QSS20: Modern Statistical Computing

Unit 11: Supervised Machine Learning, Part I (Intro and regularization)

Goals for this week

Today: Introduction to supervised machine learning

- Recap of Twitter API
- Lecture on basics of supervised ML
- Walkthrough of supervised ML in Python
- Activity on basic ML

Wednesday: Decision Trees and optimizing supervised ML models

- Recap of basic supervised ML
- Lecture on Decision Trees & optimization
- Activity on DTs & optimization

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Recap of Twitter API

What do you remember?

Recap of Twitter API

Tips:

- Twitter API much cleaner than scraping, but limited to 100 results per query and last week for recent convo (unless you request more access)
- To access Twitter, you need credentials—namely, an API key
- Wrappers like `tweepy` (pronounce how you like) let you input specific parameters instead of constructing a behemoth URL for an API call
- Three things you can track using Twitter API:
    - Topics of convo & contributors using hashtags or `conversation_id`
    - Networks of users that follow each other
    - Specific users: their posts and engagement (e.g., likes, followers)

Useful commands:

```
client = tweepy.Client(bearer_token=creds['twitter_api']['bearer_token'])
        # access credentials with my_creds.yaml
tweet_resp = client.search_recent_tweets(query =  hashtag, etc.) # call API
tweet_data = tweet_resp.data # not .json() as with NAEP/Yelp
account_id = client.get_id(username) # get account id
followers = client.get_users_followers(id = account_id, etc.) # get followers
tweets = client.get_users_tweets(id = account_id.data['id'], etc.)
        # get recent tweets by account
```

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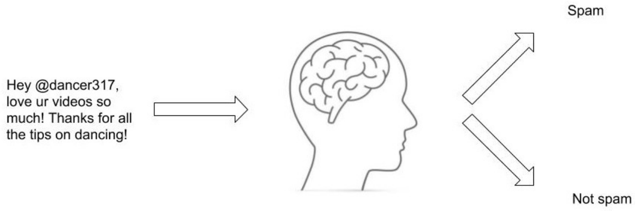
Example of supervised ML: classifying spam emails

Which of these are spam, and which aren't? What do you notice that can help make this distinction?

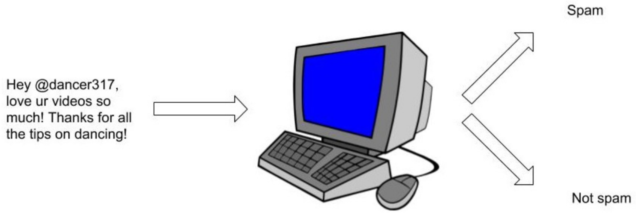
- *Hey @dancer317, love ur videos so much! Thanks for all the tips on dancing!*
- *OUR LASER PRINTER/FAX/COPIER TONER CARTRIDGE PRICES NOW AS LOW AS 39 DOLLARS. SPECIALS WEEKLY ON ALL LASER PRINTER SUPPLIES. WE CARRY MOST ALL LASER PRINTER CARTRIDGES, FAX SUPPLIES AND COPIER TONERS AT WAREHOUSE PRICES*
- *I'm not sold on your first point about crossing national boundaries, but I see what you mean about non-economic alternatives.*
- *Some of the most beautiful women in the world bare it all for you. Denise Richards, Britney Spears, Jessica Simpson, and many more. CLICK HERE FOR NUDE CELEBS*

Example of supervised ML: classifying spam emails

What you just learned to do is text classification!


Hey @dancer317, love ur videos so much! Thanks for all the tips on dancing!
Spam
Not spam

We want our machines to learn to do this, like so:


Hey @dancer317, love ur videos so much! Thanks for all the tips on dancing!
Spam
Not spam

Graphics source

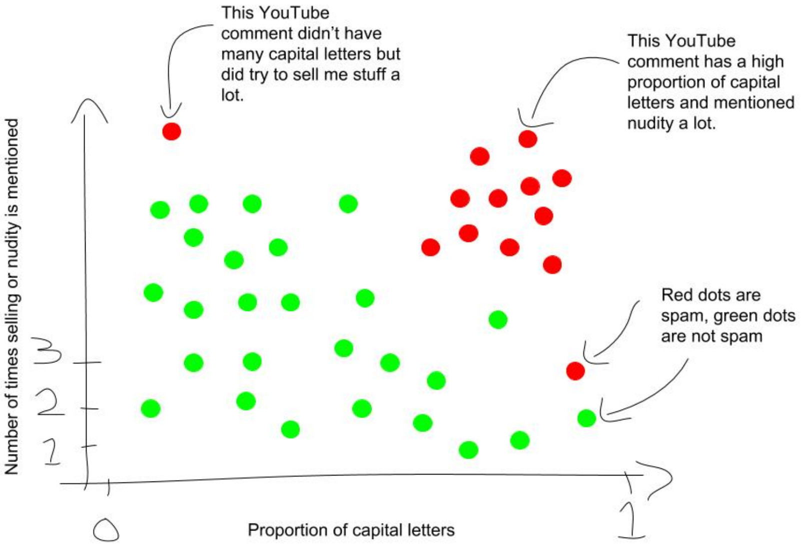
Example of supervised ML: classifying spam emails

How our machines see the data:

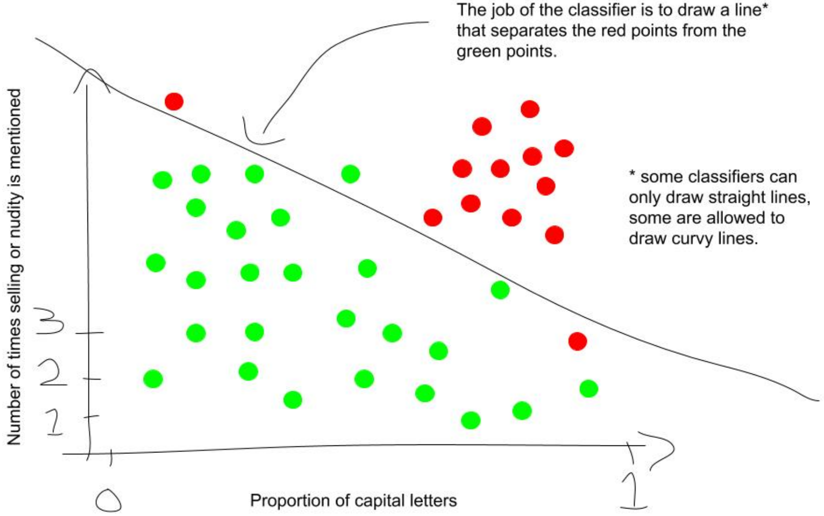
Comment	Selling or nudity	Proportion capital letters	Is it spam?
Hey @dancer317, love ur videos so much! Thanks for ...	0	0.1	No
OUR LASER PRINTER/FAX/COPIER TONER CARTRIDGE PRICES ...	4	1.0	Yes
I'm not sold on your first point ...	1	0.05	No
Some of the most beautiful women in the world ...	3	0.15	Yes

(1) Whether the comment mentions selling or nudity and (2) the proportion of capital letters here are the *features* we want to train a model to recognize when trying to recognize spam. The last column is our human-judged *label*.

Example cont'd: Plotting our features



Example cont'd: Plotting our features



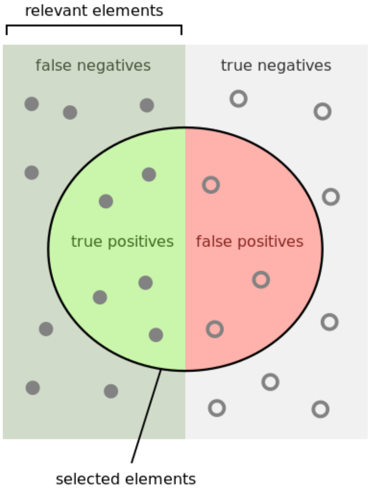
Where has machine learning come up already?

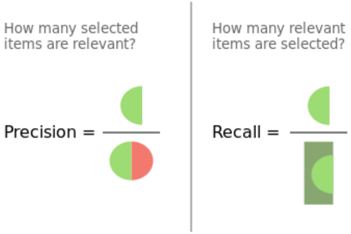
- **Sentiment classification:** `VADER` scores sentiment using a dictionary, but dictionaries work more or less well depending on the context
  - **Solution:** supervised machine learning where we:
    1. Take data labeled with positive/negative sentiment (binary) or sentiment score (continuous)
    2. Create a document-term matrix
    3. Predict sentiment using the terms as predictors
    4. Use that to score the sentiment of unlabeled data
- **Topic modeling:** LDA is a form of unsupervised machine learning that takes an unlabeled input—a document-term matrix—and returns high probability topics and words
- **Record linkage:** k-means is a form of unsupervised machine learning where we feed the algorithm a vector of 1/0 reflecting a pair's matches or not on different fuzzy variables and we cluster the pairs into "likely match" and "likely not match"

What is ‘supervised machine learning?’: Introductory terminology

- **Supervised machine learning:** Building a model to infer classifications based on features. Learning a function that maps features to outputs.
- **Unsupervised versus supervised learning:** unsupervised learning is a form of dimension reduction/clustering on unlabeled data; supervised learning is used for prediction on labeled data
- **Labeled data:** is associated with outcome/result we are interested in, also called the ‘target’ (in CS) or the ‘dependent variable’ (social science). For ex: pos/neg sentiment, spam/not spam, voting yes/no,
- **Features/predictors:** what we use to predict the label, also called ‘covariates’ or ‘independent variables’ (in social science). For images, features are often pixels. For text, features could be word counts or weighted word counts, parts of speech, proportion of capitals, etc.
- **Text vectorization:** Converting natural language documents into numbers that can be fed into a classifier. Usually this means converting a corpus into a document-term matrix (which is?).

Evaluating ML models: precision and recall




How many selected items are relevant?
Precision =
How many relevant items are selected?
Recall =

Graphics source

Evaluating ML models: how to compute metrics

Accuracy:

$$\frac{\sum \text{true positives} + \sum \text{true negatives}}{\sum \text{total population}}$$

Precision:

$$\frac{\sum \text{true positives}}{\sum \text{predicted positives}}$$

Recall::

$$\frac{\sum \text{true positives}}{\sum \text{condition positives}}$$

F1-score:

$$\frac{\sum \text{true positives}}{\sum \text{true positives} + 1/2(\sum \text{false positives} + \sum \text{false negatives})}$$

Evaluating ML: terminology

- **Train-test split:** Dividing labeled data into a training set and a test set. Often done once in supervised machine learning model training, but can be done several times independently as in cross-validation (see Wednesday)
- **Training set:** A selection of labeled data that is used to train the machine learning algorithm
- **Test set:** A selection of labeled data that is used to test the accuracy of the machine learning algorithm
- **Loss function:** Machine learning models seek to minimize this function, which measures model effectiveness at estimating the relationship between an input (features) and output variable/label. This is typically expressed as a difference between the predicted value and the actual value.
- **Accuracy:** The ratio of true positives and true negatives (the numerator) to the total number of cases (the denominator)
- **Precision:** How close a models' guesses are to the mark; the ratio of true positives to predicted positives
- **Recall:** How many actual positives a model guessed right; the ratio of true positives to condition positives

Why do supervised ML?

- Once we have a good number of labeled texts (say 200-500 cases), can use supervised ML to train a model to predict the labels
- **Two benefits:**
  1. Identifies what features (e.g., words) are most defining of each category
  2. Can scale up almost indefinitely to predict labels for unobserved cases
- **Main goal:** generalization, or a model that predicts the response on novel inputs/new data it hasn't yet seen (e.g., new or future cases)
- **Two main types:**
  1. **Regression**: predict numeric values (not the focus this week)
  2. **Classification:** predict categories
     - **Binary classification:** predict yes/no or True/false category, e.g.: fraudulent or not; experiencing homelessness or not; positive sentiment or not (focus this week)
     - **Multiclass** $>$ 2 categories

Problems with machine learning

Consider a traditional linear or logistic regression with two predictors trying to predict a sentiment label:

$$\text{positive sentiment}_i = \alpha + \beta_1 \times \text{uses word great } (1 = \text{yes})_i + \\ \beta_2 \times \text{uses word terrible } (1 = \text{yes})_i + \epsilon_i$$

What would happen if we tried to scale this to a large corpus of text data? How many terms might we end up including? How might that number compare to the number of observations?

Problems with machine learning

The problem: When a model gets overly complex (e.g., the number of terms modeled exceeds the number of observations), we risk **overfitting** because the model would pick up on language use or other idiosyncratic trends/noise particular to some observed cases but meaningless outside the observed data

For example, if you trained a linear model on reviews of fantasy movies, it might decide that the word 'hilarious' associates with negative reviews while the phrase 'hobbit_feet' indicates a positive review.

Would these words still be meaningful if you used the model you just trained to make predictions on a *broader corpus of movies?*

How to make classification better

- Two tools help us establish robust patterns/avoid overfitting:
  1. More flexible classifiers than ordinary least squares: $y = f(x)$, where f is a function mapping some input (e.g., a document-term matrix) to a label (y); go beyond OLS or generalized linear models (GLM) for the mapping function
     - One way to do this: Regularization to prevent models from overfitting on training data/decrease their sensitivity to noise (by adding a penalty term for model complexity; read more here from scikit-learn or from this blog)
     - Another way: Tree-based methods to learn non-linear relationships (we'll talk about this on Wednesday)
  2. Sample splitting: we estimate/train the model in one random split of the data; we evaluate its performance in a separate split of the data

More about regularization

- **Bias-variance tradeoff:** ordinary least squares (OLS) is guaranteed to minimize `bias` in the coefficients, but at the cost of variance (small changes in the input data can lead to large changes in $\hat{\beta}$)
- **Regularization:** add a penalty term that decreases the complexity of the model by penalizing $\hat{\beta}$ based on distance from zero
- **OLS loss function:**, where *i* indexes an observation and *j* indexes a predictor/covariate:

$$\hat{\beta}_{LS} = \sum_{i=1}^{n}(y_i - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2$$

- **LASSO/L_1 regularization**: absolute value; tends to shrink to zero

$$\hat{\beta}_{Lasso} = \sum_{i=1}^{n}(y_i - \sum_{j=1}^{p} x_{ij}\hat{\beta})^2 + \lambda \sum_{j=1}^{p}|\hat{\beta}_j|$$

- **Ridge/L_2 regularization**: squared; shrinks smaller but less likely towards zero

$$\hat{\beta}_{Ridge} = \sum_{i=1}^{n}(y_i - \sum_{j=1}^{p} x_{ij}\hat{\beta})^2 + \lambda \sum_{j=1}^{p}(\hat{\beta}_j)^2$$

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Four DataCamp chapters

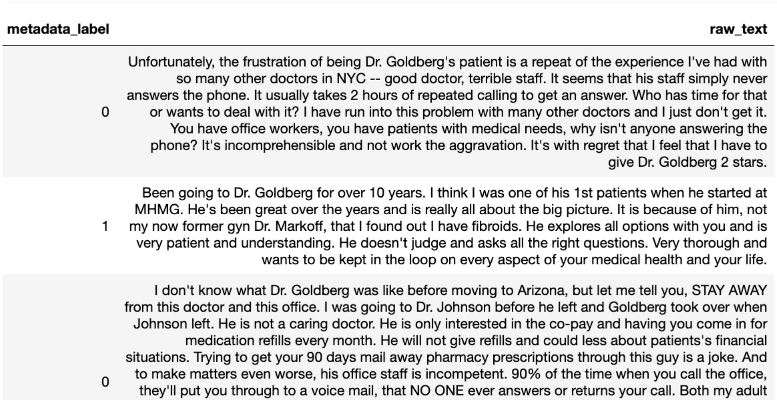
1. **Classification**: uses `k-nearest neighbors`; in activities, we'll shift to other classifiers (ridge; LASSO; Decision Tree; Random Forest)
2. **Regression**: covers K-fold cross-validation and ridge/lasso
3. **Fine-tuning your model:** ROC curve with different $\hat{y}$ thresholds for continuous logistic regression predictions; hyperparameter tuning with `GridSearchCV` and `RandomizedSearchCV`
4. **Preprocessing and pipelines:** transforming categorical features into dummy indicators; imputation; standardizing inputs

DataCamp: pros/cons of their approach

- **What I liked:**
  - Emphasis on importance of preprocessing for model accuracy
  - Start with a model where the hyperparameters (e.g., α/λ in LASSO/ridge) are fixed and move to models where we iterate over a grid of hyperparameters and choose the one that maximizes eval metric
- **What I liked less:**
  - **Reliance on black-box functions**: rather than using functions like `train_test_split` and `score`, personally believe it's better (since we're already black-boxing the algorithms) to do these steps ourselves:
    - **Splitting:** can use `random` module; increased flexibility to (1) balance features/outcomes across the splits; (2) account for temporal or row-based clustering (eg if we observe a person or employer multiple times in the data, want all their rows in one split)
    - **Evaluation:** calculate metrics using $\hat{y}$ (predicted response; binary or continuous 0-1) versus y
  - **Rationale for imputation**: less about "losing data"; more about biases if rows missing some values differ systematically from those w/ complete data

Example classification task

Predicting positive sentiment (`1 = positive`) using text of Yelp reviews



metadata_label	raw_text
0	Unfortunately, the frustration of being Dr. Goldberg's patient is a repeat of the experience I've had with so many other doctors in NYC -- good doctor, terrible staff. It seems that his staff simply never answers the phone. It usually takes 2 hours of repeated calling to get an answer. Who has time for that or wants to deal with it? I have run into this problem with many other doctors and I just don't get it. You have office workers, you have patients with medical needs, why isn't anyone answering the phone? It's incomprehensible and not work the aggravation. It's with regret that I feel that I have to give Dr. Goldberg 2 stars.
1	Been going to Dr. Goldberg for over 10 years. I think I was one of his 1st patients when he started at MHMG. He's been great over the years and is really all about the big picture. It is because of him, not my now former gyn Dr. Markoff, that I found out I have fibroids. He explores all options with you and is very patient and understanding. He doesn't judge and asks all the right questions. Very thorough and wants to be kept in the loop on every aspect of your medical health and your life.
0	I don't know what Dr. Goldberg was like before moving to Arizona, but let me tell you, STAY AWAY from this doctor and this office. I was going to Dr. Johnson before he left and Goldberg took over when Johnson left. He is not a caring doctor. He is only interested in the co-pay and having you come in for medication refills every month. He will not give refills and could less about patients's financial situations. Trying to get your 90 days mail away pharmacy prescriptions through this guy is a joke. And to make matters even worse, his office staff is incompetent. 90% of the time when you call the office, they'll put you through to a voice mail, that NO ONE ever answers or returns your call. Both my adult

Labeled Yelp data (subsample of 15k): Zhang, Zhan, Lecun, 2015. "Character-level Convolutional Networks for Text Classification"

Notebook to follow along

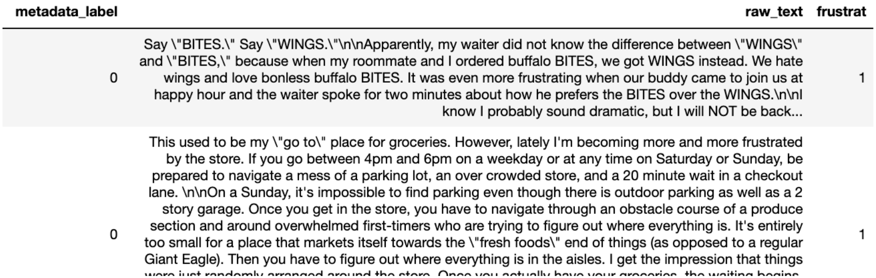
09_ML_intro_activity_blank.ipynb

Step 1: preprocess the data

See slides here for process of document-term matrix creation

Step 1: terms versus negative label

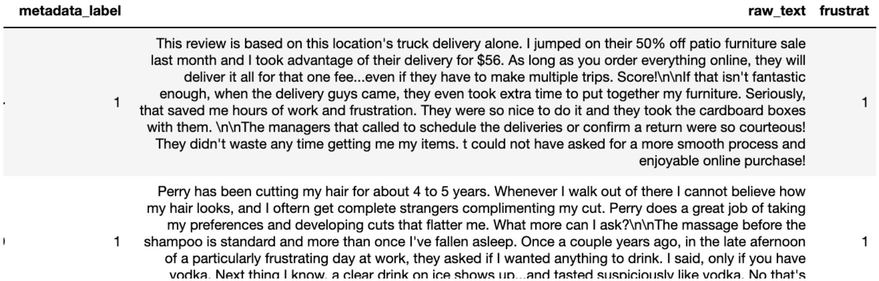
Uses word "frustrat" and negative label:



metadata_label	raw_text	frustrat
0	Say \"BITES.\" Say \"WINGS.\"\n\nApparently, my waiter did not know the difference between \"WINGS\" and \"BITES,\" because when my roommate and I ordered buffalo BITES, we got WINGS instead. We hate wings and love bonless buffalo BITES. It was even more frustrating when our buddy came to join us at happy hour and the waiter spoke for two minutes about how he prefers the BITES over the WINGS.\n\nI know I probably sound dramatic, but I will NOT be back...	1
0	This used to be my \"go to\" place for groceries. However, lately I'm becoming more and more frustrated by the store. If you go between 4pm and 6pm on a weekday or at any time on Saturday or Sunday, be prepared to navigate a mess of a parking lot, an over crowded store, and a 20 minute wait in a checkout lane. \n\nOn a Sunday, it's impossible to find parking even though there is outdoor parking as well as a 2 story garage. Once you get in the store, you have to navigate through an obstacle course of a produce section and around overwhelmed first-timers who are trying to figure out where everything is. It's entirely too small for a place that markets itself towards the \"fresh foods\" end of things (as opposed to a regular Giant Eagle). Then you have to figure out where everything is in the aisles. I get the impression that things were just randomly arranged around the store. Once you actually have your groceries, the waiting begins.	1

Step 1: terms versus positive label

Uses word "frustrat" and positive label:



metadata_label	raw_text	frustrat
1	This review is based on this location's truck delivery alone. I jumped on their 50% off patio furniture sale last month and I took advantage of their delivery for $56. As long as you order everything online, they will deliver it all for that one fee...even if they have to make multiple trips. Score!\n\nIf that isn't fantastic enough, when the delivery guys came, they even took extra time to put together my furniture. Seriously, that saved me hours of work and frustration. They were so nice to do it and they took the cardboard boxes with them. \n\nThe managers that called to schedule the deliveries or confirm a return were so courteous! They didn't waste any time getting me my items. t could not have asked for a more smooth process and enjoyable online purchase!	1
1	Perry has been cutting my hair for about 4 to 5 years. Whenever I walk out of there I cannot believe how my hair looks, and I oftern get complete strangers complimenting my cut. Perry does a great job of taking my preferences and developing cuts that flatter me. What more can I ask?\n\nThe massage before the shampoo is standard and more than once I've fallen asleep. Once a couple years ago, in the late afernoon of a particularly frustrating day at work, they asked if I wanted anything to drink. I said, only if you have vodka. Next thing I know, a clear drink on ice shows up...and tasted suspiciously like vodka. No that's	1

Step 2: split into train and test set (more manual; notebook also has `train_test_split`)

```python
## define the number of rows in training set (20\% test)
## and sample
nrows_train = round(X.shape[0]*0.8)
nrows_test = X.shape[0] - nrows_train
random.seed(221)
train_ids = random.sample(set(X['metadata_rowid']),
                nrows_train)
## function fed ids and name of id col
def my_split(train_ids, id_col):
    test_ids = set(X[id_col]).difference(train_ids)
    X_train_man = X[X[id_col].isin(train_ids)].copy()
    X_test_man = X[X[id_col].isin(test_ids)].copy()
    y_train_man = y[y.index.isin(train_ids)].iloc[:,
                        0].to_numpy()
    y_test_man = y[y.index.isin(test_ids)].iloc[:,
                        0].to_numpy()
    return(X_train_man, X_test_man, y_train_man, y_test_man)
```

Step 3: estimate model in training data (here, we're hardcoding the hyperparameters)

```python
## list of nonfeatures
non_feat = ['metadata_rowid', 'raw_text', 'process_text']

## initialize classifier
dt = DecisionTreeClassifier(random_state=0, max_depth = 10)

## estimate the model on training data/training label
dt.fit(X_train_man[[col for col in X_train.columns
                    if col not in non_feat]],
                    y_train_man)
```

Breaking things down:

- `non_feat`: want to shield things like our `id` variable from being treated as a feature; keep it in matrix for later post-modeling dx
- `dt`: initialize the decision-tree classifier; this is a `DecisionTreeClassifier` class within sklearn; telling it max tree depth is 10 features
- `dt.fit()`: use the `fit()` method from class; feed it training data and training label
- **Note:** skipped standardization bc features already on common scale

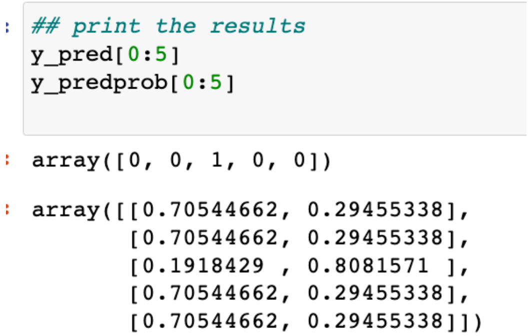
Step 4: apply the model to test set to generate binary and continuous predictions

```
y_pred = dt.predict(X_test_man[[col for col
                in X_test_man.columns if "metadata_rowid"
                not in col]])
y_predprob = dt.predict_proba(X_test_man[[col for col
                in X_test_man.columns if "metadata_rowid"
                not in col]])
```

Breaking things down:

- `predict`: predicted binary class (default cutoff $\sim$ 0.5)
- `predict_proba`: continuous predicted probability (0-1 range for classification)
- **To discuss:** why don't I need `y_test` at this stage?
- **To discuss:** what needs to be the same about the training and test set in order for me to generate these predictions? (e.g., # of rows; columns?)

Output of step 4: one or two-D array with predicted labels or probabilities



```
## print the results
y_pred[0:5]
y_predprob[0:5]
```

```
array([0, 0, 1, 0, 0])
```

```
array([[0.70544662, 0.29455338],
       [0.70544662, 0.29455338],
       [0.1918429 , 0.8081571 ],
       [0.70544662, 0.29455338],
       [0.70544662, 0.29455338]])
```

Step 5: use the $\hat{y}$ from step 4 to evaluate accuracy

```python
## dataframe of binary, continuous, and true labels
y_pred_df = pd.DataFrame({'y_pred_binary': y_pred,
                          'y_pred_continuous':
                          [one_prob[1]  for one_prob in y_predprob],
                          'y_true': y_test_man})

## use np.select to code each obs to its error cat
error_cond = [  (y_pred_df['y_true'] == 1) &
                (y_pred_df['y_pred_binary'] == 1),
                 (y_pred_df['y_true'] == 1) &
                 (y_pred_df['y_pred_binary'] == 0),
                (y_pred_df['y_true'] == 0) &
                (y_pred_df['y_pred_binary'] == 0)]
error_codeto = ["TP", "FN", "TN"]

y_pred_df['error_cat'] = np.select(error_cond,
                          error_codeto, default = "FP")

## see notebook for calculations using the error_cat column
```

Step 6: interpret the model

```
feat_imp = pd.DataFrame({'feature_imp': dt.feature_importances_,
                          'feature_name':
                         [col for col in X_train.columns
                         if col not in non_feat]})
```

Breaking it down:

- `feature_importances_` is an attribute of the estimated decision tree
- **Important note:** tree-based feature importances just have magnitude and not direction; in this case, an "important" feature might be either highly predictive of positive sentiment (1) or highly predictive of negative sentiment (0)
- `coef_` in regularized logistic regressions have both magnitude and direction

Can then generalize this basic setup in many ways:

- **Within the same model, parametrize the hyperparameters and iterate over a grid**: code has example of more manual via putting the `ridge` model into a function and parameterizing the α/λ parameter
- **Iterate over models and hyperparameters:** can create a function that takes in a sklearn classifier and then use list comprehension to iterate over classifiers
- **Parametrize the evaluation metrics:** create a function that returns different eval metrics; use that to simultaneously evaluate many models
- **Parametrize the feature sets used for prediction:** e.g., predicting product pricing using (1) historical price data versus (2) tweet sentiment versus (3) both combined

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Break for activity (section 4 in notebook)

Notebook:
https://github.com/jhaber-zz/QSS20_public/blob/main/activities/09_binaryclassification_activity_blank.ipynb

1. Read the documentation here to initialize a ridge regression (l2 penalty)- you can use the same cost parameter (C) and number of iterations as in the lasso example above: https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html
2. Fit the model using `X_train_man, y_train_main`
3. Generate binary and continuous predictions
4. Create a function that takes in a dataframe of binary predictions and true labels and calculates the F_1 score using this formula:

$$F_1 = 2 * \frac{precision * recall}{precision + recall} = \frac{TP}{TP + 0.5(FP + FN)}$$

5. Apply that function to calculate the F1 score for the decision tree and lasso (from above), and ridge regression (from the activity)
6. **Challenge exercise**: parametrize the model fitting with a function that takes in a classifier as an argument and returns coefficients or feature importances and certain eval metrics (eg precision, recall, and F1)

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Unit 11: Supervised Machine Learning, Part II (Decision Trees & Optimization)

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Learning goals

- Get comfortable with vocabulary of and rationale for model optimization
- Learn the basic mechanics of a few machine learning models: logistic regression, decision tree, and random forest models
- Understand cross-validation for model evaluation and how to interpret
- Gain experience implementing, comparing, and optimizing supervised machine learning models
- Get familiar with visualization to compare model performance

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- Lecture on Decision Trees & optimization
- Activity on DTs & optimization

Remaining five classes

- M 10/31: Introduction to SQL
- W 11/02: Web-scraping with BeautifulSoup
- M 11/07: Either:
  - geo-visualization (like pset 3 extra credit), **OR**...
  - scalable web-scraping with scrapy, **OR**...
  - Review session/Q&A
- W 11/09: Final project work session
- M 11/14: Final status-update presentations

Survey: Your feedback as of pset 3

https://forms.gle/LifYtXP3EmsRLQMM8

Goals for today

Today: Introduction to supervised machine learning

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Recap of supervised machine learning

What do you remember?

Recap of supervised machine learning: Tips

- Supervised ML builds a model on **features** (e.g., words) to predict a **label** (e.g., spam/not spam)
- Benefits: Scalable, flexible, can tell you what features matter most
- Do you care more about avoiding false negatives (e.g., detecting cancer) or false positives (e.g., detecting spam)? The former is a case for recall, the latter precision
- It often pays to use multiple metrics and try multiple hyperparameters (optimization)
- ML models try to avoid both overfitting (for generalizability) and underfitting (for accuracy); regularized models can strike a balance
- Splitting labeled data into training set (to build model) and test set (to evaluate it) reduces risk of overfitting; cross-validation even better
    - 80/20 rule is common (see Pareto principle), but depends on the amount and complexity of your data and the complexity of your model
    - with more or simpler data and/or simpler models, you can afford a smaller test set

Recap of supervised machine learning: Steps with code

1. Preprocess the data—with text data, this often means creating a DTM

```
vectorizer = CountVectorizer(lowercase = True)
dtm_sparse = vectorizer.fit_transform(list_of_strings)
```

2. Split into train and test set

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size)
```

3. Estimate model on training data

```
logit_ridge = LogisticRegression(C = 0.01, solver='liblinear')
logit_ridge.fit(X_train, y_train)
```

4. Apply model to get predictions

```
y_pred = logit_ridge.predict(X_test)
y_predprob = logit_ridge.predict_proba(X_test)
```

5. Evaluate model performance with metric(s) of choice

```
sklearn.metrics.accuracy_score(y_pred, y_test) # or metrics.f1_score
```

6. Interpret model to identify important features

```
ridge_coef = pd.DataFrame({'coef': logit_ridge.coef_[0],
             'feature_name': [col for col in X_train.columns]})
```

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Math behind logit models (from last time)

Logistic regression models fit where the probability of being positive ($y = 1$) is described by a sigmoid function of the form:

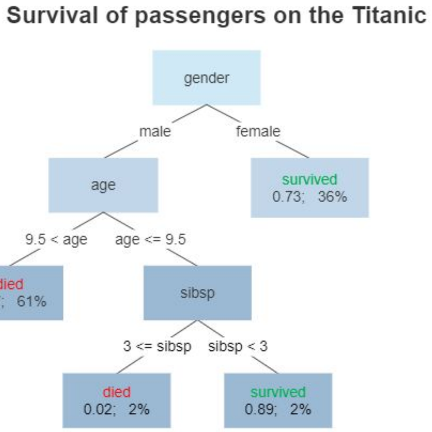
$$f(X) = P(y = 1|X) = \frac{exp(-X'\theta)}{1 + exp(-X'\theta)} \tag{1}$$

Once θ—a vector of word *weights* or *loadings*—is estimated, we can predict outcomes $\hat{y}$ conditional on observed word count X.

If $\hat{y} > 0.5$, then the observation is classified as positive. This is a *linear classifier* as the decision boundary is defined by $\frac{exp(-X'\theta)}{1+exp(-X'\theta)} = 0.5$, which after rearranging and taking logs appears equivalent to $-X'\theta = 0$—a linear function of the features X.

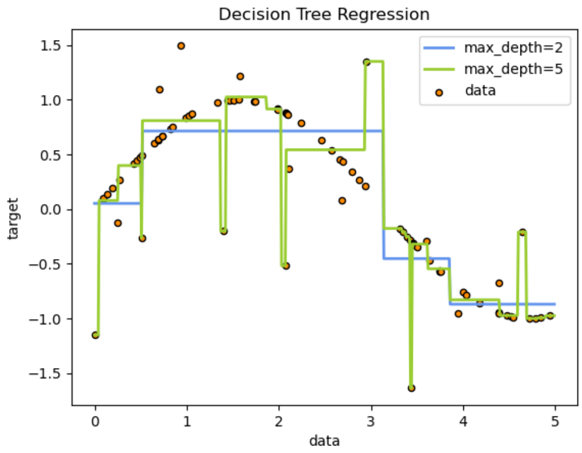
This uses penalized Maximum Likelihood as a loss function (estimates inaccuracy in relationship between X and y)

Tree-based methods use if-then-else decision rules



Graphics source

Tree-based methods learn non-linear relationships



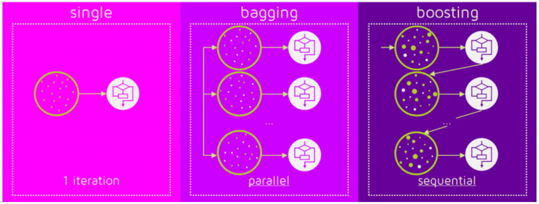
Graphics source

Logic behind classification trees/random forests

- **Classification and regression trees (CART):** take an input space—in the case of the Titanic, one comprised of gender; age; number of family on ship—and recursively partition that space into regions with different local models (in the Titanic case, binary prediction of survival or mortality)
- Decision Trees learn simple decision rules from the data features
  - A decision tree is made up of *decision nodes* (which identify feature values) and *leaf nodes* (which assign labels)
  - The former checks input features and selects a branch (usually this is binary: True/False), starting with the *root node* and continuing until arriving at a leaf node, which stops the evaluation and assigns a label
- **Growing a tree:**
  - Categorical variables (e.g., male or female): consider split on each category
  - Continuous variables (e.g., age): find sorted/unique values and consider thresholds (τ)
  - What do we use to evaluate the splits? evaluate how much a split reduces our loss/cost function (e.g., gain in "information" from split); evaluate splits against max. tree depth; ensure sufficient observations in terminal leafs
- **Random forests:** randomly sample from rows (observations) and columns (inputs/predictors), fit many trees, and take average over predictions (bagging) to aggregate over the trees; slower but less overfitting

Other extensions of trees: “boosted” trees

- Random forest is an example of the bagging approach to ensemble learning, where we fit many trees in parallel with subsets of observations/predictors



- Another form of ensemble learning is boosting, or a sequential process where we start with a shallow or “weak learner” (basically, something only slightly better than random guess) to predict the outcome, examine the predictions or residuals, and target misclassification in next iteration
  - **AdaBoost:** upweight misclassified observations from previous iteration
  - **GradientBoosting:** more general framework for boosting; calculates residuals from previous iteration ($y - \hat{y}$) and predicts those residuals in next iteration

Diagram source QuantDare

Optimization from last class: code

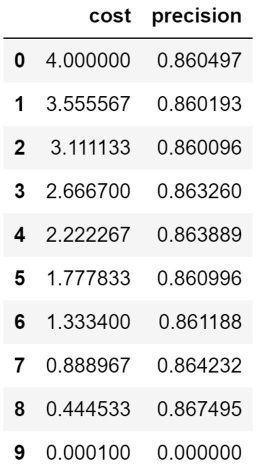
```python
def one_las(one_c):
    """takes cost parameter, estimates model, returns preds"""
    one_lasso = LogisticRegression(penalty = "l1", max_iter=100,
              C = one_c, solver='liblinear')
    one_lasso.fit(X_train_man[[col for col in X_train.columns if
                               col not in non_feat]], y_train_man)
    ...
    return(y_pred_df)

all_pred = [one_las(one_c) for one_c in c_list] # bind to DF
all_pred_df = pd.concat(all_pred)

def score_onedf(one_c, all_c): # score one cost level
    one_df = all_c[all_c.cost == one_c].copy()
    prec_onec =  precision_score(
        one_df['y_true'], one_df['y_pred'], zero_division = 0)
    return(prec_onec)

c_list = np.linspace(4, 0.0001, 10) # define range to search
pd.DataFrame({'cost': c_list,
              'precision': [score_onedf(one_c, all_pred_df)
              for one_c in c_list]})
```

Optimization from last class: output



	cost	precision
0	4.000000	0.860497
1	3.555567	0.860193
2	3.111133	0.860096
3	2.666700	0.863260
4	2.222267	0.863889
5	1.777833	0.860996
6	1.333400	0.861188
7	0.888967	0.864232
8	0.444533	0.867495
9	0.000100	0.000000

More automated approach to optimization: gridsearch

```python
# define dictionary with possible model parameters
param_grid = {'min_samples_split': [2,10],
              'min_samples_leaf': [2,10]}

# define gridsearch object
model_dt = GridSearchCV(dt_classifier,
                        param_grid,
                        cv=3,
                        return_train_score=True)

# fit model
model_dt.fit(X_train, y_train)

# find best performing candidate model over gridsearch
best_index = np.argmax(
    model.cv_results_["mean_train_score"])
```

K-fold cross-validation

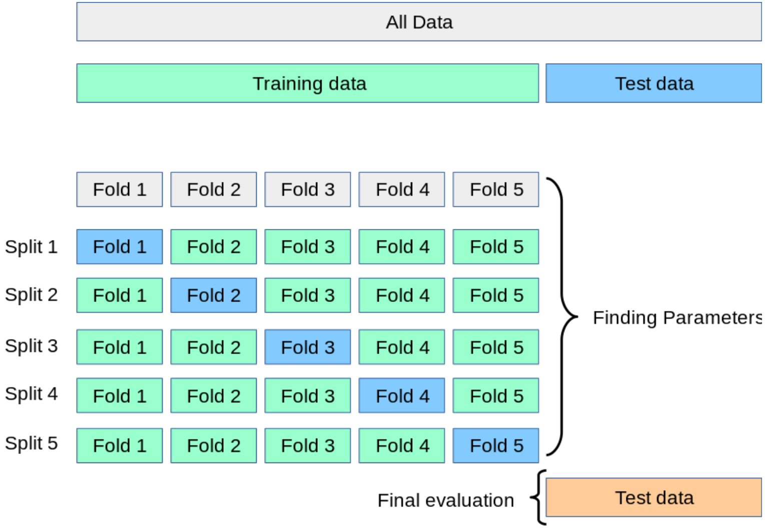
Instead of building a model from the training data in one swoop, k-fold cross-validation splits the training data into k smaller sets or "folds", trains a separate model using each fold, and averages the result. In other words, as described in the scikit-learn documentation, the procedure is:

- a model is trained using $k - 1$ of the folds as training data
- the resulting model is validated on the remaining part of the data (i.e., it is used as a test set to compute a performance measure such as accuracy)

Advantages:

- reduces risk of overfitting due to idiosyncrasies of one random split
- maximizes our available data; don't need to split into train/test/validation—this means more signal available and less risk of underfitting as well

K-Fold Cross-Validation



Optimizing ML: terminology

- **overfitting:** When a model is trained on too little data to generalize to new data, usually when trained and tested on the same sample. In this case, the model just repeats the labels of the samples that it has just seen, and is evaluated to have a perfect score–but it fails to predict anything useful on yet-unseen data.
- **underfitting:** When a model fails to adequately capture the underlying structure of the data, usually when trained on too little data
- **cross-validation:** A way to assess the performance of an algorithm on an unseen data set. Essentially this repeats a train-test split several times and averages the result of these independent slices, giving a superior estimation of model accuracy compared to a single train-test split.
- **parameter:** An algorithm setting that may be selected for performance or substantive reasons. If a parameter is not learned directly within an estimator but instead must be set explicitly (passed as an argument), then it's called a *hyper-parameter*.
- **optimization:** Selecting the best element from some set of alternatives such that the result maximizes some criterion (e.g., model accuracy)
- **grid-search:** An exhaustive search over model parameters to discover the optimal configuration, maximizing model performance

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Coding activity

Notebook: https://github.com/jhaber-zz/QSS20_public/blob/main/activities/09_ML_optimization_activity_blank.ipynb