Data Science

Introduction to Machine Learning: Random Forests, k-NN, Feature Engineering

April 21, 2021

Goals for today

A quick survey of other ML methods

- 1. We've looked at two very different ways to build predictive models:
 - 1.1 Linear Regressions
 - 1.2 Decision Trees
- 2. What else is out there?

Previously, on...

Decisions Tress are great, but...

- 1. They are very brittle (prone to over-fit)
- 2. We discussed one way of combating that (Holdout Cross Validation)
- 3. Is there any other way, specific to decision trees?
- 4. Yes, Just make more trees!

Random forests

If one DT is brittle, make a bunch of trees to do the work together.

- 1. Problem: How do we make sure that they're not all brittle in the same way?
- 2. Solution (part 1): You don't use the whole dataset to train all of them.
- 3. Solution (part 2): You don't use *all* of the features in the DTs
- 4. These parts are known as *baggin* and *random feature* selection

That's my bag

Bagging is short for Bootstrap Aggregation:

- 1. From you dataset, sample (with replacement!) n elements
- 2. For some number, B, of sample sets, train a DT for each $i \in B$
- 3. Now we need to Aggregate:
- 4. Thoughts on how?
 - 4.1 It depends on whether you need a classifier!

Aggregate 1: You don't need a classifier

For each T_i we get some prediction y_i .

- 1. For a regression, just take the average:
- 2. $\frac{1}{|B|} \sum_{j \in B} y_j$

Aggregate 2: You do need a classifier

For each T_i we get some prediction y_i.
1. For a classifier, just treat it as a vote!

Bagging ads some randomness, let's add more¹

- 1. For each tree, at every split point (where you'll put a decision node):
 - 1.1 choose a *random* subset of the available attributes (features)
 - 1.2 Use the same "most significant" attribute process as before, but only on that random subset.
- 2. This reduces the correlation *between* trees!

¹it is a *random* forest, after all

Random Trees (classifier) with SKLearn:

from sklearn.ensemble import RandomForestClassifier

```
classifier = RandomForestClassifier(n_estimators=N)
classifier = classifier.fit(X, Y)
```

Random Trees (regressor) with SKLearn:

from sklearn.ensemble import RandomForestRegressor

classifier = RandomForestRegressor(n_estimators=N)
classifier = classifier.fit(X, Y)

Other useful parameters:

Both use bootstraping by default (though you can turn it off)

- 1. max_depth: How deep of a tree you'll allow
- 2. max_samples: How many samples you'll allow for each T
- 3. min_samples_leaf: How many samples needed for a leaf node to be created.

The company you keep

What if we don't want to think too hard about what our features mean?²

- 1. The human brain is very good at pattern matching (this is good and bad)
- 2. One way we determine what 'group' something belongs to is to see what it's near!
- 3. Let's write a program to do that.

²This is a charicature!

First let's define a *neighbor*

- 1. For many types of features, we can have a notion of *distance*
- Using that notion of distance we can ask questions like:
 Is B or C closer to point A?
- 3. We can ask this for every point in the dataset, for *every* other point in the dataset
- 4. This can give us an *ordering* of the nearest neighbors.

k...

- 1. When k = 1, we only care about the closet point.
- 2. When k = 2, we only care about the two closet points, and they 'vote'.
- 3. When k = 3, we only care about the... you get it.

Discussion time.

What do we have to do in order to train this model?

1. We only have to store the dataset in a way that let's us calculate the nearest neighbor(s)

Discussion time 2.

What do we think k-NN might be good for?

Let's take a look (1NN):



Let's take a look (5NN):



$k\text{-}\mathrm{NN}$ and SKLearn

You might see a pattern developing:

- 1. sklearn.neighbors.KNeighborsClassifier
- 2. Defaults to k = 5
- 3. You can also play with the metric and p parameters to change how distance is calculated (default is Euclidean distance).

Feature Engineering (interaction terms)

- 1. Sometimes (as in the video for the make up lecture) we only want to add categorical terms
- 2. But sometimes we also want to add *interactions* between our terms.
- 3. To the notebook!

Thanks for your time!

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