COMP 204: Python programming for life sciences

Intro to machine learning with scikit-learn
Part 1

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based on materials from Christopher J.F. Cameron and Carlos G. Oliver

Problem: predicting who will live or die on the Titanic

Passenger survival data
http://biostat.mc.vanderbilt.edu/wiki/pub/Main/DataSets/titanic3.xls
See here for more info about the data

To read in the Excel '.xls' file, we will use the Pandas Python module

- **API** http://pandas.pydata.org/pandas-docs/stable/
- **tutotials** https://pandas.pydata.org/pandas-docs/stable/tutorials.html

Parsing an Excel '.xls' file with Pandas

```
import pandas as pd

# parse Excel '.xls' file
xls = pd.ExcelFile("./titanic3.xls")
# extract first sheet in Excel file
sheet_1 = xls.parse(0)
# get list of column names
print(list(sheet_1))
# prints: ['pclass', 'survived', 'name',
#   'sex', 'age', 'sibsp', 'parch', 'ticket',
#   'fare', 'cabin', 'embarked', 'boat', 'body',
#   'home.dest']
```

Passenger survival data

In the 'titanic3.xls' file:

- each row is a passenger
- each column is a **feature** describing the current passenger
- there are 14 features available in the dataset
- For example, the first passenger would be described as:

  Miss. Elisabeth Walton Allen (female - 29)

  A first class passenger staying in cabin B5 with no relatives on board that payed $211.3375 for ticket number #24160. She came aboard at the Southampton port to arrive at St Louis, MO. Mrs. Allen survived the titanic incident and was found on lifeboat #2.

Available dataset features

1. ‘pclass’ - passenger class (1 = first; 2 = second; 3 = third)
2. ‘survived’ - yes (1) or no (0)
3. ‘name’ - name of passenger (string)
4. ‘sex’ - sex of passenger (string - ‘male’ or ‘female’)
5. ‘age’ - age of passenger in years (float)
6. ‘sibsp’ - number of siblings/spouses aboard (integer)
7. ‘parch’ - number of parents/children aboard (integer)
8. ‘ticket’ - passenger ticket number (alphanumeric)
9. ‘fare’ - fare paid for ticket (float)
10. 'cabin’ - cabin number (alphanumeric - e.g. ‘B5’)
11. ‘embarked’: port of embarkation
    (C = Cherbourg; Q = Queenstown; S = Southampton)
12. ‘boat’ - lifeboat number (if survived - integer)
13. ‘body’ - body number
    (if did not survive and body was recovered - integer)
14. ‘home.dest’ - home destination (string)

Data mining

Determining passenger survival rate

```
from collections import Counter

# count passengers that survived
counter = Counter(sheet_1["survived"].values)
print(counter) # prints 'Counter({0: 809, 1: 500})'
print("survived:",counter[1]) # prints: 'survived: 500'
print("survival rate:",counter[1]/(counter[1]+counter[0]))
# prints 'survival rate: 0.3819709702062643'
```

Data mining #2

There are some obvious indicators of passenger survival in the data

```
# get the number of passengers with a body tag
# and their survival status
counter = Counter(sheet_1.loc[sheet_1["body"].notna(),
                              "survived"].values)
print(counter) # prints: 'Counter({0: 121})''
```

It appears that anyone with a body number did not survive

- this feature would be accurate at determining survival
- but, it's not too useful
  - i.e., the passenger would need to already be dead to have a number

Data mining #3

We could also look at how mean survival is affected by another feature's value

For example, passenger class:

```
print(sheet_1.groupby("pclass")["survived"].mean())
# prints:
# pclass
# 1      0.619195
# 2      0.429603
# 3      0.255289
# Name: survived, dtype: float64
```

From the mean survival rates

- first class passengers had the highest chance of surviving
- survival rates correlates nicely with passenger class

Data mining #4

With Pandas, you can also group by multiple features

For example, passenger class and sex

```
print(sheet_1.groupby(["pclass","sex"])["survived"]
      .mean())
# prints:
# pclass  sex
# 1       female     0.965278
#         male       0.340782
# 2       female     0.886792
#         male       0.146199
# 3       female     0.490741
#         male       0.152130
# Name: survived, dtype: float64
```

As a male grad student, I probably wouldn't have made it...

Why machine learning?

From basic data analysis, we can conclude

- Titanic officers followed maritime tradition
  - 'women and children first'
- if we examined the data more, we would see females
  - were on average younger than male passengers
  - paid more for their tickets
  - were more likely to travel with families

Let's now say that we wanted to determine our own survival

- we could write a long Python script to calculate survival
- but this would be tedious (lots of conditional statements)
- and would be dependent on our knowledge of the data

Instead, let's have the computer learn how to predict survival

Data preparation

Before we provide data to a **machine learning (ML)** algorithm

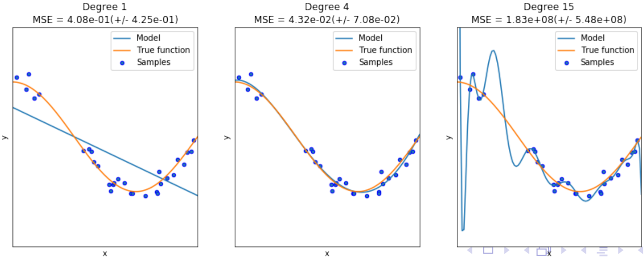
1. remove **examples** (passengers) with missing data
    - some passengers do not have a complete set of features
    - ML algorithms have difficulty with missing data
2. transform features with categorical string values to numeric representations
    - computers have an easier time interpreting numbers
3. remove features with low influence on a ML model's predictions
    - why would we want to limit the amount of features?
    - **overfitting**

Overfitting

What is overfitting?

- occurs when the ML algorithm learns a function that fits too closely to a limited set of data points
- predictions on unseen data will be biased to **training data**
  - increased error for **testing data** during **evaluation**

The true model a cosine function $y = \cos(1.5\pi x)$. We fit 3 polynomial models with 1, 4, 15 degrees to y. The model on the left has only degree 1 (**underfitting**); the model on the right has 15 degrees and go through almost every single data point but it generalizes poorly to the testing data (**overfitting**). More info here



Count the number of examples with a given feature

```
print(sheet_1.count())
# prints:
# pclass        1309
# survived      1309
# name          1309
# sex           1309
# age           1046
# sibsp         1309
# parch         1309
# ticket        1309
# fare          1308
# cabin          295
# embarked      1307
# boat           486
# body           121
# home.dest      745
```

Data preparation #2

Let's drop features with low example counts

- body, cabin, and boat numbers
- home desitnation

```
data = sheet_1.drop(["body","cabin","boat"
                      ,"home.dest"], axis=1)
print(list(data))
# prints: ['pclass', 'survived', 'name', 'sex', 'age',
# 'sibsp', 'parch', 'ticket', 'fare', 'embarked']
```

And remove any examples with missing data

```
data = data.dropna()
```

```
print(data.count())
# prints:
# pclass      1043
# survived    1043
# name        1043
# sex         1043
# age         1043
# sibsp       1043
# parch       1043
# ticket      1043
# fare        1043
# embarked    1043
# dtype: int64
```

Perfect, 1043 examples with a complete feature set

Label encoding

Some of our features are labels, not numeric values

- name, sex, and embarked
- ML algorithms expect numeric values for features

Let's encode them as numeric values

- sex = 0 (female) or 1 (male)
- embarked = 0 (C), 1 (Q), or 2 (S)

Luckily, Python's scikit-learn module has useful methods available

- **scikit-learn API**: `http://scikit-learn.org/stable/modules/classes.html`
- **scikit-learn tutorials**: `http://scikit-learn.org/stable/`

```
from sklearn import preprocessing

le = preprocessing.LabelEncoder()
data.sex = le.fit_transform(data.sex)
data.embarked = le.fit_transform(data.embarked)
print(data[:1])
# prints:
#    pclass  survived                              name  \
# 0       1         1  Allen, Miss. Elisabeth Walton
#     sex   age  sibsp  parch        ticket      fare  \
# 0     0  29.0      0      0         24160  211.3375
#    embarked
# 0         2
```

Removing unnecessary/misleading features

Unless there is some sick joke to reality

- a passenger's name plays very little importance in their survival

A passenger's ticket number is a mixture of alpha and numeric characters

- it will be difficult to represent as a feature
- may be misleading to the ML algorithm

Like before, we'll remove both from the dataset

Features vs. labels

Now that we have a prepared ML dataset

- split into two lists:
  1. **model input** (or X)
  2. **model targets/input labels** (or y)

```
X = data.drop(["survived"], axis=1).values
y = data["survived"].values
```

Why should we drop ‘survived’ from X?

Training vs testing datasets

From the ML dataset select training and testing sets

A ML algorithm will attempt to learn the training dataset

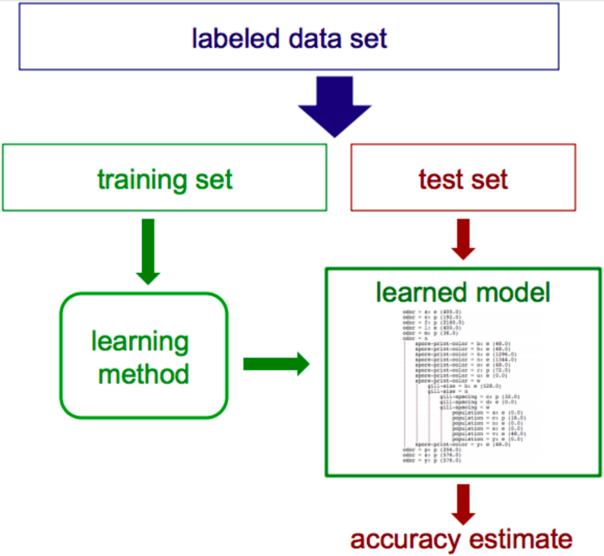
- can be as simple as selecting a random split of data
- 80% for training and 20% for testing
- or may involve more complicated sampling methods

A learned model is not exposed to the test dataset during training

Any predictions on the testing data are designed to be indicative of the performance of the model in general

- make sure the selection of your datasets are representative of the problem you are solving
- remember back to 'cat vs. bird', we want pictures of both cats and birds in the training and testing data

Model evaluation



Split the dataset into training and testing datasets

In scikit-learn, we can easily create training and testing datasets

```
from sklearn import model_selection

X = data.drop(["survived"], axis=1).values
y = data["survived"].values
results = model_selection.train_test_split(X, y,
    test_size = 0.2, shuffle = True)
X_train, X_test, y_train, y_test = results
```

Logistic regression prediction

```
logitreg = linear_model.LogisticRegression(solver='liblinear')
fit = logitreg.fit(X_train, y_train)
effect_size = pd.DataFrame(fit.coef_)
effect_size.columns = data.drop(["survived"], axis=1).columns
print(effect_size)
# pclass        sex      sibsp     parch
# 0 -0.78978 -2.514111 -0.205692  0.059857

y_train_pred = fit.predict(X_train)
y_test_pred = fit.predict(X_test)

acc_train = sum(y_train_pred==y_train)/len(y_train)
acc_test = sum(y_test_pred==y_test)/len(y_test)
print(f"train accuracy: {acc_train:.3f}; \
test accuracy: {acc_test:.3f}")
# train accuracy: 0.793; test accuracy: 0.779
```

Receiver Operator Characteristic (ROC) curve

```
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
from matplotlib import pyplot

# calculate AUC
probs = y_test_prob[:,1]
auc = roc_auc_score(y_test, probs)
print('AUC: %.3f' % auc)
pyplot.plot([0, 1], [0, 1], linestyle='--')
# plot the roc curve for the model
fpr, tpr, thresholds = roc_curve(y_test, probs)
pyplot.plot(fpr, tpr, marker='.')
pyplot.show()
```

Next time in COMP 364

More of Python's scikit-learn module:

1. ML algorithm selection
   - **support vector machines (SVM)**
2. fitting a function and creating a learned model
   - making predictions using a learned model
3. accuracy estimates
   - **true/false positive (TP/FP) rates**
   - error measures
   - **receiver operating characteristic (ROC)** curves?