Today’s Agenda

- How You’re Already Using Machine Learning Models

- 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
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 Are Already Using Machine Learning

- Have you create an OLS linear regression model?
  - Congrats; you're a data scientist.

- You may have also used more advanced machine learning algorithms without realizing it.
  - **EM imputation**
    - Utilizes an expectation-maximization algorithm to predict missing data.
Statistical Analysis vs. Machine Learning

- **Statistical Analysis**
  - Focus on interpretability
  - Assumption checking (i.e., integrity of mathematical approach)
  - Interpretability of component parts/predictors
  - "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
  - Neural networks

- **Semi-supervised Learning**

- **Unsupervised Learning**
  - K-Means clustering (which you might already know)

- **Reinforcement Learning**
Classic Machine Learning Model Cheat Sheet

Also see:
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.
- However, adjusted-$R^2$ will always reveal relatively poor prediction; sometimes extremely poor, and always poorer with more predictors.

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 $k$, you probably don't need machine learning (or rather, it won't get you much better prediction anyway).
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
- Most models are optimized to a loss function; hyperparameters
- 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.
You probably learned 1-predictor OLS linear regression as the solution to a mathematical formula

\[
Y' = b_{yx}X + a_{yx}
\]

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

\[
a_{yx} = \bar{Y} - b_{yx} \overline{X}
\]

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 tuning of hyperparameters 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

```r
model <- train(
  formula, data,
  method="lm",
  preProcess=c("center","scale","zv"),
  trControl=trainControl(method="cv", number=10, verboseIter = T)
)
```

### Basic Classification

```r
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 = ""` 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), lambda = seq(0.0001, 0.1, length = 10))` # 0 = LASSO, 1 = ridge
    # complexity penalties

- Find a full list of methods with `names(getModellInfo())`
Machine Learning: Decision Trees

- Can be regression trees or classification trees (in general: CART)

- 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](https://towardsdatascience.com/decision-trees-in-machine-learning-641b9c4e8052) and [https://computersciencesource.files.wordpress.com/2010/01/detresb.png](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
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
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. Accuracy is determined by comparing
  - 2-fold cross validation is not the same as holdout validation – why?
  - N-fold cross validation is also called leave-one-out cross validation
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 Sensitivity to 1-Specificity)

- caret will generally select the best-performing hyperparameters for you, 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?


- 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