Machine Learning

http://datascience.tntlab.org

Module 12

Today's Agenda

- Situating Machine Learning versus Artificial Intelligence and Statistics

- Overview of Statistical Analysis vs. Machine Learning
  - Terminology differences
  - Model selection

- Technical Walkthrough
  - Walkthrough of *caret*
  - Some starter algorithms: tree, random forest, LASSO, ridge
  - Cross-validation and model comparisons

Artificial Intelligence

- AI simply refers to any algorithmic system designed to mimic human functioning
  - **Weak (narrow) AI**: All modern AI systems; mimic individual examples of human activities in a tightly-defined scope
    - Object character recognition
    - Siri/Alexa
    - Video game AI
    - Natural language processing (e.g., Google Translate)
    - Machine learning
  - **Strong (general) AI:** Mimics human thoughts; has consciousness (or something approximating consciousness)
    - *2001: A Space Odyssey*
    - *AI*
    - *Her*
    - Does not currently exist and probably won't for a very long time

Key to Understanding Machine Learning

- You've already learned a lot of these concepts in statistics classes.

- A lot of new terms are used for things you already have words for.
  - "Training dataset" = "dataset"
  - "Train" = "provide data to create a predictive model"

- The key to understanding machine learning is relating it back to what you already know, and extending those ideas where concepts are genuinely new

You May Already Be Using Machine Learning

- Have you created an **OLS linear regression model**?
  - Congrats; you're a data scientist!
  - Although OLS regression isn't necessarily machine learning, it can be solved with machine learning methods.

Statistical Analysis vs. Machine Learning

- **Statistical Analysis**
  - Focus on coefficient interpretability
  - Emphasis on assumption checking (i.e., integrity of mathematical approach)
  - "Given this theoretical model, how well do the data describe y?"
  - **Goal:** Draw conclusions about predictors

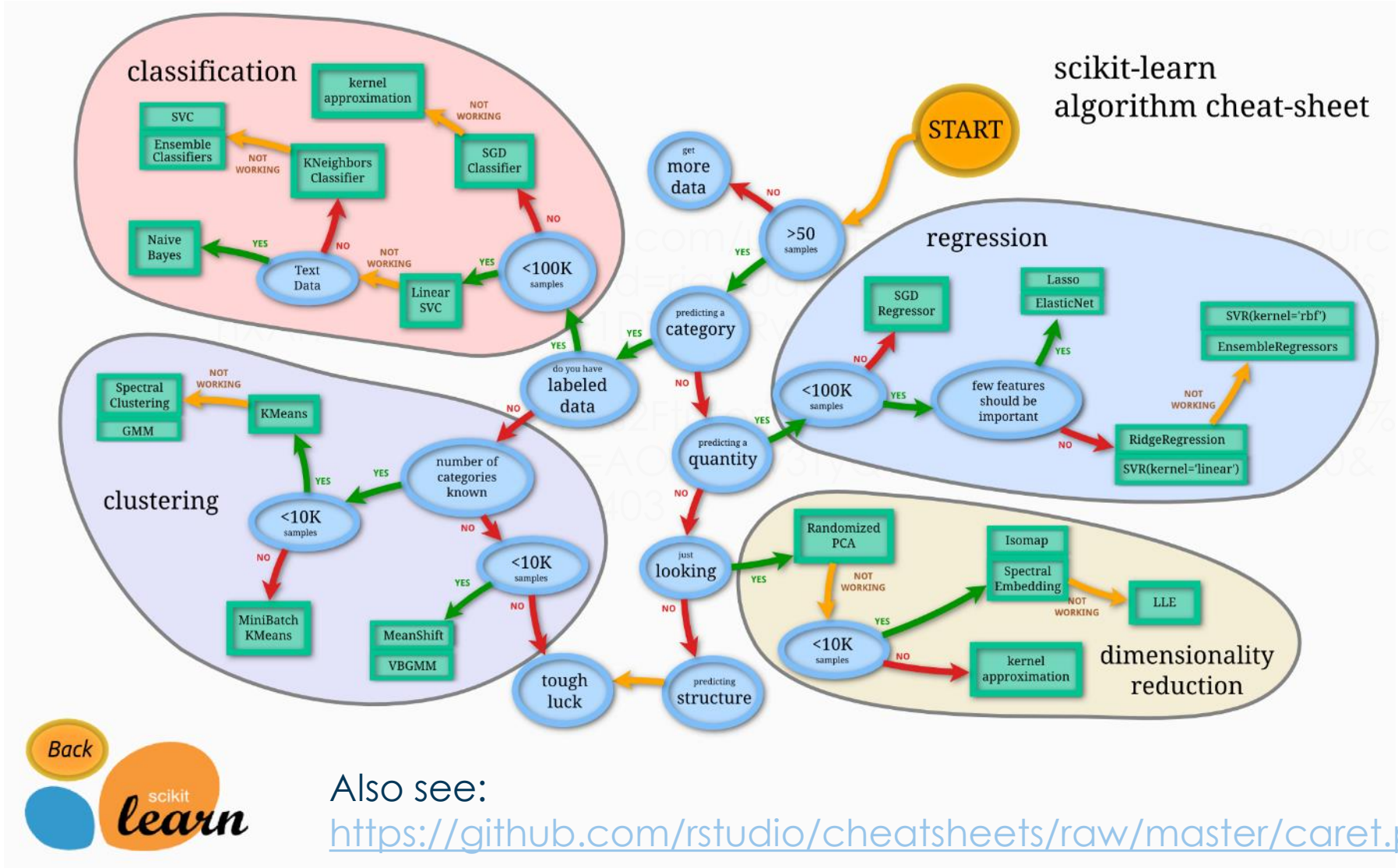
- **Machine Learning**
  - Focus on generalizable prediction
  - Intention to take an algorithm developed in one context and use it in another
  - "Given these data, what algorithm will predict y most consistently in other datasets with similar generative characteristics?"
  - **Goal:** Predict as strongly as possible equally well in the future

- *You will see many of the same predictive modeling techniques in both.*

Types of Machine Learning (by Process)

- **Supervised Learning** (the focus in Data Camp)
  - Regression models: continuous DVs
  - Classification models: discrete DVs
  - Decision tree models (e.g., random forests)
- **Unsupervised Learning**
  - Principle components analysis
  - K-Means clustering (which you might already know)
  - Gaussian mixture modeling
- **Semi-supervised Learning**
- **Reinforcement Learning**

Classic Machine Learning Model Cheat Sheet



Also see:
https://github.com/rstudio/cheatsheets/raw/master/caret.pdf

Problems Supervised Machine Learning Solves

- When you have many predictors, overall effect estimates like R^2 will be inflated
- In psychology, we usually use adjusted-R^2 to account for this
  - Predicts the amount of shrinkage in R^2 likely to be seen due to local overfitting
  - Adjusted-R^2 is ultimately a guess

- Machine learning is designed to better predict "true" variance despite the noise created by a complex predictor space

- If *N* is orders of magnitude larger than *k*, machine learning probably won't get you much better prediction

Problems Supervised Machine Learning Creates

- There are many ways to model the relationship between y and a set of x
  - Researcher degrees of freedom
    - Model selection: linear regression, random forest, support vector machines, etc.
    - Parameter selection: variable selection (ntbcw: parameter estimation)
    - Hyperparameter selection: configuration options for the model
  - Model selection itself might be considered a hyperparameter; existing statistical decision-making is a type of hyperparameter too
  - Most models are optimized to a *loss (cost) function*
  - Hyperparameters can themselves be optimized

- If you're trying to eek out every last bit of true variance, regardless of where it comes from, you're going to need to get creative
  - Comes with a distinct interpretability vs. prediction tradeoff

- Every one of these algorithms has a literature at least as if not more complex than the full courses you've taken on ANOVA or regression

Bias-Variance Tradeoff

- Increased bias in parameter estimation = decreased variance in estimates across samples

- In statistical approaches, we see decreased/increased; e.g., because bias = 0 with OLS regression, we maximize variance in R^2 out-of-sample
- In many predictive models used in machine learning, we **sacrifice bias** to achieve greater consistency in the predictive accuracy of final models
  - This renders individual coefficients less interpretable
  - Fully accepting this tradeoff means giving up interpretability altogether
  - If you give up interpretability altogether, you have even greater freedom to model high-complexity sets of predictors

- Example
  - **computer vision**: Predicting outcomes from videos/pictures

Linear Regression as Machine Learning

- You probably learned 1-predictor OLS linear regression as the solution to a mathematical formula

$$Y' = b_{yx}X + a_{yx}$$

$$b_{yx} = r_{xy}\frac{\sigma_y}{\sigma_x} = \frac{N\sum XY - (\sum X \sum Y)}{N\sum X^2 - (\sum X)^2}$$

$$a_{yx} = \overline{Y} - b_{yx}\overline{X}$$

- But what if you didn't know the formulas? What would you do?
  1. Guess the value of *b*, predict your data, and look at the mean squared residual
  2. Change *b* in one direction, predict again, and see if MSR changed
  3. If it went down, change *b* further that way; if it didn't, go the other way
  4. Repeat until you can't get MSR any smaller
- In machine learning terms, we call the MSR for regression the "cost function"
  - Iterative procedure to find a minimum cost called *stochastic gradient descent*

Why Use *caret*?

- What is *caret*?
  - Does not actually contain any machine learning algorithms
  - Provides a common framework/syntax to access many other packages that do contain machine learning algorithms
  - Centralizes approach to hyperparameter tuning across algorithms
  - Automates mathematical modeling that you'd normally need to do by hand (by code)

- You need to know how to use those packages to use their functions in *caret;* each one is slightly different

Supervised Learning with *caret*

- Basic Regression
  - **model <- train(**
    formula,
    data,
    method="lm",
    preProcess=c("center","scale","zv"),
    trControl=trainControl(method="cv", number=10, verboseIter = T)
)
- Basic Classification
  - **model <- train(**
    formula,
    data,
    method="glmnet",
    preProcess=c("center","scale","zv","conditionalX"),
    trControl=trainControl(method="cv", number=10, verboseIter = T,
    summaryFunction = twoClassSummary, classProbs = T)
)

Pre-Processing: Missing Values

- Add **preProcess = c()** to *caret* syntax

- A reminder about missing values
  - NMAR: Not missing at random
  - MAR: Missing at random
  - MCAR: Missing completely at random

- Imputation of missing values
  - **Median imputation:** Assumes MCAR, so just don't
  - **K-nearest neighbors:** Assumes MAR, so use if you're comfortable with that

Pre-Processing Options

- Centering and standardizing
  - **preProcess = c("center", "scale")**
- Box-Cox transformation for non-linearity
  - **preProcess = "boxcox"**
- Listwise deletion of non-varying predictors
  - **preProcess = "zv"** # or nearly zero with "nzv"
- Run a PCA and use components as predictors instead
  - **preProcess = "pca"**
- Remove highly correlated pairs of variables (by default, > .9)
  - **preProcess = "corr'**
- In classification, remove predictors if there is no variance within a class
  - **preProcess = "conditionalX"**

Machine Learning Models and Their Hyperparameters

- To add hyperparameters to *caret*, add
  - **tuneLength=3** # number of levels for default tuning parameter
  - **tuneGrid=expand.grid()** # change many tuning parameters

- **method="ranger"** # random forests
  - **tuneLength = 10** # changes mtry, which you could set by hand
- **method="glmnet"** # ridge and LASSO regression
  - **myGrid <- expand.grid(alpha = c(0,1),** # 0 = LASSO, 1 = ridge
    lambda = seq(0.0001, 0.1, length = 10)) # complexity penalties

- Find a full list of methods with **names(getModelInfo())**
- Find explanations at http://topepo.github.io/caret/train-models-by-tag.html including permitted hyperparamters

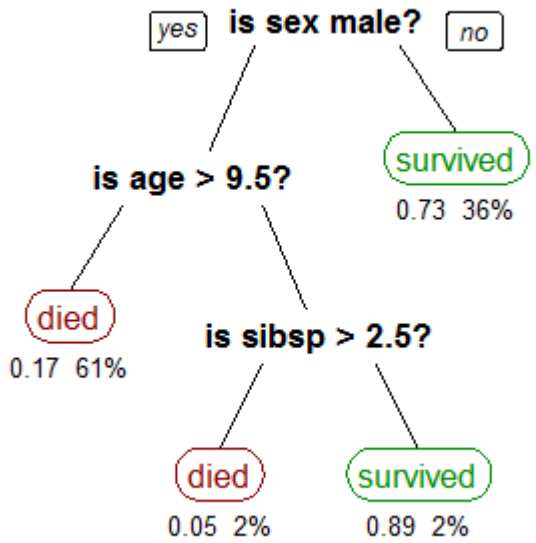
Machine Learning: Decision Trees

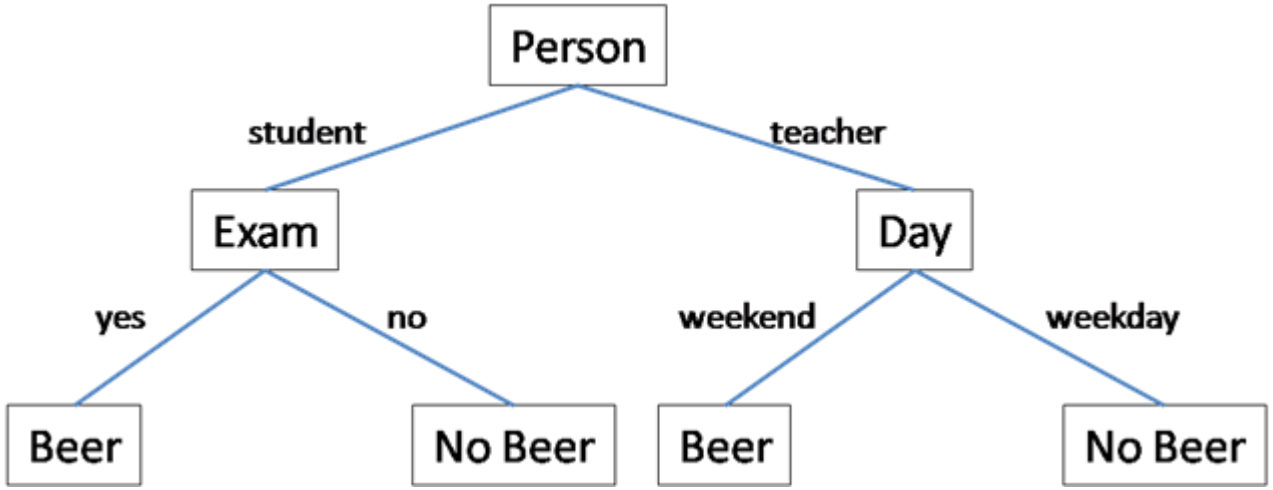
- Can be regression trees or classification trees

- A very simple classification tree roughly works like this:
  - Look at y and each x to see which creates the two most homogeneous groups
  - This becomes the *root node*
  - For each classification created by the root node, repeat homogeneity test
    - If you get better overall prediction with the new classification, create a *split*
    - If you don't, stop following this path (i.e., this is a *leaf*)
  - Continue this process (recursively) until you hit a *stopping rule*, such as too little additional variance predicted
  - Refine the model by *pruning*, which removes leaves that don't contribute much to overall prediction

- Regression trees work similarly, but creating groups is more complex

Machine Learning: Decision Trees

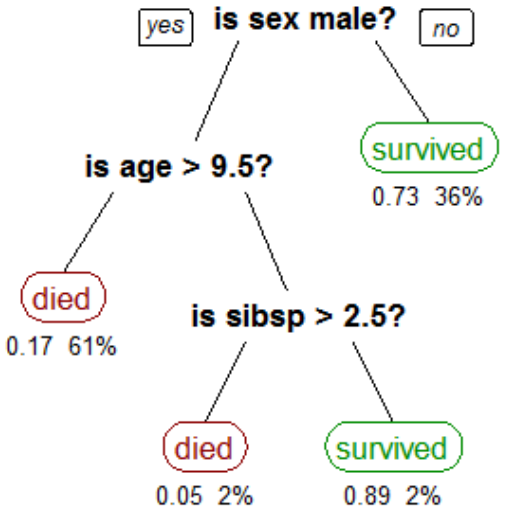




From https://towardsdatascience.com/decision-trees-in-machine-learning-641b9c4e8052
and https://computersciencesource.files.wordpress.com/2010/01/detresb.png

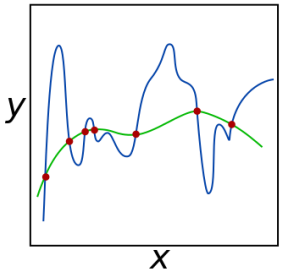
Machine Learning: Random Forests

- Many decision trees; select models from random subsets of predictors to minimize the chance of overly influential cases (and thus overfitting)
- Because they involve later predictors conditional on earlier predictors, they by definition model interactions without explicit interaction terms
- Here, see an interaction between sibsp and age and sex plus their main effects
- Thus, transformations are less important here too
- Ultimately they use an "ensemble method" to combine trees; in this case, the mode



Machine Learning: LASSO/Ridge Regression

- LASSO and ridge combine automated predictor selection with regression
  - In ML, the goal is to minimize the results of the "cost" function
    - Remember: in lm, this is the residual mean square
    - In LASSO and ridge, this is the residual mean square plus a bias term
    - Gradient descent is used to create parameter estimates



  - LASSO performs "L1 regularization," in which the bias term = the sum of lambda * the absolute values of the parameters, which can force zeros
  - Ridge performs "L2 regularization," in which the bias term = the sum of lambda * the squared parameters, which makes all parameters shrink
  - Elastic-net performs "L1/L2 regularization", i.e., lambda * the sum of both L1 & L2

- Hyperparameters
  - **alpha**: the balance between LASSO and ridge
  - **lambda**: the cost function used to either drop (LASSO) or down-weight (ridge) predictors
  - The power of ML comes from testing combinations of hyperparameters

Cost Function Changes Between OLS/Ridge/LASSO

- OLS regression

$$\text{Cost} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

- Ridge regression (also called L2 regularization)

$$\text{Cost} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{k} b_j^2$$

- LASSO regression (also called L1 regularization)

$$\text{Cost} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{k} |b_j|$$

Examples of Cost Functions

- Ridge regression (L2 regularization)

$$\text{Cost} = \sum_{i=1}^{N}(y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{k} b_j^2$$

- LASSO regression (L1 regularization)

$$\text{Cost} = \sum_{i=1}^{N}(y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{k} |b_j|$$

- Elastic Net (L1/L2 regularization)

$$\text{Cost} = \sum_{i=1}^{N}(y_i - \hat{y_i})^2 + (1-\alpha)\left(\lambda \sum_{j=1}^{k} b_j^2\right) + \alpha\left(\lambda \sum_{j=1}^{k} |b_j|\right)$$

Holdout vs. Cross Validation

- Validation does not tell you which model to choose; it gives you a generalizability estimate assuming consistent data generation.

- Holdout Validation
  - Randomly select some subset of data to use for model training (fitting) and testing (predicting). Accuracy is determined by comparing trained predictions and test values.

- k-fold Cross Validation
  - Randomly split the dataset into k datasets (folds) randomly which will be used as both training and test datasets. Each fold is used as a test set with all other folds as training sets. Generalizability is determined by examining summary statistics of prediction across folds.

Quantifying Accuracy

- Regression
  - R^2 is easy and universal; just ask for model output (or plot)

- Classification
  - **Confusion matrices:** Like Type I and Type II errors at the case level
    - **confusionMatrix(predicted, true)**
    - Accuracy: Proportion of correct predictions
    - Sensitivity: Proportion of positive predictions out of all true positives
    - Specificity: Proportion of negative predictions out of all true negatives
  - **Receiving operating characteristic (ROC) curve**
    - **colAUC(X=predicted, y=actual, plotROC=TRUE)** from *caTools*
    - Area under the curve (AUC) ranges from 0 to 1 (ratio of Sensititiy to 1-Specificity)

- *caret* will generally select the best-performing hyperparameters for you through k-fold, but you should know where they came from and what they do

Comparing Models

- If using n-fold cross validation, keep your fold composition the same within trControl
  - Inside a unique **trainControl()** definition that you run one time**:**
    - **index = createFolds(*outcomevar*, k = 10)**

- Use **resamples()** to compare output directly
  - **summary(resamples(list(model1, model2)))**

- Use plots to look at difference in AUC across models
  - **dotplot(resamples(list(model1, model2)), metric="ROC")**

Want to Practice Building Predictive Models?

- Many datasets to practice on here: http://archive.ics.uci.edu/ml/index.php

- Enter competitions on your ability to build high-quality predictive models here: http://www.kaggle.com
  - These competitions do not test your ability to use such models in a production environment, i.e., the real world