Metrics: Precision (TP/TP+FP)



Source: Wikipedia.

Model evaluation

Metrics: Recall (TP/TP+FN)



Source: Wikipedia.

Model evaluation

Metrics: F1

The F_1 score is the *harmonic mean* of precision and recall and is often used as an overall description of predictive performance for a classifier.

$$F_1 = 2\frac{precision * recall}{precision + recall} = \frac{TP}{TP + \frac{1}{2}(FP + FN)}$$

Model evaluation

Metrics: The confusion matrix

True categories \ Predicted categories	Hate	Offensive	Neither
Hate	0.61	0.31	0.09
Offensive	0.05	0.91	0.04
Neither	0.02	0.03	0.95

Davidson, Thomas, Dana Warmsley, Michael Macy, and Ingmar Weber. 2017. "Automated Hate Speech Detection and the Problem of Offensive Language." In Proceedings of the 11th International Conference on Web and Social Media (ICWSM), 512–15.

Model evaluation

Metrics: Receiver Operating Characteristic (ROC) curve

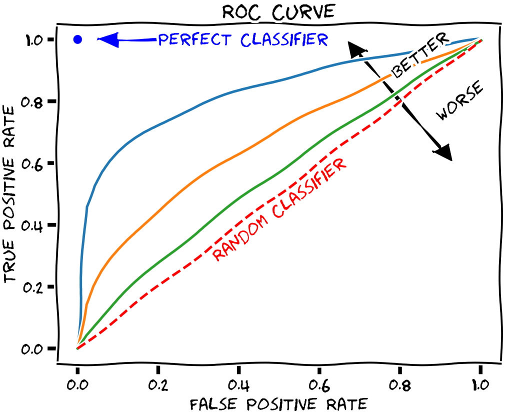
- If an algorithm returns a predicted probability then we must identify a *threshold* for class assignment
- In the binary case,

$$Class(Y) = \begin{cases} 1, & P(\hat{Y}|X) \geq threshold \\ 0, & P(\hat{Y}|X) < threshold \end{cases}$$

- Plot the true positive rate ($TPR = TP/TP + FN$) against false positive rate ($FPR = FP/FP + TN$) for different predicted probability thresholds to identify the optimal value. This is known as the *ROC* curve.
- The area under the ROC curve (*AUC*) provides an overall measure of classifier performance.

Model evaluation

Metrics: Receiver Operating Characteristic (ROC) curve



Source: Wikipedia

Model evaluation

Metrics

- The choice of metric depends on the outcome of interest and what you want to optimize for. Often we might want to use a metric like ROC or F1 to find a compromise.
- Consider a carbon monoxide alarm:

	Alarm	No alarm
CO present	TP	FN
CO absent	FP	TN

- False negatives are really bad and should be avoided at all costs.
- Too many false positives will also be bad, as it may lead people to remove the batteries from the alarm, but a low level will be tolerated.

Classification algorithms*

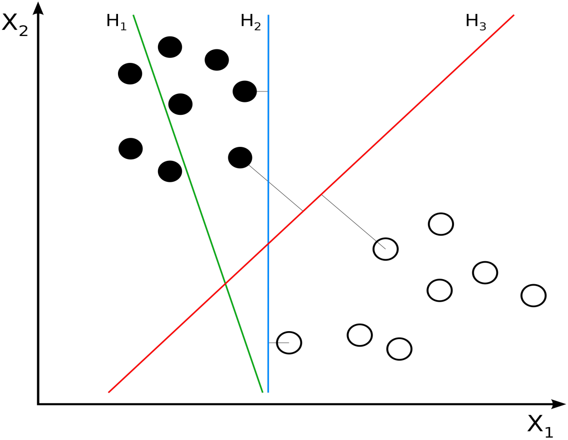
Logistic regression

- Logistic regression is a regression model for binary outcomes (although there is some debate about when we should estimate a standard linear probability model using OLS).
- Uses a logit function to estimate the log-odds of an event ($Y = 1$) given predictors X.
- Multinomial logistic regression can be used if you have a multi-class outcome.
    - e.g. A model predicting level of education.

*Many of these algorithms can also be used for regression problems where the outcome is continuous.

Classification algorithms

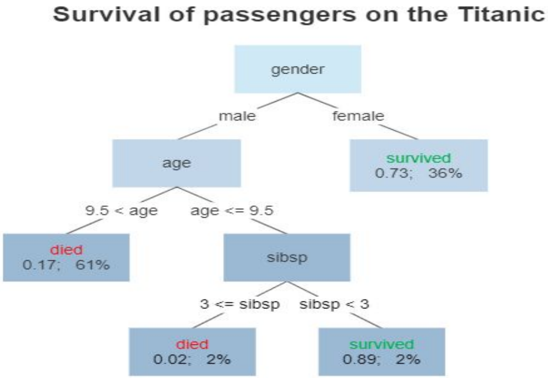
Support Vector Machines



Source: Wikipedia

Classification algorithms

Decision Trees



Source: Wikipedia. See this website for an excellent visual introduction to decision trees.

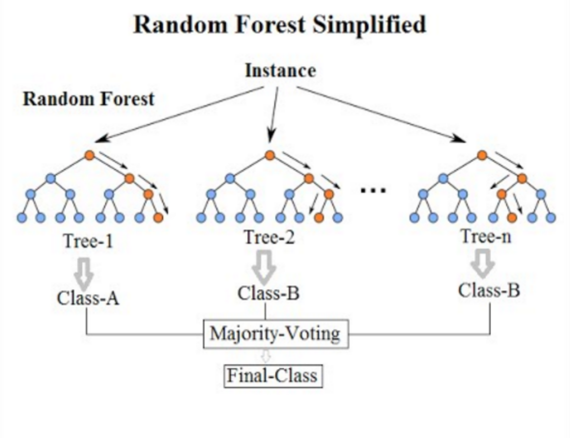
Classification algorithms

Random Forests

- Decision trees tend to overfit the training data
- Solution: Grow lots of trees and average over them
  - Using a procedure called *bootstrap aggregating* or *bagging* for short we can sample from our data and generate a *forest* consisting of many decision trees. This is known as an *ensemble* method because it involves more than one model.
  - The approach is effective because the algorithm randomly splits the data into leaf nodes based on different features, hence it is a *random* forest.
  - The final classification is an average across the different decision trees.

Classification algorithms

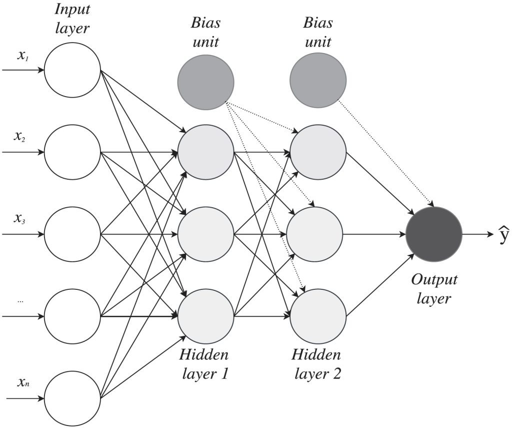
Random Forests



Source: Wikipedia

Classification algorithms

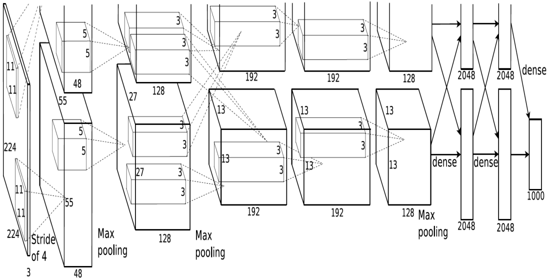
Neural networks



Davidson 2019.

Classification algorithms

Neural networks



Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. 2012. "Imagenet Classification with Deep Convolutional Neural Networks." In Advances in Neural Information Processing Systems, 1097–1105.

Classification algorithms

Hyperparameters

- Each algorithm has hyperparameters that can adjust how it works.
  - e.g. Regularization type for logistic regression and SVM.
  - e.g. Number of trees, tree depth, and splitting criterion for random forest.
  - e.g. Number of layers, activation function, and optimization routine for neural networks.
- Often we want to find the algorithm that best fits the data so we conduct a search over different hyperparameters and compare many different models.
  - In many cases we also want to test the effect of different pre-processing or feature construction steps.

Classification algorithms

Hyperparameter search and computational complexity.

- Davidson (2019) uses neural network models to predict high school GPA.
  - Three model hyperparameters with 40 different combinations
    - Number of hidden layers (depth)
    - Number of neurons per hidden layer (breadth)
    - Activation function
  - Each model is trained using 5-fold cross-validation, resulting in 200 different model fits
- These models took over 12 hours to estimate on a high-end Macbook Pro.

Python code and output is available here.

Classification algorithms

Black-box models and interpretability

- In contrast to standard explanatory models, which are considered to be interpretable, many of these algorithms are described as "black boxes," meaning that we are unable to observe their workings.
- There is a trade-off between model complexity (often associated with better predictions) and human interpretability
  - Watts (2014) argues that it may be worth sacrificing some interpretability in the interest of better predictions.
- But there are lots of developments in the field of ML interpretability

Classification algorithms

Black-box models

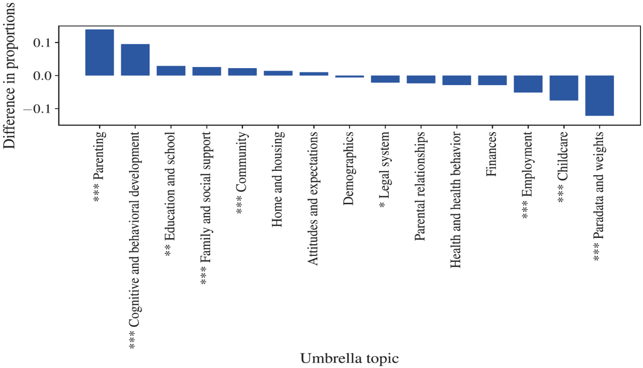
(a) Original Image (b) Explaining *Electric guitar* (c) Explaining *Acoustic guitar* (d) Explaining *Labrador*

Figure 4: Explaining an image classification prediction made by Google's Inception network, highlighting positive pixels. The top 3 classes predicted are "Electric Guitar" ($p = 0.32$)**, "Acoustic guitar"** ($p = 0.24$) **and "Labrador"** ($p = 0.21$)

Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. 2016. "'Why Should I Trust You?': Explaining the Predictions of Any Classifier." In Proceedings of the 22nd ACM SIGKDD, 1135–44. ACM. https://doi.org/10.1145/2939672.2939778.

Classification algorithms

Black-box models



Davidson 2019.

Summary

- Machine learning techniques allow us to "automate discovery from data"
- Supervised and unsupervised ML techniques
- Prediction vs. explanation
- Over and under-fitting
- Regularization
- Common algorithms