

Machine Learning

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In this notebook, we'll discuss how to formulate a research question in the machine learning framework; how to build, evaluate, compare, and select models; and how to reasonably and accurately interpret model results. You'll also get hands-on experience using the `scikit-learn` package in Python.

This tutorial is based on chapter 6 of [Big Data and Social Science](#) (<https://github.com/BigDataSocialScience/>).

Glossary of Terms

There are a number of terms specific to Machine Learning that you will find repeatedly in this notebook.

- **Features:** These are what you probably know as *independent variables*, *attributes*, *predictors*, or *explanatory variables*.
- **Underfitting:** This happens when a model is too simple and does not capture the structure of the data well enough.
- **Overfitting:** This happens when a model is too complex or too sensitive to the noise in the data; this can result in poor generalization performance, or applicability of the model to new data.
- **Regularization:** This is a general method to avoid overfitting by applying additional constraints to the model. For example, you can limit the number of features present in the final model, or the weight coefficients applied to the (standardized) features are small.
- **Supervised learning** involves problems with one target or outcome variable (continuous or discrete) that we want to predict, or classify data into. Classification, prediction, and regression fall into this category. We call the set of explanatory variables **X features**, and the outcome variable of interest **Y** the **label**.

Setup

We'll be using `scikit-learn` (<http://scikit-learn.org>) for the machine learning models.

```
In [1]: %pylab inline
import os
import glob
import pandas as pd
import time
import sklearn
import seaborn as sns
from sklearn.metrics import precision_recall_curve,roc_curve, auc
from sklearn.metrics import accuracy_score, precision_score, recall_score
from sklearn.ensemble import (RandomForestClassifier, ExtraTreesClassifier,
                               GradientBoostingClassifier,
                               AdaBoostClassifier)
from sklearn.linear_model import LogisticRegression, SGDClassifier
from sklearn import svm
from sklearn.model_selection import train_test_split

from sklearn.linear_model import LogisticRegression
from sklearn.metrics import precision_recall_curve, roc_auc_score, auc
from sklearn import preprocessing

import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline

import warnings
warnings.filterwarnings('ignore')
```

Populating the interactive namespace from numpy and matplotlib

The Machine Learning Process

The Machine Learning Process is as follows:

- **Understand the problem and goal.** *This sounds obvious but is often nontrivial.* Problems typically start as vague descriptions of a goal - improving health outcomes, increasing graduation rates, understanding the effect of a variable X on an outcome Y , etc. It is really important to work with people who understand the domain being studied to dig deeper and define the problem more concretely. What is the analytical formulation of the metric that you are trying to optimize?
- **Formulate it as a machine learning problem.** Is it a classification problem or a regression problem? Is the goal to build a model that generates a ranked list prioritized by risk, or is it to detect anomalies as new data come in? Knowing what kinds of tasks machine learning can solve will allow you to map the problem you are working on to one or more machine learning settings and give you access to a suite of methods.
- **Data exploration and preparation.** Next, you need to carefully explore the data you have. What additional data do you need or have access to? What variable will you use to match records for integrating different data sources? What variables exist in the data set? Are they continuous or categorical? What about missing values? Can you use the variables in their original form, or do you need to alter them in some way?
- **Feature engineering.** In machine learning language, what you might know as independent variables or predictors or factors or covariates are called "features." Creating good features is

probably the most important step in the machine learning process. This involves doing transformations, creating interaction terms, or aggregating over data points or over time and space.

- **Method selection.** Having formulated the problem and created your features, you now have a suite of methods to choose from. It would be great if there were a single method that always worked best for a specific type of problem. Typically, in machine learning, you take a variety of methods and try them, empirically validating which one is the best approach to your problem.
- **Evaluation.** As you build a large number of possible models, you need a way choose the best among them. We'll cover methodology to validate models on historical data and discuss a variety of evaluation metrics.
- **Deployment.** Once you have selected the best model and validated it using historical data as well as a field trial, you are ready to put the model into practice. You still have to keep in mind that new data will be coming in, and the model might change over time.

You're probably used to fitting models in social science classes. In those cases, you probably had a hypothesis or theory about the underlying process that gave rise to your data, chose an appropriate model based on prior knowledge and fit it using least squares, and used the resulting parameter or coefficient estimates (or confidence intervals) for inference. This type of modeling is very useful for *interpretation*.

In machine learning, our primary concern is *generalization*. This means that:

- **We care less about the structure of the model and more about the performance** This means that we'll try out a whole bunch of models at a time and choose the one that works best, rather than determining which model to use ahead of time. We can then choose to select a *suboptimal* model if we care about a specific model type.
- **We don't (necessarily) want the model that best fits the data we've already seen**, but rather the model that will perform the best on *new data*. This means that we won't gauge our model's performance using the same data that we used to fit the model (e.g., sum of squared errors or R^2), and that "best fit" or accuracy will most often *not* determine the best model.
- **We can include a lot of variables in to the model.** This may sound like the complete opposite of what you've heard in the past, and it can be hard to swallow.

Problem Formulation

First, turning something into a real objective function. What do you care about? Do you have data on that thing? What action can you take based on your findings? Do you risk introducing any bias based on the way you model something?

Four Main Types of ML Tasks for Policy Problems

- **Description:** [How can we identify and respond to the most urgent online government petitions? \(<https://dssg.uchicago.edu/project/improving-government-response-to-citizen-requests-online/>\)](https://dssg.uchicago.edu/project/improving-government-response-to-citizen-requests-online/)
- **Prediction:** [Which students will struggle academically by third grade? \(<https://dssg.uchicago.edu/project/predicting-students-that-will-struggle-academically-by-third-grade/>\)](https://dssg.uchicago.edu/project/predicting-students-that-will-struggle-academically-by-third-grade/)

- **Detection:** [Which police officers are likely to have an adverse interaction with the public? \(<https://dssg.uchicago.edu/project/expanding-our-early-intervention-system-for-adverse-police-interactions/>\)](https://dssg.uchicago.edu/project/expanding-our-early-intervention-system-for-adverse-police-interactions/)
- **Behavior Change:** [How can we prevent juveniles from interacting with the criminal justice system? \(<https://dssg.uchicago.edu/project/preventing-juvenile-interactions-with-the-criminal-justice-system/>\)](https://dssg.uchicago.edu/project/preventing-juvenile-interactions-with-the-criminal-justice-system/)

Our Machine Learning Problems

Data Exploration and Preparation

During the first classes, we have explored the data, linked different data sources, and created new variables. The first steps of creating a machine learning model are exactly that.

1. **Creating the label:** The Label is the dependent variable, or Y variable, that we are trying to predict. In the machine learning framework, labels are often *binary*: true or false, encoded as 1 or 0.
2. **Decide on features:** Our features are our independent variables or predictors. Good features make machine learning systems effective. The better the features the easier it is to capture the structure of the data. You generate features using domain knowledge. In general, it is better to have more complex features and a simpler model rather than vice versa. Keeping the model simple makes it faster to train and easier to understand rather than extensively searching for the "right" model and "right" set of parameters. Machine Learning Algorithms learn a solution to a problem from sample data. The set of features is the best representation of the sample data to learn a solution to a problem.
3. **Feature engineering** is the process of transforming raw data into features that better represent the underlying problem/data/structure to the predictive models, resulting in improved model accuracy on unseen data." (from [Discover Feature Engineering \(<http://machinelearningmastery.com/discover-feature-engineering-how-to-engineer-features-and-how-to-get-good-at-it/>\)](http://machinelearningmastery.com/discover-feature-engineering-how-to-engineer-features-and-how-to-get-good-at-it/)). Example of feature engineering are:
 - **Transformations**, such as log, square, and square root.
 - **Dummy (binary) variables**, sometimes known as *indicator variables*, often done by taking categorical variables (such as industry) which do not have a numeric value, and adding them to models as a binary value.
 - **Aggregation**. Aggregate features often constitute the majority of features for a given problem. These use different aggregation functions (*count, min, max, average, standard deviation, etc.*) which summarize several values into one feature, aggregating over varying windows of time and space. For example, we may want to calculate the *number* (and *min, max, mean, variance, etc.*) of crimes within an *m*-mile radius of an address in the past *t* months for varying values of *m* and *t*, and then use all of them as features.
4. **Cleaning data:** To run the `scikit-learn` set of models your input dataset must have no missing variables.
5. **Imputing values to missing or irrelevant data:** Once the features are created, always check to make sure the values make sense. You might have some missing values, or impossible values for a given variable (negative values, major outliers). If you have missing values you

should think hard about what makes the most sense for your problem; you may want to replace with 0, the median or mean of your data, or some other value.

6. Normalization: Certain models will have an issue with features on different scales. For example, an individual's age is typically a number between 0 and 100 while earnings can be a number between 0 and 1000000 (or higher). In order to circumvent this problem, we can scale

Load the 2014 Data

```
In [2]: # Specify a path with the data folder
# Change "NAME" to your name as recorded on your computer
# path = 'C:/Users/NAME/PADM-GP_2505/Data/'
Path = '/Users/wsq/Desktop/Advanced Data Analytics and Evidence Building/PA'
# use the chdir function from the os package to set your working directory
os.chdir(Path + "/Projects")
```



```
In [3]: # Read-in the 2014 projects file
grants_2014 = pd.read_csv(Path + '/Projects/RePORTER_PRJ_C_FY2014_new.csv',
```

Clean the PI IDs

Clean the PI IDs for 2014. We are going to clean the PI ID just like we cleaned the PI names in previous Notebooks. We will be using the PI ID instead of the Name, because it is a better way to identify a unique individual. We used the names in previous notebooks for pedagogical purposes, because it is more intuitive.

```
In [4]: grants_2014 = grants_2014.reset_index()

# First we need to convert PI_IDS into a string variable
grants_2014['PI_IDS'] = grants_2014['PI_IDS'].astype(str)

# Make a temporary dataframe that creates an observation for each PI.
# Use the explode function to split the PI_IDS at the ;
temp = grants_2014['PI_IDS'].str.split(';').explode().reset_index()

# Rename the PI_IDS variable
temp = temp.rename(columns = {'PI_IDS': 'PI_ID'})

# Replace " " with an empty string
temp['PI_ID'] = temp['PI_ID'].str.replace(' ', '')

# Only keep observations in the temp dataframe where PI_ID is not an empty
temp = temp[temp['PI_ID'] != ""]
temp = temp[temp['PI_ID'] != " "]
temp = temp[temp['PI_ID'] != ""]

# For the the PI_ID variable, use the str.replace function to replace ` (co
temp['PI_ID'] = temp['PI_ID'].str.replace('\(contact\)', '')

# Merge this temporary dataframe with df_NYU
grants_2014B = grants_2014.merge(temp, on = 'index')

# Filter for NCI projects
grants_2014B = grants_2014B[grants_2014B['IC_NAME'] == 'NATIONAL CANCER INS

# view the select variables for the first 5 observations
grants_2014B[['APPLICATION_ID', 'PI_NAMES', 'PI_ID', 'PI_IDS', 'FY', 'FULL_PROJECT_NUM', 'PROJECT_TITLE']]
```

		APPLICATION_ID	PI_NAMES	PI_ID	PI_IDS	FY	FULL_PROJECT_NUM	PROJECT_TITLE
1	8715629	BURDETTE, EVERETTE C (contact); DIEDERICH, CHR...		8495898 8495898 (contact); 1888559;	8495898 (contact); 1888559;	2014	2R44CA121740-02	Minimally Invasive High Intensity Ultrasound T...
2	8715629	BURDETTE, EVERETTE C (contact); DIEDERICH, CHR...		8495898 8495898 (contact); 1888559;	8495898 (contact); 1888559;	2014	2R44CA121740-02	Minimally Invasive High Intensity Ultrasound T...
3	8676705	BICKELL, NINA A;		3150322 3150322;	3150322; 2014		5R01CA149025-05	Implementing a Tracking & Feedback Registry to...
17	8616355	TUSCHL, THOMAS ;		7337985 7337985;	7337985; 2014		5R01CA159227-04	Development of quantitative multiplex RNA in s...
19	8585032	BESSLER, MONICA ;		3144163 3144163;	3144163; 2014		5R01CA105312-09	MOLECULAR STUDIES OF BONE MARROW FAILURE

Creating Labels

Labels are the dependent variables, or Y variables, that we are trying to predict. In the machine learning framework, your labels are usually binary: true or false, encoded as 1 or 0. In this case, our label will identify all people who started working on a Brain Cancer project between FY 2016 and FY 2020

- Note the cohort of people we are studying are all people who worked on NCI projects on 2014

Read in the data

When reading in the data we will do several things

- **Create a loop that will read in project data from 2016-2020**
- **Select only the columns we need**
- **Filter for NCI projects**
- **Filter for having a spending category of Brain Cancer**
- **Convert PROJECT_START into a datetime variable**

```
In [5]: # Identify the files you want to read in
years = ('RePORTER_PRJ_C_FY2016_new.csv', 'RePORTER_PRJ_C_FY2017_new.csv',
```

```
In [6]: # Generate an empty dataframe that will hold all the patent data we have
NCI_2016_2020 = pd.DataFrame([])

# Now loop through each file identified in the years vector
# Read that file using only the columns we need
# And append it to the dataframe that we created above
# This might take a little while to run (no more than 1 minute)
for counter, file in enumerate(years):
    print(counter,file)
    projects = pd.read_csv(file, usecols=['APPLICATION_ID', 'FY', 'IC_NAME',
                                           encoding='latin-1'])
    # Filter for NCI projects
    projects = projects[projects['IC_NAME'] == 'NATIONAL CANCER INSTITUTE']
    # Select Brain Cancer NCI projects
    projects = projects[projects['NIH_SPENDING_CATS'].str.contains('Brain C

    # convert PROJECT_START into a date variable
    projects['PROJECT_START'] = pd.to_datetime(projects['PROJECT_START'])

    NCI_2016_2020 = NCI_2016_2020.append(projects)

NCI_2016_2020 = NCI_2016_2020.reset_index(drop=True)
NCI_2016_2020.head(20)
```

0 RePORTER_PRJ_C_FY2016_new.csv
 1 RePORTER_PRJ_C_FY2017_new.csv
 2 RePORTER_PRJ_C_FY2018_new.csv
 3 RePORTER_PRJ_C_FY2019_new.csv
 4 RePORTER_PRJ_C_FY2020_new.csv

	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START
0	9344016	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Neurosc...	11142396;	NaT
1	9067335	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Genetic...	1870316;	2015-05-15
2	9149712	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Clinica...	9076342;	NaT
3	9338858	2016	NATIONAL CANCER	Aging; Brain Cancer; Brain Disorders; Breast C	9294195; 1888652; 1873010	2014-04-17

Clean the PI IDs

```
In [7]: # First we need to convert PI_IDS into a string variable
NCI_2016_2020['PI_IDS'] = NCI_2016_2020['PI_IDS'].astype(str)

# Make a temporary dataframe that creates an observation for each PI.
# Use the explode function to split the PI_IDS at the ;
temp = NCI_2016_2020['PI_IDS'].str.split(';').explode().reset_index()

# Rename the PI_IDS variable
temp = temp.rename(columns = {'PI_IDS': 'PI_ID'})

# Replace " " with and empty string
temp['PI_ID'] = temp['PI_ID'].str.replace(' ', '')

# Only keep observations in the temp dataframe where PI_ID is not an empty
temp = temp[temp['PI_ID'] != ""]
temp = temp[temp['PI_ID'] != " "]

# For the the PI_ID variable, use the str.replace fundtion to replace ` (co
temp['PI_ID'] = temp['PI_ID'].str.replace('\(contact\)', '')

temp.head()
```

Out[7]:

	index	PI_ID
0	0	11142396
2	1	1870316
4	2	9076342
6	3	9294195
7	3	1888652

```
In [8]: # reset the index
NCI_2016_2020 = NCI_2016_2020.reset_index()

# view the first 5 observations
NCI_2016_2020.head()
```

Out[8]:

	index	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START
0	0	9344016	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Neurosc...	11142396;	NaT
1	1	9067335	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Genetic...	1870316;	2015-05-15
2	2	9149712	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Clinica...	9076342;	NaT
3	3	9338858	2016	NATIONAL CANCER INSTITUTE	Aging; Brain Cancer; Brain Disorders; Breast C...	9294195; 1888652; 1873940 (contact);	2014-04-17
4	4	9128413	2016	NATIONAL CANCER INSTITUTE	Bioengineering; Brain Cancer; Brain Disorders;...	10363645;	2014-09-01

```
In [9]: # Merge this temporary dataframe with grants_2017
NCI_2016_2020B = NCI_2016_2020.merge(temp, on = 'index')

# view the first 5 observations
NCI_2016_2020B.head(10)
```

Out[9]:

	index	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START	
0	0	9344016	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Neurosc...	11142396;	NaT	111...
1	1	9067335	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Genetic...	1870316;	2015-05-15	18...
2	2	9149712	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Clinica...	9076342;	NaT	90...
3	3	9338858	2016	NATIONAL CANCER INSTITUTE	Aging; Brain Cancer; Brain Disorders; Breast C...	9294195; 1888652; 1873940 (contact);	2014-04-17	92...
4	3	9338858	2016	NATIONAL CANCER INSTITUTE	Aging; Brain Cancer; Brain Disorders; Breast C...	9294195; 1888652; 1873940 (contact);	2014-04-17	18...

Filter for new projects

We want to identify all PIs that had a Brain Cancer project start after the 2016 fiscal year began

```
In [10]: # Define the start as the pridr day in Fiscal year 2016
State_date = pd.to_datetime('10/01/2015')

# select all nre procjects (that started after FY 2016)
New_NCI_PI = NCI_2016_2020B[NCI_2016_2020B['PROJECT_START'] >= State_date]

# Reset index
New_NCI_PI = New_NCI_PI.reset_index()

# view the firts 5 observations
New_NCI_PI.head()
```

Out[10]:

	level_0	index	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_ST
0	9	7	9049804	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Neurosc...	11021607;	2016-0
1	17	11	9003765	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Genetic...	7075834;	2015-1
2	21	14	9029909	2016	NATIONAL CANCER INSTITUTE	Brain Cancer; Brain Disorders; Cancer; Genetic...	1893276;	2015-1
3	25	17	9210945	2016	NATIONAL CANCER INSTITUTE	Bioengineering; Biotechnology; Brain Cancer; B...	1965067 (contact); 1951886;	2016-0
4	26	17	9210945	2016	NATIONAL CANCER INSTITUTE	Bioengineering; Biotechnology; Brain Cancer; B...	1965067 (contact); 1951886;	2016-0

```
In [11]: New_NCI_PI = New_NCI_PI[['PI_ID']].drop_duplicates()
New_NCI_PI["New_BC"] = 1

# view the select variables for the firts 4 observations
New_NCI_PI.head(8)
```

Out[11]:

	PI_ID	New_BC
0	11021607	1
1	7075834	1
2	1893276	1
3	1965067	1
4	1951886	1
5	11951932	1
6	11873857	1
7	14271813	1

Join the data

We will create a new dataframe by joining the grants_2014B and New_NCI_PI dataframes. We will continue using this data frame to store all the features we create.

```
In [12]: # Merge the temp dataframe into the DF_2015 data frame
# Use an left merge
# keep only the PI_ID and NCI_2017 variables and then drop duplicates. This
DF = pd.merge(grants_2014B, New_NCI_PI, on='PI_ID', how = 'left')[['PI_ID'],
DF.head()
```

Out[12]:

	PI_ID	New_BC
0	8495898	NaN
1	1888559	NaN
2	3150322	NaN
3	7337985	NaN
4	3144163	NaN

The observations that have an Nan for NCI_2017, means they did not have a new NCI project in 2017, so we will replace that NaN value with a 0

```
In [13]: DF['New_BC'] = DF['New_BC'].fillna(0)

DF.head()
```

Out[13]:

	PI_ID	New_BC
0	8495898	0.0
1	1888559	0.0
2	3150322	0.0
3	7337985	0.0
4	3144163	0.0

In [14]:

DF.shape

Out[14]:

(7741, 2)

In [15]:

sum(DF['New_BC'])

Out[15]:

195.0

There are 7741 PIs who had NCI project in 2017, of whom 2750 started a new Brain Cancer NCI project between 2016-2020

Feature Generation

Our features are our independent variables or predictors. Good features make machine learning systems effective. The better the features the easier it is to capture the structure of the data. You generate features using domain knowledge. In general, it is better to have more complex features and a simpler model rather than vice versa. Keeping the model simple makes it faster to train and easier to understand rather than extensively searching for the "right" model and "right" set of parameters.

Our features are the following

- NIH_SPENDING_CATS: We need to identify each spending category each PI has grants in then make dummies
- State: The state in which the applicant organization is located (we need to make dummies)
- Number of NCI projects in 2014
- Number of projects that will still be active in 2016, 2017, 2018, 2019, and 2020
- Total Cost of 2014 Projects
- brain cancer activity of organizations (creating binary variables for different levels of activity)

Spending Category

In [16]: grants_2014B[['NIH_SPENDING_CATS']].head()

Out[16]:

NIH_SPENDING_CATS

- | | NIH_SPENDING_CATS |
|----|---|
| 1 | Bioengineering; Cancer; Contraception/Reprodu... |
| 2 | Bioengineering; Cancer; Contraception/Reprodu... |
| 3 | Breast Cancer; Cancer; Clinical Research; Clin... |
| 17 | Biotechnology; Cancer; Clinical Research; Gene... |
| 19 | Cancer; Clinical Research; Genetics; Hematolog... |

Separate up the Spending Category

```
In [17]: # First we need to convert PI_IDS into a string variable
grants_2014B['PI_IDS'] = grants_2014B['NIH_SPENDING_CATS'].astype(str)

# Make a temporary dataframe that creates an observation for each spending
# Use the explode function to split the NIH_SPENDING_CATS at the ;
temp = grants_2014B['NIH_SPENDING_CATS'].str.split(';').explode().reset_index()

# Rename the NIH_SPENDING_CATS variable
temp = temp.rename(columns = {'NIH_SPENDING_CATS': 'NIH_SPENDING_CAT'})

# Replace " " with an empty string
temp['NIH_SPENDING_CAT'] = temp['NIH_SPENDING_CAT'].str.replace(' ', '')

# Only keep observations in the temp dataframe where PI_ID is not an empty
temp = temp[temp['NIH_SPENDING_CAT'] != ""]

temp.head(10)
```

Out[17]:

	index	NIH_SPENDING_CAT
0	1	Bioengineering
1	1	Cancer
2	1	Contraception/Reproduction
3	1	DiagnosticRadiology
4	1	FibroidTumors(Uterine)
6	2	Bioengineering
7	2	Cancer
8	2	Contraception/Reproduction
9	2	DiagnosticRadiology
10	2	FibroidTumors(Uterine)

```
In [18]: # Select the relevant columns
Cat = grants_2014B[['index', 'PI_ID', 'NIH_SPENDING_CATS']]

Cat.head()
```

Out[18]:

	index	PI_ID	NIH_SPENDING_CATS
1	1	8495898	Bioengineering; Cancer; Contraception/Reprodu...
2	1	1888559	Bioengineering; Cancer; Contraception/Reprodu...
3	2	3150322	Breast Cancer; Cancer; Clinical Research; Clin...
17	13	7337985	Biotechnology; Cancer; Clinical Research; Gene...
19	15	3144163	Cancer; Clinical Research; Genetics; Hematolog...

```
In [19]: # Merge this temporary dataframe with the spending catagory dataframe
Cat2 = Cat.merge(temp, on = 'index')

# Remove the index and NIH_SPENDING_CATS variables
Cat2 = Cat2.drop(columns=['index', 'NIH_SPENDING_CATS'])

# Drop duplicate observations
Cat2 = Cat2.drop_duplicates()

# Drop duplicate observations
Cat2['Cat'] = 1

# View the first 10 observations
Cat2.head(10)
```

Out[19]:

	PI_ID	NIH_SPENDING_CAT	Cat
0	8495898	Bioengineering	1
1	8495898	Cancer	1
2	8495898	Contraception/Reproduction	1
3	8495898	DiagnosticRadiology	1
4	8495898	FibroidTumors(Uterine)	1
5	1888559	Bioengineering	1
6	1888559	Cancer	1
7	1888559	Contraception/Reproduction	1
8	1888559	DiagnosticRadiology	1
9	1888559	FibroidTumors(Uterine)	1

Create Dummy variables for each of the spending catagories

To create these Dummy variables, we will transform the dataframe from long to wide

```
In [20]: # use the pivot function to transform the dataframe from long to wide
Cat3 = pd.pivot(Cat2, index='PI_ID', columns = 'NIH_SPENDING_CAT',values =
#Re-arange the new columns in the correct order
cols = Cat2['NIH_SPENDING_CAT'].unique()
Cat3=Cat3[cols]

# Replace missing values with 0
Cat3 = Cat3.fillna(0)

# View the first 5 observations
Cat3.head()
```

Out[20]:

	NIH_SPENDING_CAT	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibr
PI_ID						
10012000	1.0	1.0		0.0		1.0
10021262	0.0	1.0		0.0		0.0
10021476	0.0	1.0		0.0		0.0
10108300	0.0	1.0		0.0		0.0
10113370	0.0	1.0		0.0		0.0

5 rows × 122 columns

Join the data

Join the features we just created with the DF fataframe

```
In [21]: # Join Cat3 with the DF fataframe using a left join
DF = pd.merge(DF, Cat3, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[21]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibr
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 124 columns

State

We will create dummy variables for state

```
In [22]: state = grants_2014B[['PI_ID', 'ORG_STATE']]

# Drop duplicate observations
state = state.drop_duplicates()

# Only keep the first state recorded for each PI
state = state.groupby(['PI_ID']).first()

# View the first 5 observations
state.head()
```

Out[22]:

ORG_STATE

PI_ID	ORG_STATE
10000506	None
10011128	AZ
10012000	MA
10021262	ON
10021476	NY

```
In [23]: # We need to create dummy variables for state and organization name
state2 = pd.get_dummies(state, columns=['ORG_STATE'])

state2.head()
```

Out[23]:

ORG_STATE_AK ORG_STATE_AL ORG_STATE_AR ORG_STATE_AZ ORG_STATE_BC ORG_

PI_ID	ORG_STATE_AK	ORG_STATE_AL	ORG_STATE_AR	ORG_STATE_AZ	ORG_STATE_BC	ORG_
10000506	0	0	0	0	0	0
10011128	0	0	0	1	0	0
10012000	0	0	0	0	0	0
10021262	0	0	0	0	0	0
10021476	0	0	0	0	0	0

5 rows × 53 columns

There are a few states PIs that are with organizations from different states, we have to identify them and then collapse the State dummy variable for them

In [24]:

state2.shape

Out[24]:

(7741, 53)

Check point 1

I wanted to provide code to make simple dummy variables, however, to do this for the state data, we needed to select a single state for each person. It is better to identify every ORG_STATE a person is associated with in 2014. Using the long to wide transfer we did when creating the dummy variables for spending catagories, create state dummy variables that identify every ORG_STATE a person is associated with. You should write over the state2 data frame so that the code to join the DF data with the states data runs. (1 points)

```
In [25]: # Select the relavant columns  
State_temp = grants_2014B[['index', 'PI_ID', 'ORG_STATE']]  
State_temp.head()
```

```
Out[25]:
```

	index	PI_ID	ORG_STATE
1	1	8495898	IL
2	1	1888559	IL
3	2	3150322	NY
17	13	7337985	NY
19	15	3144163	PA

```
In [26]: # Merge this temporary dataframe with the spending catagory dataframe
State_temp2 = State_temp.merge(temp, on = 'index')

# Remove the index and NIH_SPENDING_CATS variables
State_temp2 = State_temp2.drop(columns=['index', 'NIH_SPENDING_CAT'])

# Drop duplicate observations
State_temp2 = State_temp2.drop_duplicates()

# Drop duplicate observations
State_temp2['State_temp'] = 1

# View the first 10 observations
State_temp2.head(10)
```

Out[26]:

	PI_ID	ORG_STATE	State_temp
0	8495898	IL	1
5	1888559	IL	1
10	3150322	NY	1
15	6265424	NY	1
19	12448156	NaN	1
23	1869066	HI	1
27	12430520	CA	1
34	8590003	TN	1
36	1877317	TN	1
38	7284983	WA	1

```
In [27]: # use the pivot function to transform the dataframe from long to wide
State_temp3 = pd.pivot(State_temp2, index='PI_ID', columns = 'ORG_STATE', values='Value')

#Re-arange the new columns in the correct order
cols = State_temp2['ORG_STATE'].unique()
State_temp3=State_temp3[cols]

# Replace missing values with 0
State_temp3 = State_temp3.fillna(0)

# View the first 5 observations
State_temp3.head()
```

Out[27]:

	ORG_STATE	IL	NY	NaN	HI	CA	TN	WA	MA	KS	OR	...	VT	MS	QC	LA	SD	PR	NV	D
PI_ID																				
10012000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0	
10021262	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0	
10021476	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0	
10108300	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0	
10113370	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0	

5 rows × 50 columns

```
In [28]: # Join Cat3 with the DF fataframe using a left join
DF = pd.merge(DF, State_temp3, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[28]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0	1.0	1.0	1.0
1	1888559	0.0	1.0	1.0	1.0	1.0	1.0
2	3150322	0.0	1.0	1.0	1.0	1.0	1.0
3	7337985	0.0	NaN	NaN	NaN	NaN	NaN
4	3144163	0.0	NaN	NaN	NaN	NaN	NaN

5 rows × 174 columns

```
In [29]: # We need to create dummy variables for state and organization name  
state2 = pd.get_dummies(state, columns=['ORG_STATE'])  
  
state2.head()
```

Out[29]:

PI_ID	ORG_STATE_AK	ORG_STATE_AL	ORG_STATE_AR	ORG_STATE_AZ	ORG_STATE_BC	ORG_STATE_CO
10000506	0	0	0	0	0	0
10011128	0	0	0	1	0	0
10012000	0	0	0	0	0	0
10021262	0	0	0	0	0	0
10021476	0	0	0	0	0	0

5 rows × 53 columns

```
In [30]: state2.shape
```

Out[30]: (7741, 53)

Join the DF data with the States data

```
In [31]: # Merge this temporary dataframe with the spending catagory dataframe
State_temp2 = State_temp.merge(temp, on = 'index')

# Remove the index and NIH_SPENDING_CATS variables
#State_temp2 = State_temp2.drop(columns=['index', 'ORG_STATE'])

# Drop duplicate observations
State_temp2 = State_temp2.drop_duplicates()

# Drop duplicate observations
State_temp2['State_temp'] = 1

# View the first 10 observations
State_temp2.head(10)
```

Out[31]:

	index	PI_ID	ORG_STATE	NIH_SPENDING_CAT	State_temp
0	1	8495898	IL	Bioengineering	1
1	1	8495898	IL	Cancer	1
2	1	8495898	IL	Contraception/Reproduction	1
3	1	8495898	IL	DiagnosticRadiology	1
4	1	8495898	IL	FibroidTumors(Uterine)	1
5	1	1888559	IL	Bioengineering	1
6	1	1888559	IL	Cancer	1
7	1	1888559	IL	Contraception/Reproduction	1
8	1	1888559	IL	DiagnosticRadiology	1
9	1	1888559	IL	FibroidTumors(Uterine)	1

```
In [32]: # use a left join nerge to join the state2 data witht the DF dataframe
DF = pd.merge(DF, state2, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[32]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 227 columns

Number of projects in 2014

```
In [33]: # Calculate how many Projects each PI has
projects = grants_2014B.groupby(['PI_ID'])['APPLICATION_ID'].nunique().sort

# Convert into a dataframe and reset index
projects = projects.to_frame().reset_index()

# Rename APPLICATION_ID to Total_NCI_Projects_2014
projects.rename(columns={'APPLICATION_ID': 'Total_NCI_Projects_2014'}, inplace=True)

# View the first 2 observations
projects.head(2)
```

Out[33]:

	PI_ID	Total_NCI_Projects_2014
0	14267998	58
1	1875698	40

Join the DF data with the projects data

```
In [34]: DF = pd.merge(DF, projects, on = 'PI_ID', how = 'inner')

# View the first 5 observations
DF.head()
```

Out[34]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 228 columns

Number of projects what will still be active in FY 2016

```
In [35]: # convert PROJECT_END into a date variable
grants_2014B['PROJECT_END'] = pd.to_datetime(grants_2014B['PROJECT_END'])
```

```
In [36]: # Identity the end of FY 2015
FY_2016 = pd.to_datetime('09/30/2015')

# Filter for projects that will still be active in 2016
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2016]

# select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2016' that is equal to one for all observations
ongoing['active_2016'] = 1

# View the first 2 observations
ongoing.head(2)
```

Out[36]:

	PI_ID	active_2016
1	8495898	1
2	1888559	1

```
In [37]: # Sum up the number of projects that will still be active in 2016 for each
ongoing = ongoing.groupby('PI_ID')['active_2016'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# View the first 2 observations
ongoing.head(2)
```

Out[37]:

	PI_ID	active_2016
0	10000506	1
1	10011128	1

```
In [38]: # convert PROJECT_END into a date variable
grants_2014B['PROJECT_END'] = pd.to_datetime(grants_2014B['PROJECT_END'])
```

```
In [39]: # Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2017 with 0
DF['active_2016'] = DF['active_2016'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[39]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0		1.0	1.0		1.0
1	1888559	0.0		1.0	1.0		1.0
2	3150322	0.0		1.0	1.0		1.0
3	7337985	0.0		NaN	NaN		NaN
4	3144163	0.0		NaN	NaN		NaN

5 rows × 229 columns

Number of projects what will still be active in FY 2017

```
In [40]: # Identify the end of FY 2016
FY_2017 = pd.to_datetime('09/30/2016')

# Filter for projects that will still be active in 2017
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2017]

# Select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2017' that is equal to one for all observations
ongoing['active_2017'] = 1

# Sum up the number of projects that will still be active in 2017 for each
ongoing = ongoing.groupby('PI_ID')['active_2017'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2017 with 0
DF['active_2017'] = DF['active_2017'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[40]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	Nan	Nan		Nan	Nan
4	3144163	0.0	Nan	Nan		Nan	Nan

5 rows × 230 columns

Number of projects what will still be active in FY 2018

```
In [41]: # Identify the end of FY 2017
FY_2018 = pd.to_datetime('09/30/2017')

# Filter for projects that will still be active in 2016
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2018]

# select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2018' that is equal to one for all observations
ongoing['active_2018'] = 1

# Sum up the number of projects that will still be active in 2018 for each
ongoing = ongoing.groupby('PI_ID')['active_2018'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2018 with 0
DF['active_2018'] = DF['active_2018'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[41]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	Nan	Nan		Nan	Nan
4	3144163	0.0	Nan	Nan		Nan	Nan

5 rows × 231 columns

Number of projects what will still be active in FY 2019

```
In [42]: # Identify the end of FY 2018
FY_2019 = pd.to_datetime('09/30/2018')

# Filter for projects that will still be active in 2019
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2019]

# Select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2019' that is equal to one for all observations
ongoing['active_2019'] = 1

# Sum up the number of projects that will still be active in 2019 for each
ongoing = ongoing.groupby('PI_ID')['active_2019'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2019 with 0
DF['active_2019'] = DF['active_2019'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[42]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	Nan	Nan		Nan	Nan
4	3144163	0.0	Nan	Nan		Nan	Nan

5 rows × 232 columns

Number of projects what will still be active in FY 2020

```
In [43]: # Identify the end of FY 2019
FY_2020 = pd.to_datetime('09/30/2019')

# Filter for projects that will still be active in 2020
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2020]

# select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2020' that is equal to one for all observations
ongoing['active_2020'] = 1

# Sum up the number of projects that will still be active in 2020 for each
ongoing = ongoing.groupby('PI_ID')['active_2020'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2020 with 0
DF['active_2020'] = DF['active_2020'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[43]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	Nan	Nan		Nan	Nan
4	3144163	0.0	Nan	Nan		Nan	Nan

5 rows × 233 columns

Total Cost of Projects

```
In [44]: # Calculate how many Projects each PI has
Cost = grants_2014B.groupby(['PI_ID'])['TOTAL_COST'].sum()

# Convert into a dataframe and reset index
Cost = Cost.to_frame().reset_index()

# drop first row
Cost = Cost.iloc[1:, :]

# View the first 5 observations
Cost.head()
```

Out[44]:

	PI_ID	TOTAL_COST
1	10011128	750566.0
2	10012000	85785.0
3	10021262	217377.0
4	10021476	278247.0
5	10027192	310470.0

```
In [45]: DF = pd.merge(DF, Cost, on = 'PI_ID', how = 'left')
DF.head()
```

Out[45]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 234 columns

Number of NCI projects by organization

```
In [46]: # Use a conditional statement do create a new dataframe were there are only
BC = grants_2014B[grants_2014B['NIH_SPENDING_CATS'].str.contains('Brain Can

# Calculate how many NCI Projects each ORG has
BC = BC.groupby(['ORG_NAME'])['APPLICATION_ID'].nunique().sort_values(ascen

# Convert into a dataframe and reset index
BC = BC.to_frame().reset_index()

# Rename APPLICATION_ID to Total_BC_Projects_by_ORG
BC.rename(columns={'APPLICATION_ID': 'Total_BC_Projects_by_ORG'}, inplace = True

# View the first 5 observations
BC.head()
```

Out[46]:

	ORG_NAME	Total_BC_Projects_by_ORG
0	UNIVERSITY OF CALIFORNIA, SAN FRANCISCO	49
1	BASIC SCIENCES	44
2	MASSACHUSETTS GENERAL HOSPITAL	33
3	DUKE UNIVERSITY	24
4	UNIVERSITY OF TX MD ANDERSON CAN CTR	21

	ORG_NAME	Total_BC_Projects_by_ORG
0	UNIVERSITY OF CALIFORNIA, SAN FRANCISCO	49
1	BASIC SCIENCES	44
2	MASSACHUSETTS GENERAL HOSPITAL	33
3	DUKE UNIVERSITY	24
4	UNIVERSITY OF TX MD ANDERSON CAN CTR	21

```
In [47]: BC2 = pd.merge(grants_2014B, BC, on = 'ORG_NAME', how = 'left')[['PI_ID',
# Fill the NaN values for Total_BC_Projects_by_ORG with 0
BC2['Total_BC_Projects_by_ORG'] = BC2['Total_BC_Projects_by_ORG'].fillna(0)

#Drop duplicate observations
BC2 = BC2.drop_duplicates()

# View the first 5 observations
BC2.head()
```

Out[47]:

	PI_ID	Total_BC_Projects_by_ORG	ORG_NAME
0	8495898	0.0	ACOUSTIC MEDSYSTEMS, INC.
1	1888559	0.0	ACOUSTIC MEDSYSTEMS, INC.
2	3150322	3.0	ICAHN SCHOOL OF MEDICINE AT MOUNT SINAI
3	7337985	0.0	ROCKEFELLER UNIVERSITY
4	3144163	1.0	CHILDREN'S HOSP OF PHILADELPHIA

```
In [48]: # Sum up the number of projects for people who worked for more than one org
BC3 = BC2.groupby(['PI_ID'])['Total_BC_Projects_by_ORG'].sum()

# Convert into a dataframe and reset index
BC3 = BC3.to_frame().reset_index()

# View the first 5 observations
BC3.head()
```

Out[48]:

	PI_ID	Total_BC_Projects_by_ORG
0	10000506	47.0
1	10011128	0.0
2	10012000	10.0
3	10021262	0.0
4	10021476	3.0

We will look at the distribution of the Total_BC_Projects_by_ORG variable to understand better how to split it up

```
In [49]: # use the describe to look at the distribution
BC3['Total_BC_Projects_by_ORG'].describe()
```

Out[49]:

count	7741.000000
mean	7.962796
std	12.097469
min	0.000000
25%	0.000000
50%	3.000000
75%	9.000000
max	76.000000
Name:	Total_BC_Projects_by_ORG, dtype: float64

Looking at this distribution, we will break the organizations into the following groups:

- No brain cancer projects.
- A few brain cancer projects (1-3)
- A Moderate number of brain cancer projects (5-9)
- Several brain cancer projects (10-20)
- A large number of brain cancer projects (over 20)

No brain cancer projects

```
In [50]: # Identify observations where the PI is from an org with no brain cancer pr
No = BC3[BC3['Total_BC_Projects_by_ORG'] == 0]

# Create a variable "Org_No" that is equal to 1
No['Org_No'] = 1

# Select the two variables we need
No = No[['PI_ID', 'Org_No']]

# Merge with the DF dataframe
DF = pd.merge(DF, No, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_No'] = DF['Org_No'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[50]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	Nan	Nan		Nan	Nan
4	3144163	0.0	Nan	Nan		Nan	Nan

5 rows × 235 columns

A few brain cancer projects (1-3)

```
In [51]: # Identify observations where the PI is from an org with 1-3 brain cancer p
Few = BC3[BC3['Total_BC_Projects_by_ORG'] >= 1]
Few = Few[Few['Total_BC_Projects_by_ORG'] <= 3]

# Create a variable "Org_No" that is equal to 1
Few['Org_Few'] = 1

# Select the two variable we need
Few = Few[['PI_ID', 'Org_Few']]

# Merge with the DF dataframe
DF = pd.merge(DF, Few, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_Few'] = DF['Org_Few'].fillna(0)

DF.head()
```

Out[51]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 236 columns

A Moderate number of brain cancer projects (5-9)

```
In [52]: # Identify observations where the PI is from an org with 5-9 brain cancer p
Moderate = BC3[BC3['Total_BC_Projects_by_ORG'] >= 5]
Moderate = Moderate[Moderate['Total_BC_Projects_by_ORG'] <= 9]

# Create a variable "Org_No" that is equal to 1
Moderate['Org_Mod'] = 1

# Select the two variables we need
Moderate = Moderate[['PI_ID', 'Org_Mod']]

# Merge with the DF dataframe
DF = pd.merge(DF, Moderate, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_Mod'] = DF['Org_Mod'].fillna(0)

DF.head()
```

Out[52]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	Nan	Nan		Nan	Nan
4	3144163	0.0	Nan	Nan		Nan	Nan

5 rows × 237 columns

Several brain cancer projects (10-15)

```
In [53]: # Identify observations where the PI is from an org with 10-20 brain cancer
Several = BC3[BC3['Total_BC_Projects_by_ORG'] >= 10]
Several = Several[Several['Total_BC_Projects_by_ORG'] <= 20]

# Create a variable "Org_No" that is equal to 1
Several['Org_Several'] = 1

# Select the two variable we need
Several = Several[['PI_ID', 'Org_Several']]

# Merge with the DF dataframe
DF = pd.merge(DF, Several, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_Several'] = DF['Org_Several'].fillna(0)

DF.head()
```

Out[53]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibi
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 238 columns

Large number of brain cancer projects (over 20)

```
In [54]: # Identify observations where the PI is from an org with more than brain capacity
large = BC3[BC3['Total_BC_Projects_by_ORG'] > 20]

# Create a variable "Org_No" that is equal to 1
large['Org_large'] = 1

# Select the two variables we need
large = large[['PI_ID', 'Org_large']]

# Merge with the DF dataframe
DF = pd.merge(DF, large, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_large'] = DF['Org_large'].fillna(0)

DF.head()
```

Out[54]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibrosis
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	NaN	NaN		NaN	NaN
4	3144163	0.0	NaN	NaN		NaN	NaN

5 rows × 239 columns

Replace all missing values with 0

```
In [55]: DF = DF.fillna(0)
```

Normalization

We need to normalize our non-binary features. To Normalize the data, we will apply a linear transformation so that the values are between 0 and 1. Normalization makes the features more consistent with each other, which allows the model to predict outputs more accurately.

```
In [56]: features_to_normalize = ['active_2016', 'active_2017', 'active_2018', 'active_2019']

DF[features_to_normalize] = DF[features_to_normalize].apply(lambda x:(x-x.mean())/(x.std()))

DF.head()
```

Out[56]:

	PI_ID	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibroid
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	0.0	0.0	0.0		0.0	0.0
4	3144163	0.0	0.0	0.0		0.0	0.0

5 rows × 239 columns

Building a Model

We need to divide our dataframe into a training data and test data. We will train our model on the training set and then test it on the test set. We will assign 80% of our data to training set and the remaining 20% to the test set

```
In [57]: # use the train_test_split to split the data into the training and test set
df_train, df_test = train_test_split(DF, test_size=0.2)
```

```
In [58]: # Look at the distribution of the variables for the training data set
df_train.describe()
```

Out[58]:

	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	I
count	6192.000000	6192.000000	6192.000000	6192.000000	6192.000000	
mean	0.025517	0.034076	0.219800	0.001130	0.020995	
std	0.157701	0.181440	0.414144	0.033606	0.143378	
min	0.000000	0.000000	0.000000	0.000000	0.000000	
25%	0.000000	0.000000	0.000000	0.000000	0.000000	
50%	0.000000	0.000000	0.000000	0.000000	0.000000	
75%	0.000000	0.000000	0.000000	0.000000	0.000000	
max	1.000000	1.000000	1.000000	1.000000	1.000000	

8 rows × 238 columns

In [59]: # Look at the distribution of the variables for the test data set
df_test.describe()

Out[59]:

	New_BC	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	I
count	1549.000000	1549.000000	1549.000000	1549.000000	1549.000000	1549.000000
mean	0.023886	0.029051	0.210458	0.000646	0.018076	
std	0.152744	0.168004	0.407766	0.025408	0.133270	
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
50%	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
75%	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
max	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000

8 rows × 238 columns

Class Balancing

Let's check how much data we still have and how many are for PIs with new brain cancer projects in our training dataset. We don't necessarily need to have a perfect 50-50 balance, but it's good to know what the "baseline" is in our dataset, to be able to intelligently evaluate our performance. If you look at our New_BC you can see that not about 38% are for PIs that will have a new brain cancer project between 2016-2020

In [60]: print('Number of rows: {}'.format(df_train.shape[0]))
df_train['New_BC'].value_counts(normalize=True)

Number of rows: 6192

Out[60]: 0.0 0.974483
1.0 0.025517
Name: New_BC, dtype: float64

Let's take a look at our testing set.

In [61]: print('Number of rows: {}'.format(df_test.shape[0]))
df_test['New_BC'].value_counts(normalize=True)

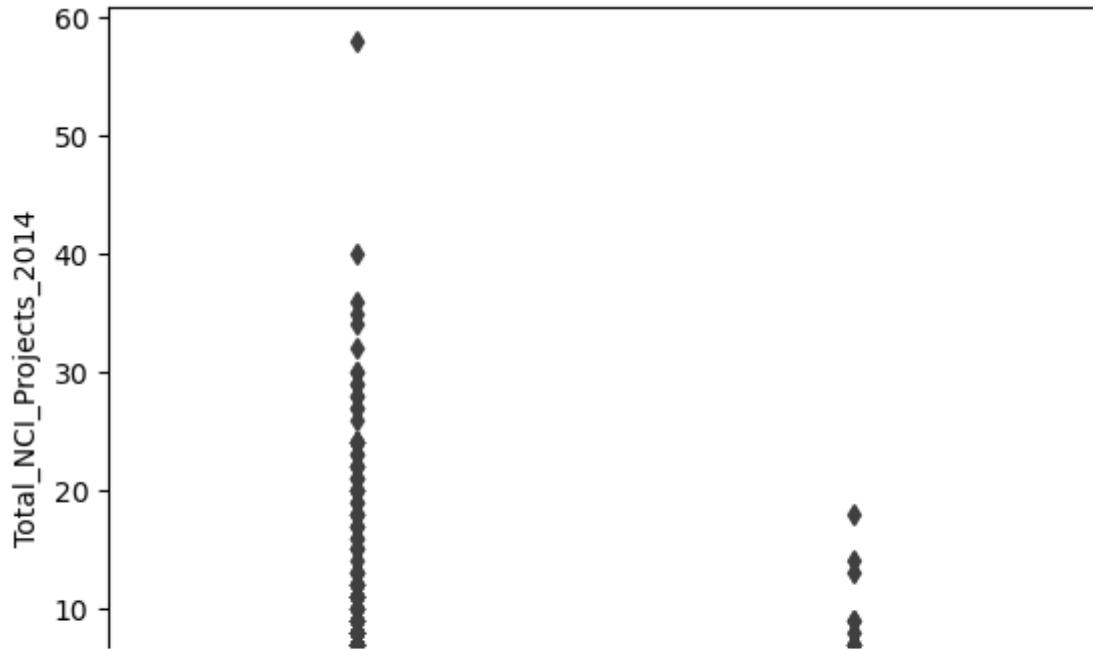
Number of rows: 1549

Out[61]: 0.0 0.976114
1.0 0.023886
Name: New_BC, dtype: float64

Investigate our data

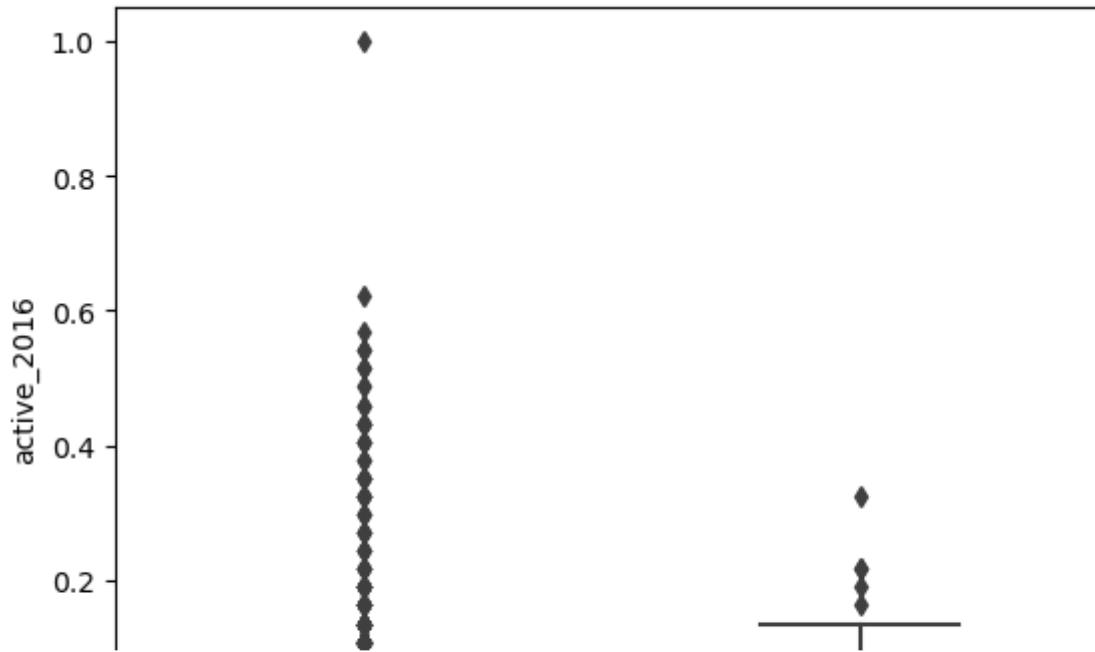
We can use visualizations to find trends and patterns in our data. We will start by looking at the Total number of NCI projects in 2014, then we will look at the number of projects that will still be active in 2016

```
In [62]: ax = sns.boxplot(x="New_BC", y="Total_NCI_Projects_2014", data=df_train)
```



We can see that PIs who will have a new brain cancer project between 2016-2020 have more NCI projects on average in 2014

```
In [63]: ax = sns.boxplot(x="New_BC", y="active_2016", data=df_train)
```



We can see that PIs who will have a new brain cancer project between 2016-2020 have more active projects in 2016.

Identify the features and lable

We need to identify the **features** and **label** for both the trainig and test datasets

```
In [64]: # use conventions typically used in python scikitlearn
x_train = df_train.drop(columns=['New_BC'])
y_train = df_train['New_BC']
x_test = df_test.drop(columns=['New_BC'])
y_test = df_test['New_BC']
```

Model Selection

Model Evaluation

In this phase, you take the predictors from your test set and apply your model to them, then assess the quality of the model by comparing the *predicted values* to the *actual values* for each record in your testing data set.

- **Performance Estimation:** How well will our model do once it is deployed and applied to new data?

Now let's use the model we just fit to make predictions on our test dataset, and see what our accuracy score is:

We will start with the simplest [LogisticRegression](http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) (http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) model and see how well that does.

You can use any number of metrics to judge your models, but we'll use [accuracy_score\(\)](http://scikit-learn.org/stable/modules/generated/sklearn.metrics.accuracy_score.html) (http://scikit-learn.org/stable/modules/generated/sklearn.metrics.accuracy_score.html) (ratio of correct predictions to total number of predictions) as our measure.

```
In [65]: from sklearn import linear_model

model = linear_model.LogisticRegression(max_iter = 100, intercept_scaling =
model.fit( x_train, y_train)

print(model)
#https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Log
LogisticRegression(intercept_scaling=2)
```

When we print the model results, we see different parameters we can adjust as we refine the model based on running it against test data (values such as `intercept_scaling`, `max_iters`, `penalty`, and `solver`).

Penalty L1: Lasso shrinks the less important feature's coefficient to zero thus, removing some feature altogether. So, this works well for feature selection in case we have a huge number of features.

C: Inverse of regularization strength; must be a positive float. Smaller values specify stronger regularization.

To adjust these parameters, one would alter the call that creates the `LogisticRegression()` model instance, passing it one or more of these parameters with a value other than the default. So, to re-fit the model with `max_iter` of 1000, `intercept_scaling` of 2, and `solver` of "lbfgs" (pulled from thin air as an example), you'd create your model as follows:

```
model = LogisticRegression( max_iter = 1000, intercept_scaling = 2,
                            solver = "lbfgs" )
```

The basic way to choose values for, or "tune," these parameters is the same as the way you choose a model: fit the model to your training data with a variety of parameters, and see which perform the best on the test set. An obvious drawback is that you can also *overfit* to your test set; in this case, you can alter your method of cross-validation.

Model Evaluation

Machine learning models usually do not produce a prediction (0 or 1) directly. Rather, models produce a score between 0 and 1 (that can sometimes be interpreted as a probability), which lets you more finely rank all of the examples from *most likely* to *least likely* to have label 1 (positive). This score is then turned into a 0 or 1 based on a user-specified threshold. For example, you might label all examples that have a score greater than 0.5 (1/2) as positive (1), but there's no reason that has to be the cutoff.

```
In [66]: # from our "predictors" using the model.
y_scores = model.predict_proba(x_test)[:, 1]
```

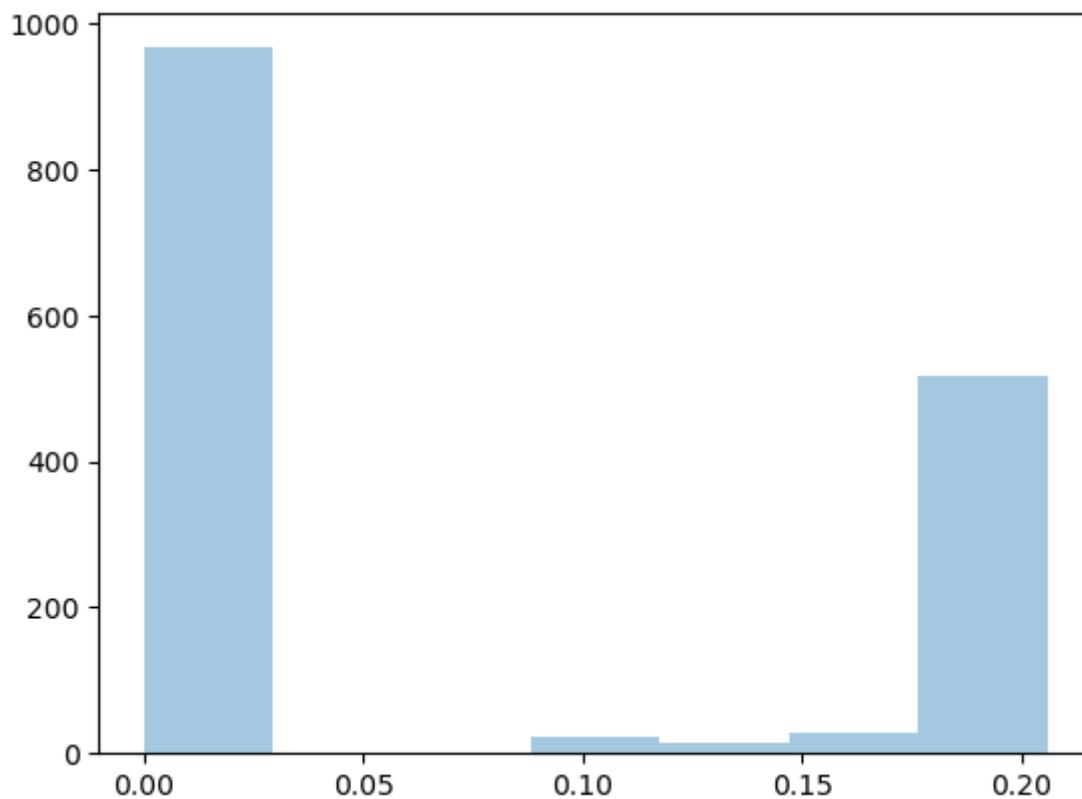
```
In [67]: y_scores
```

```
Out[67]: array([2.04182963e-01, 2.04557973e-01, 1.17792380e-04, ...,
   1.01290015e-03, 1.65683802e-01, 1.33308408e-03])
```

Let's take a look at the distribution of scores and see if it makes sense to us.

```
In [68]: sns.distplot(y_scores, kde=False, rug=False)
```

```
Out[68]: <AxesSubplot:>
```

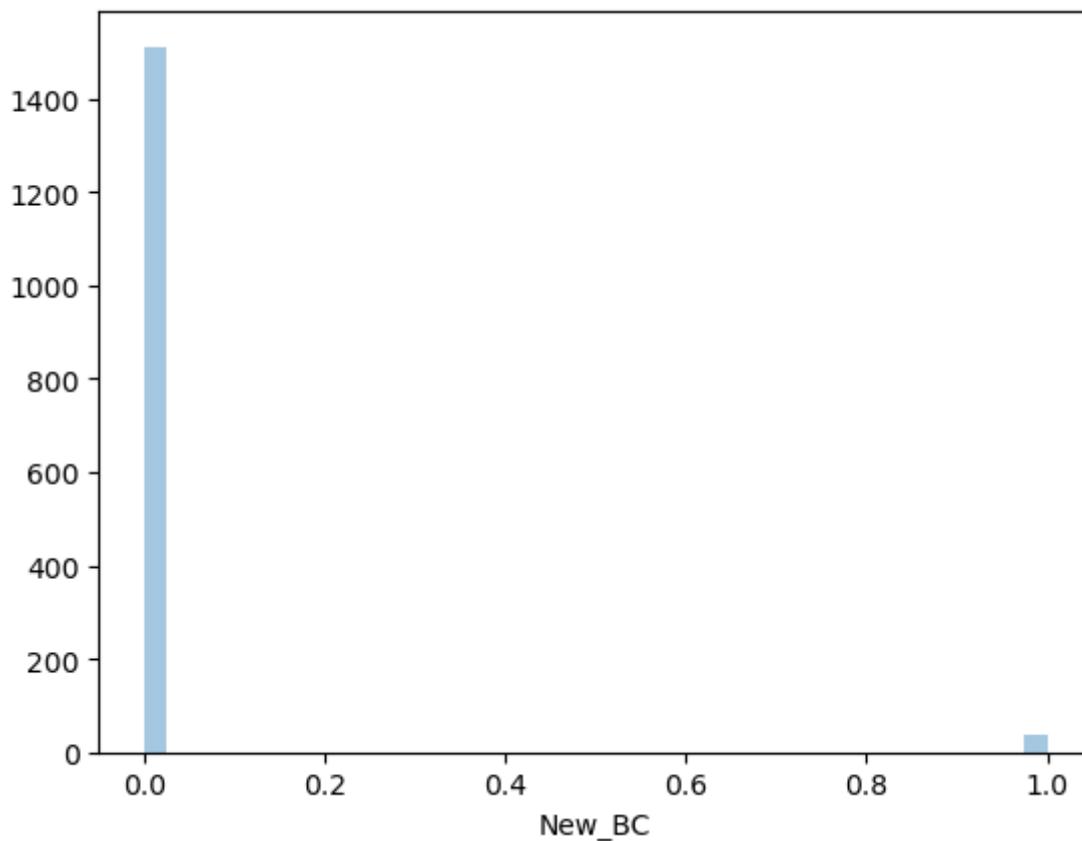


Tools like `sklearn` often have a default threshold of 0.5, but a good threshold is selected based on the data, model and the specific problem you are solving. Looking at the distribution above, we can see that our model rarely assigns a value greater than 0.45, so as a trial run, let's set a threshold of 0.45

```
In [69]: calc_threshold = lambda x,y: 0 if x < y else 1
predicted = np.array( [calc_threshold(score,0.45) for score in y_scores] )
expected = y_test
```

```
In [70]: sns.distplot(expected, kde=False, rug=False)
```

```
Out[70]: <AxesSubplot:xlabel='New_BC'>
```



Confusion Matrix

Once we have tuned our scores to 0 or 1 for classification, we create a *confusion matrix*, which has four cells: true negatives, true positives, false negatives, and false positives. Each data point belongs in one of these cells, because it has both a ground truth and a predicted label. If an example was predicted to be negative and is negative, it's a true negative. If an example was predicted to be positive and is positive, it's a true positive. If an example was predicted to be negative and is positive, it's a false negative. If an example was predicted to be positive and is negative, it's a false positive.

Actual Values

Positive (1) Negative (0)

S

--	--

```
In [71]: from sklearn.metrics import confusion_matrix
conf_matrix = confusion_matrix(expected,predicted)
print(conf_matrix)
```

```
[[1512    0]
 [ 37    0]]
```

Accuracy

Accuracy is the ratio of the correct predictions (both positive and negative) to all predictions.

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

```
In [72]: # generate an accuracy score by comparing expected to predicted.
from sklearn.metrics import accuracy_score
accuracy = accuracy_score(expected, predicted)
print( "Accuracy = " + str( accuracy ) )
```

```
Accuracy = 0.9761136216914138
```

Precision and Recall.

Two additional metrics that are often used are **precision** and **recall**.

Precision measures the accuracy of the classifier when it predicts an example to be positive. It is the ratio of correctly predicted positive examples to examples predicted to be positive.

$$Precision = \frac{TP}{TP + FP}$$

Recall measures the accuracy of the classifier to find positive examples in the data.

$$Recall = \frac{TP}{TP + FN}$$

By selecting different thresholds we can vary and tune the precision and recall of a given classifier. A conservative classifier (threshold 0.99) will classify a case as 1 only when it is *very sure*, leading to high precision. On the other end of the spectrum, a low threshold (e.g. 0.01) will lead to higher recall.

```
In [73]: from sklearn.metrics import precision_score, recall_score
precision = precision_score(expected, predicted)
recall = recall_score(expected, predicted)
print( "Precision = " + str(precision) )
print( "Recall= " + str(recall))
```

```
Precision = 0.0
Recall= 0.0
```

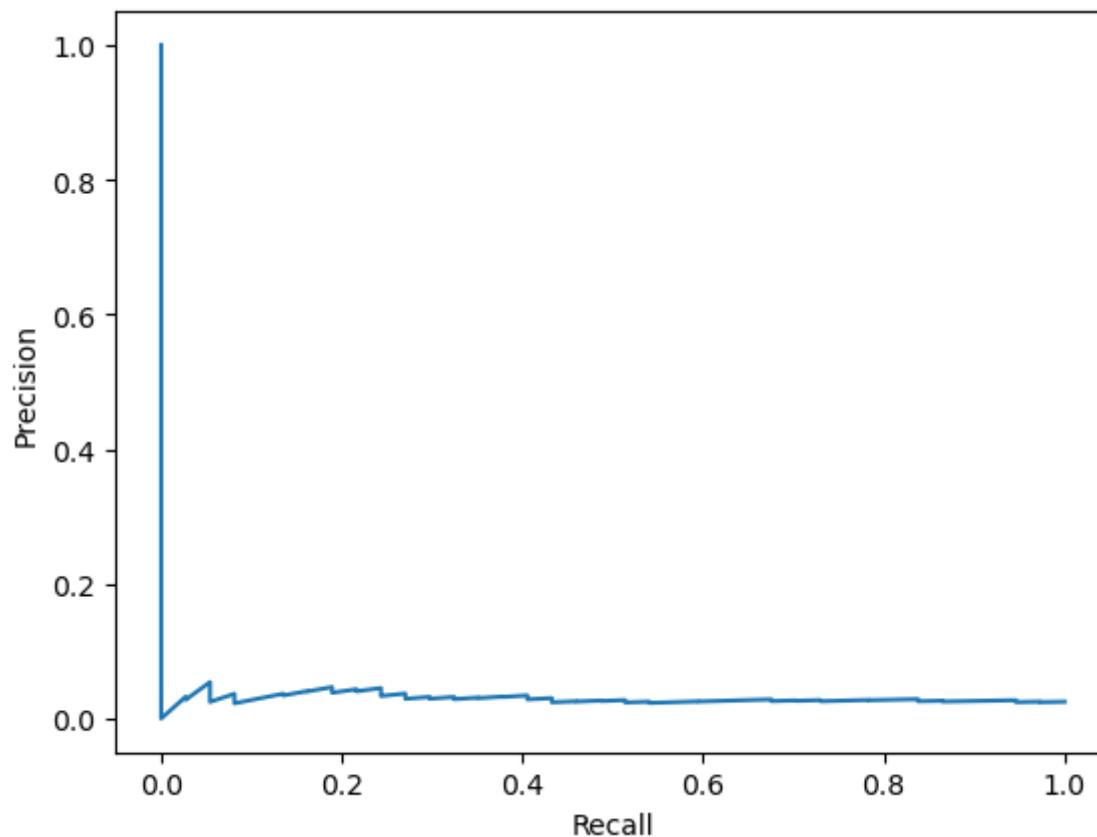
If we care about our whole precision-recall space, we can optimize for a metric known as the **area under the curve (AUC-PR)**, which is the area under the precision-recall curve. The maximum AUC-PR is 1.

```
In [74]: def plot_precision_recall(y_true,y_score):
    """
    Plot a precision recall curve

    Parameters
    -----
    y_true: ls
        ground truth labels
    y_score: ls
        score output from model
    """
    precision_curve, recall_curve, pr_thresholds = precision_recall_curve(y_true, y_score)
    plt.plot(recall_curve, precision_curve)
    plt.xlabel('Recall')
    plt.ylabel('Precision')
    auc_val = auc(recall_curve,precision_curve)
    print('AUC-PR: {:.1f}'.format(auc_val))
    plt.show()
    plt.clf()
```

```
In [75]: plot_precision_recall(expected, y_scores)
```

AUC-PR: 0.029165



<Figure size 640x480 with 0 Axes>

Precision and Recall at k%

If we only care about a specific part of the precision-recall curve we can focus on more fine-grained metrics. For instance, say NIH wants to host a workshop for people they think are likely to do brain cancer research in the future. The workshop is expensive so they only want to select the top 1% of people who are likely to do brain cancer research in the future. In that case, we would want to prioritize the 1% of applicants who are *most likely* to have future brain cancer research, and it doesn't matter too much how accurate we are on the ones who aren't very likely to have brain cancer research in the future. We can then focus on optimizing our **precision at 1%**.

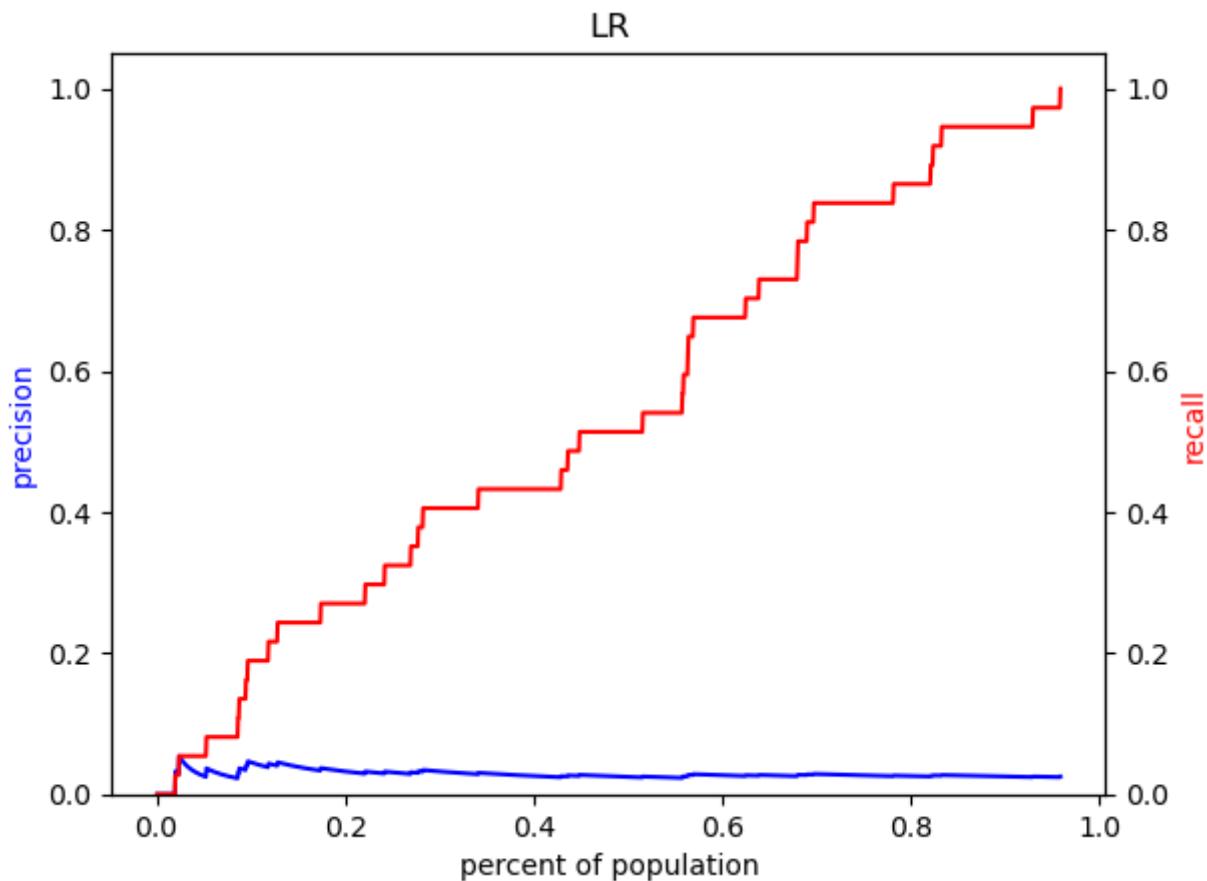
```
In [76]: def plot_precision_recall_n(y_true, y_prob, model_name):
    """
    y_true: ls
        ls of ground truth labels
    y_prob: ls
        ls of predic proba from model
    model_name: str
        str of model name (e.g, LR_123)
    """
    from sklearn.metrics import precision_recall_curve
    y_score = y_prob
    precision_curve, recall_curve, pr_thresholds = precision_recall_curve(y_true, y_score)
    precision_curve = precision_curve[:-1]
    recall_curve = recall_curve[:-1]
    pct_above_per_thresh = []
    number_scored = len(y_score)
    for value in pr_thresholds:
        num_above_thresh = len(y_score[y_score >= value])
        pct_above_thresh = num_above_thresh / float(number_scored)
        pct_above_per_thresh.append(pct_above_thresh)
    pct_above_per_thresh = np.array(pct_above_per_thresh)
    plt.clf()
    fig, ax1 = plt.subplots()
    ax1.plot(pct_above_per_thresh, precision_curve, 'b')
    ax1.set_xlabel('percent of population')
    ax1.set_ylabel('precision', color='b')
    ax1.set_ylim(0, 1.05)
    ax2 = ax1.twinx()
    ax2.plot(pct_above_per_thresh, recall_curve, 'r')
    ax2.set_ylabel('recall', color='r')
    ax2.set_ylim(0, 1.05)

    name = model_name
    plt.title(name)
    plt.show()
    plt.clf()
```

```
In [77]: def precision_at_k(y_true, y_scores, k):
    threshold = np.sort(y_scores)[::-1][int(k * len(y_scores))]
    y_pred = np.asarray([1 if i >= threshold else 0 for i in y_scores])
    return precision_score(y_true, y_pred)
```

```
In [78]: plot_precision_recall_n(expected,y_scores, 'LR')
```

<Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

```
In [79]: p_at_1 = precision_at_k(expected,y_scores, 0.01)
print('Precision at 1%: {:.2f}'.format(p_at_1))
```

Precision at 1%: 0.00

Assess Model Against Baselines

It is important to check our model against a reasonable **baseline** to know how well our model is doing. Without any context, .57% accuracy does not sound great... but that really depends on how well you would do by declaring everyone will not no Cancer researcher in the future, which would be stupid (not to mention useless) model.

A good place to start is checking against a *random* baseline, assigning every example a label (positive or negative) completely at random.

```
In [80]: random_score = [random.uniform(0,1) for i in enumerate(y_test)]
random_predicted = np.array([calc_threshold(score,0.5) for score in random_score])
random_p_at_5 = precision_at_k(expected[random_predicted], 0.01)
print('Precision at 1% (random): {:.2f}'.format(random_p_at_5))
```

Precision at 1% (random): 0.02

Check point 2

1) Formulate a prediction problem that is relevant to your project (2 points)

My Machine Learning Problem

In the following notebook, I will build a model to predict what PIs who work on NCI projects in 2014 will NOT begin a new project researching HPV after the Cancer moonshot initiative.

MG comment: It is not clear to me why it is valuable to predict which of the PIs who work on NCI projects in 2014 will NOT begin a new project researching HPV after the Cancer moonshot initiative. I appreciate that you tried to change things up a bit, but this needed further explanation to convince me it was a worthwhile prediction problem. (-1 point)

2) Read in your own data and select the appropriate subset of variables and observations(1 point)

```
In [81]: # Specify a path with the data folder
# Change "NAME" to your name as recorded on your computer
# path = 'C:/Users/NAME/PADM-GP_2505/Data/'
Path = "/Users/wsq/Desktop/Advanced Data Analytics and Evidence Building/PA"

# use the chdir function from the os package to set your working directory
os.chdir(Path + "/Projects")
```

```
In [82]: # Read-in the 2014 projects file
grants_2014 = pd.read_csv('/Users/wsq/Desktop/Advanced Data Analytics and Evidence Building/PA/Projects/grants_2014.csv')
```

```
In [83]: grants_2014.head()
```

	APPLICATION_ID	ACTIVITY	ADMINISTERING_IC	APPLICATION_TYPE	ARRA_FUNDED	AWARD_N
0	8759648	U2G		PS	3.0	N
1	8715629	R44		CA	2.0	N
2	8676705	R01		CA	5.0	N
3	8627980	R44		HL	5.0	N
4	8609633	UM1		AI	2.0	N

5 rows × 46 columns

In [84]: grants_2014[['APPLICATION_ID', 'FY', 'IC_NAME', 'PI_IDS', 'PROJECT_START', 'NIH_SPENDING_CATS']]

Out[84]:	APPLICATION_ID	FY	IC_NAME	PI_IDS	PROJECT_START	NIH_SPENDING_CATS
0	8759648	2014	National Center for HIV/AIDS, Viral Hepatitis,...	11600459;	9/30/2009	NaN
1	8715629	2014	NATIONAL CANCER INSTITUTE	8495898 (contact); 1888559;	2/1/2006	Bioengineering; Cancer; Contraception/Reproduct...
2	8676705	2014	NATIONAL CANCER INSTITUTE	3150322;	8/1/2010	Breast Cancer; Cancer; Clinical Research; Clin...
3	8627980	2014	NATIONAL HEART, LUNG, AND BLOOD INSTITUTE	8079908 (contact); 9243547;	7/5/2012	Bioengineering; Brain Disorders; Cardiovascula...
4	8609633	2014	NATIONAL INSTITUTE OF ALLERGY AND INFECTIOUS D...	1874862; 1985665 (contact); 1944840;	2/1/2007	Clinical Research; Clinical Trials; HIV/AIDS; ...

```
In [85]: grants_2014 = grants_2014.reset_index()

# First we need to convert PI_IDS into a string variable
grants_2014['PI_IDS'] = grants_2014['PI_IDS'].astype(str)

# Make a temporary dataframe that creates an observation for each PI.
# Use the explode function to split the PI_IDS at the ;
temp = grants_2014['PI_IDS'].str.split(';').explode().reset_index()

# Rename the PI_IDS variable
temp = temp.rename(columns = {'PI_IDS': 'PI_ID'})

# Replace " " with and empty string
temp['PI_ID'] = temp['PI_ID'].str.replace(' ', '')

# Only keep observations in the temp dataframe where PI_ID is not an empty
temp = temp[temp['PI_ID'] != ""]
temp = temp[temp['PI_ID'] != " "]
temp = temp[temp['PI_ID'] != ""]

# For the the PI_ID variable, use the str.replace function to replace ` (co
temp['PI_ID'] = temp['PI_ID'].str.replace('\(contact\)', '')

# Merge this temporary dataframe with grants_2014
grants_2014B = grants_2014.merge(temp, on = 'index')

# Filter for NCI prjects
grants_2014B = grants_2014B[grants_2014B['IC_NAME'] == 'NATIONAL CANCER INS

# Exclude HPV NCI projects
#grants_2014B = grants_2014B[~grants_2014B['NIH_SPENDING_CATS'].str.contains

# view the select variables for the firts 5 observations
grants_2014B[['APPLICATION_ID', 'PI_NAMES', 'PI_ID', 'PI_IDS', 'FY', 'FULL_PRO
```

Out[85]:

	APPLICATION_ID	PI_NAMES	PI_ID	PI_IDS	FY	FULL_PROJECT_NUM	PROJECT_TITLE
1	8715629	BURDETTE, EVERETTE C (contact); DIEDERICH, CHR...	8495898	8495898 (contact); 1888559;	2014	2R44CA121740-02	Minimally Invasive High Intensity Ultrasound T...
2	8715629	BURDETTE, EVERETTE C (contact); DIEDERICH, CHR...	1888559	8495898 (contact); 1888559;	2014	2R44CA121740-02	Minimally Invasive High Intensity Ultrasound T...
3	8676705	BICKELL, NINA A;	3150322	3150322;	2014	5R01CA149025-05	Implementing a Tracking & Feedback Registry to...
17	8616355	TUSCHL, THOMAS ;	7337985	7337985;	2014	5R01CA159227-04	Development of quantitative multiplex RNA in s...
19	8585032	BESSLER, MONICA ;	3144163	3144163;	2014	5R01CA105312-09	MOLECULAR STUDIES OF BONE MARROW FAILURE

3) Create a label that will allow you to address the problem you stated in #1 (1 point)

In [86]:

```
# Identify the files you want to read in
years = ('RePORTER_PRJ_C_FY2016_new.csv', 'RePORTER_PRJ_C_FY2017_new.csv',
```

```
In [87]: # Generate an empty dataframe that will hold all the patent data we have
NCI_2016_2020 = pd.DataFrame([])

# Now loop through each file identified in the years vector
# Read that file using only the columns we need
# And append it to the dataframe that we created above
# This might take a little while to run (no more than 1 minute)
for counter, file in enumerate(years):
    print(counter,file)
    projects = pd.read_csv(file, usecols=['APPLICATION_ID', 'FY', 'IC_NAME',
                                           encoding='latin-1')
    # Filter for NCI projects
    projects = projects[projects['IC_NAME'] == 'NATIONAL CANCER INSTITUTE']

    # Select HPV NCI projects
    #projects = projects[projects['NIH_SPENDING_CATS'].str.contains('HPV', n=1, case=False)]

    # Exclude HPV NCI projects
    projects = projects[projects['NIH_SPENDING_CATS'].str.contains('HPV', n=1, case=False) == False]

    # convert PROJECT_START into a date variable
    projects['PROJECT_START'] = pd.to_datetime(projects['PROJECT_START'])

    NCI_2016_2020 = NCI_2016_2020.append(projects)

NCI_2016_2020 = NCI_2016_2020.reset_index(drop=True)
NCI_2016_2020.head(20)
```

0 RePORTER_PRJ_C_FY2016_new.csv
1 RePORTER_PRJ_C_FY2017_new.csv
2 RePORTER_PRJ_C_FY2018_new.csv
3 RePORTER_PRJ_C_FY2019_new.csv
4 RePORTER_PRJ_C_FY2020_new.csv

	1003	1795	3161	4070	4677	6718	9325	12737	13272	15289	...	74049	75678	75691	760
0	NaT	2015-08-15	2005-04-08	2016-07-15	2016-08-01	NaT	NaT	2016-09-15	NaT	2016-04-14	...	NaT	NaT	NaT	NaT
1	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	...	NaT	NaT	NaT	NaT
2	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	...	NaT	NaT	NaT	NaT
3	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	...	NaT	NaT	NaT	NaT
4	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	NaT	...	2020-09-18	2017-02-03	2020-03-01	2020-08

5 rows × 275 columns

```
In [88]: # Generate an empty dataframe that will hold all the patent data we have
NCI_2016_2020 = pd.DataFrame([])

# Now loop through each file identified in the years vector
# Read that file using only the columns we need
# And append it to the dataframe that we created above
# This might take a little while to run (no more than 1 minute)
for counter, file in enumerate(years):
    print(counter,file)
    projects = pd.read_csv(file, usecols=['APPLICATION_ID', 'FY', 'IC_NAME',
                                           encoding='latin-1'])
    # Filter for NCI projects
    projects = projects[projects['IC_NAME'] == 'NATIONAL CANCER INSTITUTE']
    # Select HPV NCI projects
    projects = projects[~projects['NIH_SPENDING_CATS'].str.contains('HPV')]

    # convert PROJECT_START into a date variable
    projects['PROJECT_START'] = pd.to_datetime(projects['PROJECT_START'])

    NCI_2016_2020 = NCI_2016_2020.append(projects)

NCI_2016_2020 = NCI_2016_2020.reset_index(drop=True)
NCI_2016_2020.head(20)
```

```
0 RePORTER_PRJ_C_FY2016_new.csv
1 RePORTER_PRJ_C_FY2017_new.csv
2 RePORTER_PRJ_C_FY2018_new.csv
3 RePORTER_PRJ_C_FY2019_new.csv
4 RePORTER_PRJ_C_FY2020_new.csv
```

Out[88]:

	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START
0	9036357	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Clinical Research; Prostate Can...	1866031; 1880492 (contact); 9197685; 6667892;	2015-04-01
1	9047257	2016	NATIONAL CANCER INSTITUTE	Cancer; Diagnostic Radiology;	1858946 (contact); 9880120;	2015-04-06
2	9264070	2016	NATIONAL CANCER INSTITUTE	Cancer; Complementary and Alternative Medicine...	1860747 (contact); 2026105;	2012-08-14
3	9057474	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Prostate Cancer; Regenerative M...	2564393;	2012-08-01
4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-09-20
5	9178971	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; Prevention;	1912832;	1997-01-01
6	9109590	2016	NATIONAL CANCER INSTITUTE	Aging; Bioengineering; Cancer; Clinical Resear...	6375366; 6060960 (contact);	2015-07-14
7	9353540	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; Prevention; Rural H...	1860389; 7008046 (contact); 7809558;	2005-09-30
8	9132671	2016	NATIONAL CANCER INSTITUTE	Breast Cancer; Cancer; Clinical Research; Clin...	11184125 (contact); 10433776; 2423744; 7821138...	2010-05-01
9	9127093	2016	NATIONAL CANCER INSTITUTE		NaN	1921608; 1860749 (contact);
10	9212214	2016	NATIONAL CANCER INSTITUTE		NaN	1860389; 7008046; 7809558 (contact);
11	9105247	2016	NATIONAL CANCER INSTITUTE	Biotechnology; Cancer; Genetics;	2201860;	2001-07-01
12	9128679	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; Urologic Diseases;	11776601;	2014-09-16
13	9155094	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Clinical Research; Genetics; Pr...	12300579;	2016-08-26
14	9118700	2016	NATIONAL CANCER INSTITUTE	Biotechnology; Cancer; Cancer Genomics; Colo-R...	11649269;	2015-08-01

	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START
15	9172374	2016	NATIONAL CANCER INSTITUTE	Cancer; Digestive Diseases; Neurosciences;	1890362;	2016-09-07
16	9337154	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; (contact);	10468677; 9164004; 10879957; 3116287	2015-09-24
17	8998415	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; Clinical Trials and...	8183362;	1997-01-15
18	9042963	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; Clinical Trials and...	9294195;	NaT
19	9343609	2016	NATIONAL CANCER INSTITUTE	Cancer; Genetics;	2411391;	NaT

```
In [89]: # reset the index
NCI_2016_2020 = NCI_2016_2020.reset_index()

# view the first 5 observations
NCI_2016_2020.head()
```

	index	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START
0	0	9036357	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Clinical Research; Prostate Can...	1866031; 1880492 (contact); 9197685; 6667892;	2015-04-01
1	1	9047257	2016	NATIONAL CANCER INSTITUTE	Cancer; Diagnostic Radiology;	1858946 (contact); 9880120;	2015-04-06
2	2	9264070	2016	NATIONAL CANCER INSTITUTE	Cancer; Complementary and Alternative Medicine...	1860747 (contact); 2026105;	2012-08-14
3	3	9057474	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Prostate Cancer; Regenerative M...	2564393;	2012-08-01
4	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-09-20

```
In [90]: # Merge this temporary dataframe with grants_2017
NCI_2016_2020B = NCI_2016_2020.merge(temp, on = 'index')

# view the first 5 observations
NCI_2016_2020B.head(10)
```

Out[90]:

	index	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_START	
0	0	9036357	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Clinical Research; Prostate Can...	1866031; 1880492 (contact); 9197685; 6667892;	2015-04-01	116
1	1	9047257	2016	NATIONAL CANCER INSTITUTE	Cancer; Diagnostic Radiology;	1858946 (contact); 9880120;	2015-04-06	84
2	1	9047257	2016	NATIONAL CANCER INSTITUTE	Cancer; Diagnostic Radiology;	1858946 (contact); 9880120;	2015-04-06	18
3	2	9264070	2016	NATIONAL CANCER INSTITUTE	Cancer; Complementary and Alternative Medicine...	1860747 (contact); 2026105;	2012-08-14	31
4	3	9057474	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Prostate Cancer; Regenerative M...	2564393;	2012-08-01	80
5	3	9057474	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Prostate Cancer; Regenerative M...	2564393;	2012-08-01	92
6	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-09-20	18
7	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-09-20	19
8	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-09-20	19
9	5	9178971	2016	NATIONAL CANCER INSTITUTE	Cancer; Clinical Research; Prevention;	1912832;	1997-01-01	86

```
In [91]: # Define the start as the pridr day in Fiscal year 2016
Start_date = pd.to_datetime('10/01/2015')

# select all nci projects (that started after FY 2016)
New_NCI_PI = NCI_2016_2020B[NCI_2016_2020B['PROJECT_START'] >= Start_date]

# Reset index
New_NCI_PI = New_NCI_PI.reset_index()

# view the firts 5 observations
New_NCI_PI.head()
```

Out[91]:

	level_0	index	APPLICATION_ID	FY	IC_NAME	NIH_SPENDING_CATS	PI_IDS	PROJECT_ST
0	6	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-0
1	7	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-0
2	8	4	9125588	2016	NATIONAL CANCER INSTITUTE	Aging; Behavioral and Social Science; Cancer; ...	2429035; 6802765; 1942894 (contact);	2016-0
3	17	13	9155094	2016	NATIONAL CANCER INSTITUTE	Aging; Cancer; Clinical Research; Genetics; Pr...	12300579;	2016-0
4	19	15	9172374	2016	NATIONAL CANCER INSTITUTE	Cancer; Digestive Diseases; Neurosciences;	1890362;	2016-0

```
In [92]: New_NCI_PI = New_NCI_PI[['PI_ID']].drop_duplicates()
New_NCI_PI["New HPV"] = 1

# view the select variables for the firts 4 observations
New_NCI_PI.head(8)
```

Out[92]:

	PI_ID	New HPV
0	1874862	1
1	1985665	1
2	1944840	1
3	7337985	1
4	3144163	1
5	6666441	1
6	6579212	1
7	1898902	1

```
In [93]: # Merge the temp dataframe into the DF_2015 data frame
# Use an left merge
# keep only the PI_ID and NCI_2017 variables and then drop duplicates. This
DF = pd.merge(grants_2014B, New_NCI_PI, on='PI_ID', how = 'left')[['PI_ID'],
DF.head()
```

Out[93]:

	PI_ID	New_HPV
0	8495898	NaN
1	1888559	NaN
2	3150322	NaN
3	7337985	1.0
4	3144163	1.0

```
In [94]: DF['New_HPV'] = DF['New_HPV'].fillna(0)
DF.head()
```

Out[94]:

	PI_ID	New_HPV
0	8495898	0.0
1	1888559	0.0
2	3150322	0.0
3	7337985	1.0
4	3144163	1.0

In [95]: DF.shape

Out[95]: (7741, 2)

In [96]: sum(DF['New_HPV'])

Out[96]: 3691.0

- 4) Create at least 5 different feature groups (a group can be a single feature like normalized total cost, or a group of dummy variables like spending catagory variables) (2 point)

Spending Category

In [97]: grants_2014B[['NIH_SPENDING_CATS']].head()

Out[97]: NIH_SPENDING_CATS

- | | NIH_SPENDING_CATS |
|----|---|
| 1 | Bioengineering; Cancer; Contraception/Reprodu... |
| 2 | Bioengineering; Cancer; Contraception/Reprodu... |
| 3 | Breast Cancer; Cancer; Clinical Research; Clin... |
| 17 | Biotechnology; Cancer; Clinical Research; Gene... |
| 19 | Cancer; Clinical Research; Genetics; Hematolog... |

Separate up the Spending Category

```
# First we need to convert PI_IDS into a string variable
grants_2014B['PI_IDS'] = grants_2014B['NIH_SPENDING_CATS'].astype(str)

# Make a temporary dataframe that creates an observation for each spending
# Use the explode function to split the NIH_SPENDING_CATS at the ;
temp = grants_2014B['NIH_SPENDING_CATS'].str.split(';').explode().reset_index()

# Rename the NIH_SPENDING_CATS variable
temp = temp.rename(columns = {'NIH_SPENDING_CATS': 'NIH_SPENDING_CAT'})

# Replace " " with an empty string
temp['NIH_SPENDING_CAT'] = temp['NIH_SPENDING_CAT'].str.replace(' ', '')

# Only keep observations in the temp dataframe where PI_ID is not an empty
temp = temp[temp['NIH_SPENDING_CAT'] != ""]

temp.head(10)
```

Out[98]:

	index	NIH_SPENDING_CAT
0	1	Bioengineering
1	1	Cancer
2	1	Contraception/Reproduction
3	1	DiagnosticRadiology
4	1	FibroidTumors(Uterine)
6	2	Bioengineering
7	2	Cancer
8	2	Contraception/Reproduction
9	2	DiagnosticRadiology
10	2	FibroidTumors(Uterine)

```
In [99]: # Select the relevant columns
Cat = grants_2014B[['index', 'PI_ID', 'NIH_SPENDING_CATS']]

Cat.head()
```

Out[99]:

	index	PI_ID	NIH_SPENDING_CATS
1	1	8495898	Bioengineering; Cancer; Contraception/Reprodu...
2	1	1888559	Bioengineering; Cancer; Contraception/Reprodu...
3	2	3150322	Breast Cancer; Cancer; Clinical Research; Clin...
17	13	7337985	Biotechnology; Cancer; Clinical Research; Gene...
19	15	3144163	Cancer; Clinical Research; Genetics; Hematolog...

```
In [100]: # Merge this temporary dataframe with the spending category dataframe
Cat2 = Cat.merge(temp, on = 'index')

# Remove the index and NIH_SPENDING_CATS variables
Cat2 = Cat2.drop(columns=['index', 'NIH_SPENDING_CATS'])

# Drop duplicate observations
Cat2 = Cat2.drop_duplicates()

# Drop duplicate observations
Cat2['Cat'] = 1

# View the first 10 observations
Cat2.head(10)
```

Out[100]:

	PI_ID	NIH_SPENDING_CAT	Cat
0	8495898	Bioengineering	1
1	8495898	Cancer	1
2	8495898	Contraception/Reproduction	1
3	8495898	DiagnosticRadiology	1
4	8495898	FibroidTumors(Uterine)	1
5	1888559	Bioengineering	1
6	1888559	Cancer	1
7	1888559	Contraception/Reproduction	1
8	1888559	DiagnosticRadiology	1
9	1888559	FibroidTumors(Uterine)	1

```
In [101]: # use the pivot function to transform the dataframe from long to wide
Cat3 = pd.pivot(Cat2, index='PI_ID', columns = 'NIH_SPENDING_CAT',values =
#Re-arange the new columns in the correct order
cols = Cat2['NIH_SPENDING_CAT'].unique()
Cat3=Cat3[cols]

# Replace missing values with 0
Cat3 = Cat3.fillna(0)

# View the first 5 observations
Cat3.head()
```

Out[101]:

	NIH_SPENDING_CAT	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fibr
PI_ID						
10012000	1.0	1.0		0.0		1.0
10021262	0.0	1.0		0.0		0.0
10021476	0.0	1.0		0.0		0.0
10108300	0.0	1.0		0.0		0.0
10113370	0.0	1.0		0.0		0.0

5 rows × 122 columns

```
In [102]: # Join Cat3 with the DF fataframe using a left join
DF = pd.merge(DF, Cat3, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[102]:

	PI_ID	New HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 124 columns

State

```
In [103]: state = grants_2014B[['PI_ID', 'ORG_STATE']]

# Drop duplicate observations
state = state.drop_duplicates()

# Only keep the first state recorded for each PI
state = state.groupby(['PI_ID']).first()

# View the first 5 observations
state.head()
```

Out[103]: ORG_STATE

PI_ID	
10000506	None
10011128	AZ
10012000	MA
10021262	ON
10021476	NY

```
In [104]: # We need to create dummy variables for state and organization name
state2 = pd.get_dummies(state, columns=['ORG_STATE'])

state2.head()
```

Out[104]: ORG_STATE_AK ORG_STATE_AL ORG_STATE_AR ORG_STATE_AZ ORG_STATE_BC ORG_

PI_ID	ORG_STATE_AK	ORG_STATE_AL	ORG_STATE_AR	ORG_STATE_AZ	ORG_STATE_BC	ORG_
10000506	0	0	0	0	0	0
10011128	0	0	0	1	0	0
10012000	0	0	0	0	0	0
10021262	0	0	0	0	0	0
10021476	0	0	0	0	0	0

5 rows × 53 columns

In [105]: state2.shape

Out[105]: (7741, 53)

```
In [106]: # Select the relevant columns
State_temp = grants_2014B[['index', 'PI_ID', 'ORG_STATE']]
State_temp.head()
```

Out[106]:

	index	PI_ID	ORG_STATE
1	1	8495898	IL
2	1	1888559	IL
3	2	3150322	NY
17	13	7337985	NY
19	15	3144163	PA

```
In [107]: # Merge this temporary dataframe with the spending catagory dataframe
State_temp2 = State_temp.merge(temp, on = 'index')

# Remove the index and NIH_SPENDING_CATS variables
State_temp2 = State_temp2.drop(columns=['index', 'NIH_SPENDING_CAT'])

# Drop duplicate observations
State_temp2 = State_temp2.drop_duplicates()

# Drop duplicate observations
State_temp2['State_temp'] = 1

# View the first 10 observations
State_temp2.head(10)
```

Out[107]:

	PI_ID	ORG_STATE	State_temp
0	8495898	IL	1
5	1888559	IL	1
10	3150322	NY	1
15	6265424	NY	1
19	12448156	NaN	1
23	1869066	HI	1
27	12430520	CA	1
34	8590003	TN	1
36	1877317	TN	1
38	7284983	WA	1

```
In [108]: # use the pivot function to transform the dataframe from long to wide
State_temp3 = pd.pivot(State_temp2, index='PI_ID', columns = 'ORG_STATE', values='Value')

#Re-arange the new columns in the correct order
cols = State_temp2['ORG_STATE'].unique()
State_temp3=State_temp3[cols]

# Replace missing values with 0
State_temp3 = State_temp3.fillna(0)

# View the first 5 observations
State_temp3.head()
```

Out[108]:

PI_ID	ORG_STATE	IL	NY	NaN	HI	CA	TN	WA	MA	KS	OR	...	VT	MS	QC	LA	SD	PR	NV	D
10012000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
10021262	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
10021476	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
10108300	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
10113370	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

5 rows × 50 columns

```
In [109]: # Join Cat3 with the DF fataframe using a left join
DF = pd.merge(DF, State_temp3, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[109]:

PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0	1.0	1.0
1	1888559	0.0	1.0	1.0	1.0	1.0
2	3150322	0.0	1.0	1.0	1.0	1.0
3	7337985	1.0	NaN	NaN	NaN	NaN
4	3144163	1.0	NaN	NaN	NaN	NaN

5 rows × 174 columns

```
In [110]: # Join Cat3 with the DF fataframe using a left join
DF = pd.merge(DF, State_temp3, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[110]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 224 columns

```
In [111]: # We need to creat dummy variables for state and organization name
state2 = pd.get_dummies(state, columns=['ORG_STATE'])

state2.head()
```

Out[111]:

PI_ID	ORG_STATE_AK	ORG_STATE_AL	ORG_STATE_AR	ORG_STATE_AZ	ORG_STATE_BC	ORG_
10000506	0	0	0	0	0	0
10011128	0	0	0	1	0	0
10012000	0	0	0	0	0	0
10021262	0	0	0	0	0	0
10021476	0	0	0	0	0	0

5 rows × 53 columns

```
In [112]: state2.shape
```

Out[112]: (7741, 53)

```
In [113]: # use a left join nerge to join the state2 data witht the DF dataframe
DF = pd.merge(DF, state2, on = 'PI_ID', how = 'left')

# View the first 5 observations
DF.head()
```

Out[113]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 277 columns

```
In [114]: # Calculate how many Projects each PI has
projects = grants_2014B.groupby(['PI_ID'])['APPLICATION_ID'].nunique().sort

# Convert into a dataframe and reset index
projects = projects.to_frame().reset_index()

# Rename APPLICATION_ID to Total_NCI_Projects_2014
projects.rename(columns={'APPLICATION_ID':'Total_NCI_Projects_2014'}, inplace=True)

# View the first 2 observations
projects.head(2)
```

Out[114]:

	PI_ID	Total_NCI_Projects_2014
0	14267998	58
1	1875698	40

Number of projects in 2014

```
In [115]: # Calculate how many Projects each PI has
projects = grants_2014B.groupby(['PI_ID'])['APPLICATION_ID'].nunique().sort

# Convert into a dataframe and reset index
projects = projects.to_frame().reset_index()

# Rename APPLICATION_ID to Total_NCI_Projects_2014
projects.rename(columns={'APPLICATION_ID':'Total_NCI_Projects_2014'}, inplace=True)

# View the first 2 observations
projects.head(2)
```

Out[115]:

	PI_ID	Total_NCI_Projects_2014
0	14267998	58
1	1875698	40

```
In [116]: DF = pd.merge(DF, projects, on = 'PI_ID', how = 'inner')

# View the first 5 observations
DF.head()
```

Out[116]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 278 columns

Number of projects what will still be active in FY 2016

```
In [117]: # convert PROJECT_END into a date variable
grants_2014B['PROJECT_END'] = pd.to_datetime(grants_2014B['PROJECT_END'])
```

```
In [118]: # Identity the end of FY 2015
FY_2016 = pd.to_datetime('09/30/2015')

# Filter for projects that will still be active in 2016
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2016]

# select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2016' that is equal to one for all observations
ongoing['active_2016'] = 1

# View the first 2 observations
ongoing.head(2)
```

Out[118]:

	PI_ID	active_2016
1	8495898	1
2	1888559	1

```
In [119]: # Sum up the number of projects that will still be active in 2016 for each
ongoing = ongoing.groupby('PI_ID')['active_2016'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# View the first 2 observations
ongoing.head(2)
```

Out[119]:

	PI_ID	active_2016
0	10000506	1
1	10011128	1

```
In [120]: # convert PROJECT_END into a date variable
grants_2014B['PROJECT_END'] = pd.to_datetime(grants_2014B['PROJECT_END'])
```

```
In [121]: # Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2017 with 0
DF['active_2016'] = DF['active_2016'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[121]:

	PI_ID	New HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0		NaN	NaN	NaN	NaN
4	3144163	1.0		NaN	NaN	NaN	NaN

5 rows × 279 columns

Number of projects what will still be active in FY 2017

```
In [122]: # Identify the end of FY 2016
FY_2017 = pd.to_datetime('09/30/2016')

# Filter for projects that will still be active in 2017
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2017]

# Select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2017' that is equal to one for all observations
ongoing['active_2017'] = 1

# Sum up the number of projects that will still be active in 2017 for each
ongoing = ongoing.groupby('PI_ID')['active_2017'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2017 with 0
DF['active_2017'] = DF['active_2017'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[122]:

	PI_ID	New HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 280 columns

Number of projects what will still be active in FY 2018

```
In [123]: # Identify the end of FY 2017
FY_2018 = pd.to_datetime('09/30/2017')

# Filter for projects that will still be active in 2016
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2018]

# select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2018' that is equal to one for all observations
ongoing['active_2018'] = 1

# Sum up the number of projects that will still be active in 2018 for each
ongoing = ongoing.groupby('PI_ID')['active_2018'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2018 with 0
DF['active_2018'] = DF['active_2018'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[123]:

	PI_ID	New HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 281 columns

Number of projects what will still be active in FY 2019

```
In [124]: # Identify the end of FY 2018
FY_2019 = pd.to_datetime('09/30/2018')

# Filter for projects that will still be active in 2019
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2019]

# Select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2019' that is equal to one for all observations
ongoing['active_2019'] = 1

# Sum up the number of projects that will still be active in 2019 for each
ongoing = ongoing.groupby('PI_ID')['active_2019'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2019 with 0
DF['active_2019'] = DF['active_2019'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[124]:

	PI_ID	New HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 282 columns

Number of projects what will still be active in FY 2020

```
In [125]: # Identify the end of FY 2019
FY_2020 = pd.to_datetime('09/30/2019')

# Filter for projects that will still be active in 2020
ongoing = grants_2014B[grants_2014B['PROJECT_END'] > FY_2020]

# select only the PI_ID variable
ongoing = ongoing[['PI_ID']]

# Create a new variable 'active_2020' that is equal to one for all observations
ongoing['active_2020'] = 1

# Sum up the number of projects that will still be active in 2020 for each
ongoing = ongoing.groupby('PI_ID')['active_2020'].sum()

# Convert into a dataframe and reset index
ongoing = ongoing.to_frame().reset_index()

# Merge the temp dataframe into the DF data frame
# Use an left merge
DF = pd.merge(DF, ongoing, on='PI_ID', how = 'left')

# Fill the NaN values for active_2020 with 0
DF['active_2020'] = DF['active_2020'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[125]:

	PI_ID	New HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 283 columns

Total Cost of Projects

```
In [126]: # Calculate how many Projects each PI has
Cost = grants_2014B.groupby(['PI_ID'])['TOTAL_COST'].sum()

# Convert into a dataframe and reset index
Cost = Cost.to_frame().reset_index()

# drop first row
Cost = Cost.iloc[1:, :]

# View the first 5 observations
Cost.head()
```

Out[126]:

	PI_ID	TOTAL_COST
1	10011128	750566.0
2	10012000	85785.0
3	10021262	217377.0
4	10021476	278247.0
5	10027192	310470.0

```
In [127]: DF = pd.merge(DF, Cost, on = 'PI_ID', how = 'left')
DF.head()
```

Out[127]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 284 columns

Number of NCI projects by organization

```
In [128]: # Use a conditional statement do create a new dataframe were there are only
HPV = grants_2014B[grants_2014B['NIH_SPENDING_CATS'].str.contains('HPV', na

# Calculate how many NCI Projects each ORG has
HPV = HPV.groupby(['ORG_NAME'])['APPLICATION_ID'].nunique().sort_values(asc

# Convert into a dataframe and reset index
HPV = HPV.to_frame().reset_index()

# Rename APPLICATION_ID to Total_BC_Projects_by_ORG
HPV.rename(columns={'APPLICATION_ID': 'Total_HPV_Projects_by_ORG'}, inplace=True

# View the first 5 observations
HPV.head()
```

Out[128]:

	ORG_NAME	Total_HPV_Projects_by_ORG
0	JOHNS HOPKINS UNIVERSITY	7
1	CANCER EPIDEMIOLOGY AND GENETICS	5
2	UT SOUTHWESTERN MEDICAL CENTER	3
3	UNIVERSITY OF CALIFORNIA, SAN FRANCISCO	3
4	ALBERT EINSTEIN COLLEGE OF MEDICINE	2

	ORG_NAME	Total_HPV_Projects_by_ORG
0	JOHNS HOPKINS UNIVERSITY	7
1	CANCER EPIDEMIOLOGY AND GENETICS	5
2	UT SOUTHWESTERN MEDICAL CENTER	3
3	UNIVERSITY OF CALIFORNIA, SAN FRANCISCO	3
4	ALBERT EINSTEIN COLLEGE OF MEDICINE	2

```
In [129]: HPV2 = pd.merge(grants_2014B, HPV, on = 'ORG_NAME', how = 'left')[['PI_ID']

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
HPV2['Total_HPV_Projects_by_ORG'] = HPV2['Total_HPV_Projects_by_ORG'].fillna(0)

#Drop duplicate observations
HPV2 = HPV2.drop_duplicates()

# View the first 5 observations
HPV2.head()
```

Out[129]:

	PI_ID	Total_HPV_Projects_by_ORG	ORG_NAME
0	8495898	0.0	ACOUSTIC MEDSYSTEMS, INC.
1	1888559	0.0	ACOUSTIC MEDSYSTEMS, INC.
2	3150322	0.0	ICAHN SCHOOL OF MEDICINE AT MOUNT SINAI
3	7337985	0.0	ROCKEFELLER UNIVERSITY
4	3144163	0.0	CHILDREN'S HOSP OF PHILADELPHIA

```
In [130]: # Sum up the number of projects for people who worked for more than one org
HPV3 = HPV2.groupby(['PI_ID'])['Total_HPV_Projects_by_ORG'].sum()

# Convert into a dataframe and reset index
HPV3 = HPV3.to_frame().reset_index()

# View the first 5 observations
HPV3.head()
```

Out[130]:

	PI_ID	Total_HPV_Projects_by_ORG
0	10000506	2.0
1	10011128	0.0
2	10012000	0.0
3	10021262	0.0
4	10021476	0.0

```
In [131]: # use the describe to look at the distribution
HPV3['Total_HPV_Projects_by_ORG'].describe()
```

Out[131]:

count	7741.000000
mean	0.546053
std	1.290736
min	0.000000
25%	0.000000
50%	0.000000
75%	0.000000
max	8.000000

Name: Total_HPV_Projects_by_ORG, dtype: float64

Looking at this distribution, we will break the organizations into the following groups:

- No HPV projects.
- A few HPV projects (1-3)
- A Moderate number of HPV projects (5-9)
- Several HPV projects (10-20)
- A large number of HPV projects (over 20)

No HPV cancer projects

```
In [132]: # Identify observations where the PI is from an org with no brain cancer pr
No = HPV3[HPV3['Total_HPV_Projects_by_ORG'] == 0]

# Create a variable "Org_No" that is equal to 1
No['Org_No'] = 1

# Select the two variables we need
No = No[['PI_ID', 'Org_No']]

# Merge with the DF dataframe
DF = pd.merge(DF, No, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_No'] = DF['Org_No'].fillna(0)

# View the first 5 observations
DF.head()
```

Out[132]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 285 columns

A few HPV projects (1-3)

```
In [133]: # Identify observations where the PI is from an org with 1-3 brain cancer p
Few = HPV3[HPV3['Total_HPV_Projects_by_ORG'] >= 1]
Few = Few[Few['Total_HPV_Projects_by_ORG'] <= 3]

# Create a variable "Org_No" that is equal to 1
Few['Org_Few'] = 1

# Select the two variable we need
Few = Few[['PI_ID', 'Org_Few']]

# Merge with the DF dataframe
DF = pd.merge(DF, Few, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_Few'] = DF['Org_Few'].fillna(0)

DF.head()
```

Out[133]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 286 columns

A Moderate number of HPV cancer projects (5-9)

```
In [134]: # Identify observations where the PI is from an org with 5-9 brain cancer p
Moderate = HPV3[HPV3['Total_HPV_Projects_by_ORG'] >= 5]
Moderate = Moderate[Moderate['Total_HPV_Projects_by_ORG'] <= 9]

# Create a variable "Org_No" that is equal to 1
Moderate['Org_Mod'] = 1

# Select the two variables we need
Moderate = Moderate[['PI_ID', 'Org_Mod']]

# Merge with the DF dataframe
DF = pd.merge(DF, Moderate, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_Mod'] = DF['Org_Mod'].fillna(0)

DF.head()
```

Out[134]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 287 columns

Several HPV cancer projects (10-15)

```
In [135]: # Identify observations where the PI is from an org with 10-20 brain cancer
Several = HPV3[HPV3['Total_HPV_Projects_by_ORG'] >= 10]
Several = Several[Several['Total_HPV_Projects_by_ORG'] <= 20]

# Create a variable "Org_No" that is equal to 1
Several['Org_Several'] = 1

# Select the two variable we need
Several = Several[['PI_ID', 'Org_Several']]

# Merge with the DF dataframe
DF = pd.merge(DF, Several, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_Several'] = DF['Org_Several'].fillna(0)

DF.head()
```

Out[135]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 288 columns

In [136]: #### Large number of HPV projects (over 20)

```
In [137]: # Identify observations where the PI is from an org with more than brain capacity
large = HPV3[HPV3['Total_HPV_Projects_by_ORG'] > 20]

# Create a variable "Org_No" that is equal to 1
large['Org_large'] = 1

# Select the two variables we need
large = large[['PI_ID', 'Org_large']]

# Merge with the DF dataframe
DF = pd.merge(DF, large, on = 'PI_ID', how = 'left')

# Fill the NaN values for Total_BC_Projects_by_ORG with 0
DF['Org_large'] = DF['Org_large'].fillna(0)

DF.head()
```

Out[137]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	NaN	NaN		NaN	NaN
4	3144163	1.0	NaN	NaN		NaN	NaN

5 rows × 289 columns

```
In [138]: DF = DF.fillna(0)
```

MG comment: I appreciate that you came up with some new features :)

Normalization

We need to normalize our non-binary features. To Normalize the data, we will apply a linear transformation so that the values are between 0 and 1. Normalization makes the features more consistent with each other, which allows the model to predict outputs more accurately.

```
In [139]: features_to_normalize = ['active_2016', 'active_2017', 'active_2018', 'active_2019']

DF[features_to_normalize] = DF[features_to_normalize].apply(lambda x:(x-x.mean())/(x.std()))

DF.head()
```

Out[139]:

	PI_ID	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	Fil
0	8495898	0.0	1.0	1.0		1.0	1.0
1	1888559	0.0	1.0	1.0		1.0	1.0
2	3150322	0.0	1.0	1.0		1.0	1.0
3	7337985	1.0	0.0	0.0		0.0	0.0
4	3144163	1.0	0.0	0.0		0.0	0.0

5 rows × 289 columns

Building a Model

We need to divide our dataframe into a training data and test data. We will train our model on the training set and then test it on the test set. We will assign 70% of our data to training set and the remaining 30% to the test set.

5) Split your data into a training and test set (0 point)

```
In [140]: # use the train_test_split to split the data into the training and test set
df_train, df_test = train_test_split(DF, test_size=0.3)
```

```
In [141]: # Look at the distribution of the variables for the training data set
df_train.describe()
```

Out[141]:

	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	I
count	5418.000000	5418.000000	5418.000000		5418.000000	5418.000000
mean	0.471945	0.031561	0.215393		0.000738	0.019749
std	0.499258	0.174846	0.411133		0.027164	0.139149
min	0.000000	0.000000	0.000000		0.000000	0.000000
25%	0.000000	0.000000	0.000000		0.000000	0.000000
50%	0.000000	0.000000	0.000000		0.000000	0.000000
75%	1.000000	0.000000	0.000000		0.000000	0.000000
max	1.000000	1.000000	1.000000		1.000000	1.000000

8 rows × 288 columns

```
In [142]: # Look at the distribution of the variables for the test data set
df_test.describe()
```

Out[142]:

	New_HPV	Bioengineering	Cancer	Contraception/Reproduction	DiagnosticRadiology	I
count	2323.000000	2323.000000	2323.000000	2323.000000	2323.000000	2323.000000
mean	0.488162	0.036591	0.223848	0.001722	0.021954	
std	0.499967	0.187795	0.416911	0.041469	0.146566	
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
50%	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
75%	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
max	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000

8 rows × 288 columns

Class Balancing

Let's check how much data we still have and how many are for PIs with new HPV projects in our training dataset. We don't necessarily need to have a perfect 50-50 balance, but it's good to know what the "baseline" is in our dataset, to be able to intelligently evaluate our performance. If you look at our New_HPV you can see that not about 29% are for PIs that will have a new brain cancer project between 2016-2020

```
In [143]: print('Number of rows: {}'.format(df_train.shape[0]))
df_train['New_HPV'].value_counts(normalize=True)
```

Number of rows: 5418

Out[143]:

0.0	0.528055
1.0	0.471945
Name: New_HPV, dtype:	float64

Let's take a look at our testing set.

```
In [144]: print('Number of rows: {}'.format(df_test.shape[0]))
df_test['New_HPV'].value_counts(normalize=True)
```

Number of rows: 2323

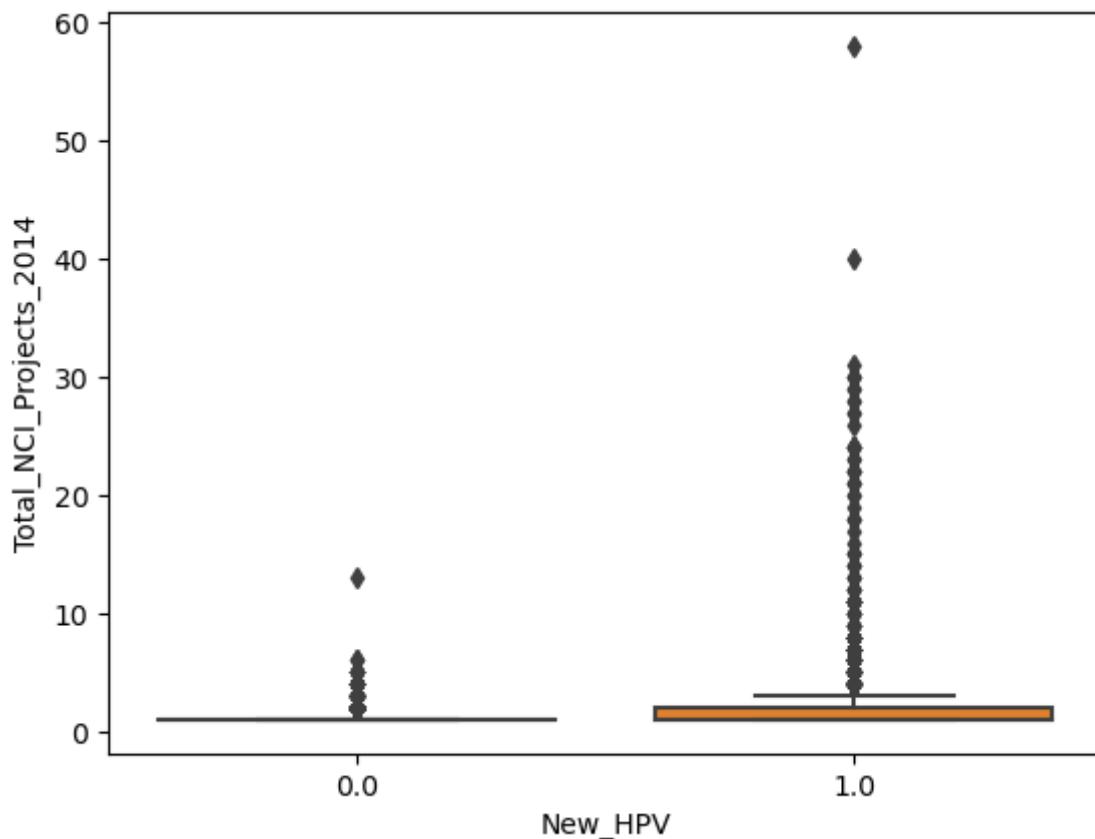
Out[144]:

0.0	0.511838
1.0	0.488162
Name: New_HPV, dtype:	float64

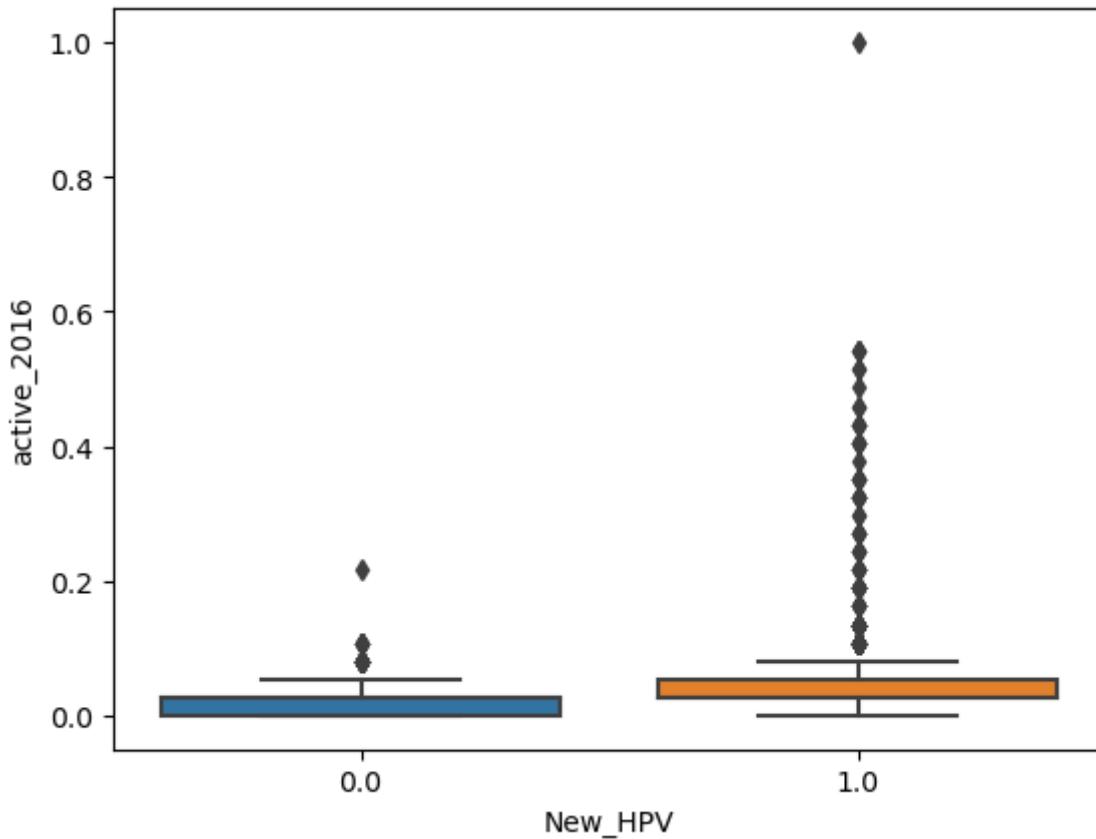
Investigate our data

We can use visualizations to find trends and patterns in our data. We will start by looking at the Total number of NCI projects in 2014, then we will look at the number of projects that will still be active in 2016

```
In [145]: ax = sns.boxplot(x="New_HPV", y="Total_NCI_Projects_2014", data=df_train)
```



```
In [146]: ax = sns.boxplot(x="New_HPV", y="active_2016", data=df_train)
```



Identify the features and label

We need to identify the **features** and **label** for both the training and test datasets

```
In [147]: # use conventions typically used in python scikitlearn
x_train = df_train.drop(columns=['New_HPV'])
y_train = df_train['New_HPV']
x_test = df_test.drop(columns=['New_HPV'])
y_test = df_test['New_HPV']
```

Model Selection

Model Evaluation

In this phase, you take the predictors from your test set and apply your model to them, then assess the quality of the model by comparing the *predicted values* to the *actual values* for each record in your testing data set.

- **Performance Estimation:** How well will our model do once it is deployed and applied to new data?

Now let's use the model we just fit to make predictions on our test dataset, and see what our accuracy score is:

We will start with the simplest [LogisticRegression](http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) (http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) model and see how well that does.

You can use any number of metrics to judge your models, but we'll use [accuracy_score\(\)](http://scikit-learn.org/stable/modules/generated/sklearn.metrics.accuracy_score.html) (http://scikit-learn.org/stable/modules/generated/sklearn.metrics.accuracy_score.html) (ratio of correct predictions to total number of predictions) as our measure.

Type *Markdown* and *LaTeX*: α^2

```
In [148]: from sklearn import linear_model
model = linear_model.LogisticRegression(max_iter = 100, intercept_scaling =
model.fit( X_train, y_train)
print(model)
#https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Log
LogisticRegression(intercept_scaling=2)
```

Model Evaluation

Machine learning models usually do not produce a prediction (0 or 1) directly. Rather, models produce a score between 0 and 1 (that can sometimes be interpreted as a probability), which lets you more finely rank all of the examples from *most likely* to *least likely* to have label 1 (positive). This score is then turned into a 0 or 1 based on a user-specified threshold. For example, you might label all examples that have a score greater than 0.5 (1/2) as positive (1), but there's no reason that has to be the cutoff.

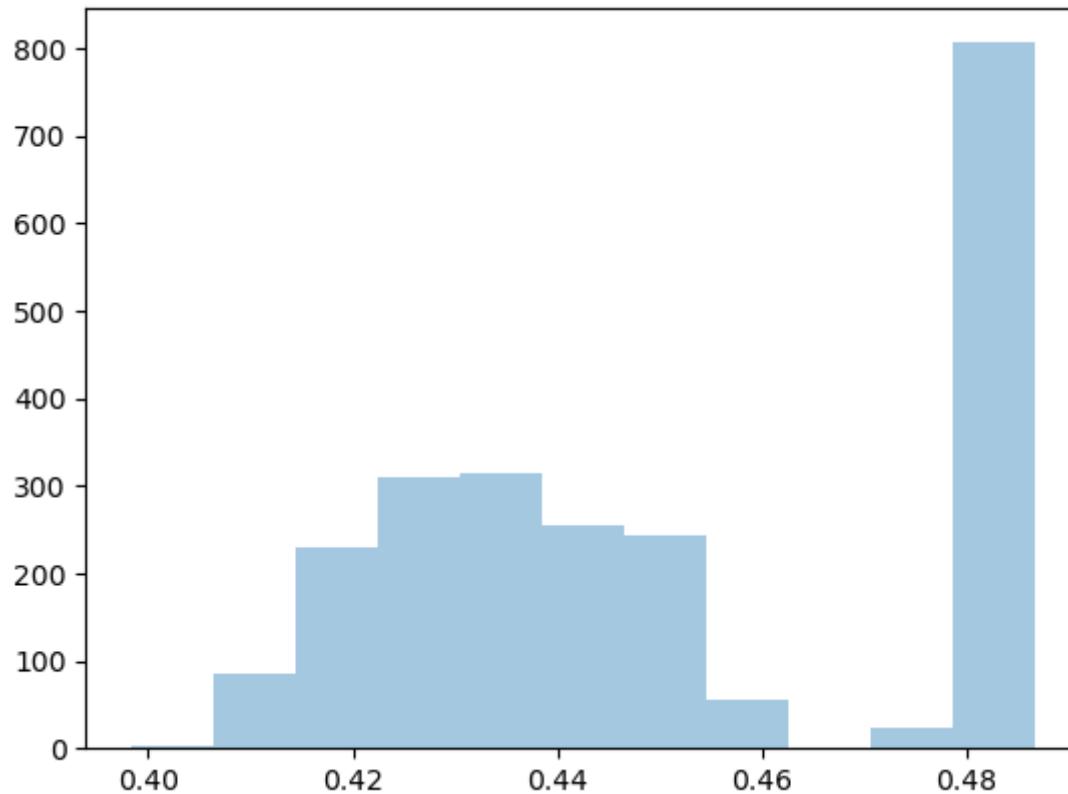
```
In [149]: # from our "predictors" using the model.
y_scores = model.predict_proba(X_test)[:,1]
```

```
In [150]: y_scores
```

```
Out[150]: array([0.48603122, 0.44795924, 0.48592788, ..., 0.44963829, 0.43665631,
0.44259546])
```

```
In [151]: sns.distplot(y_scores, kde=False, rug=False)
```

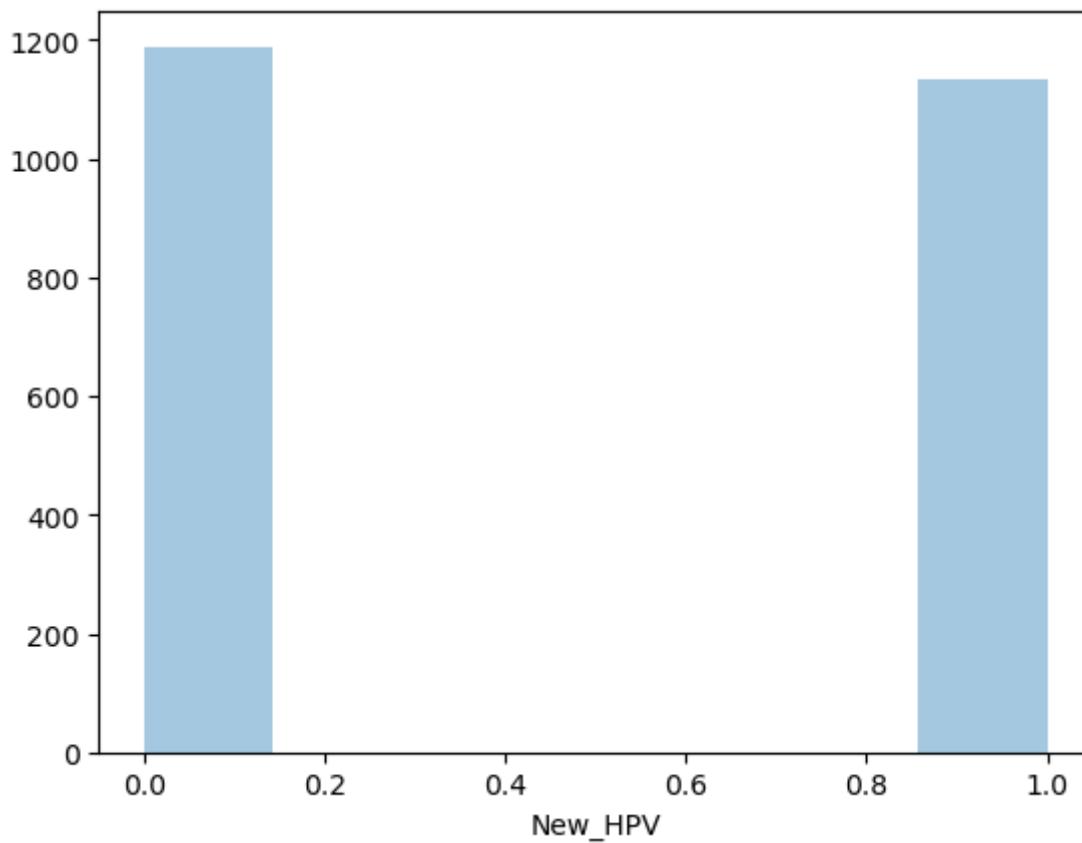
```
Out[151]: <AxesSubplot:>
```



```
In [152]: calc_threshold = lambda x,y: 0 if x < y else 1
predicted = np.array( [calc_threshold(score,0.45) for score in y_scores] )
expected = y_test
```

```
In [153]: sns.distplot(expected, kde=False, rug=False)
```

```
Out[153]: <AxesSubplot:xlabel='New_HPV'>
```



Confusion Matrix

Once we have tuned our scores to 0 or 1 for classification, we create a *confusion matrix*, which has four cells: true negatives, true positives, false negatives, and false positives. Each data point belongs in one of these cells, because it has both a ground truth and a predicted label. If an example was predicted to be negative and is negative, it's a true negative. If an example was predicted to be positive and is positive, it's a true positive. If an example was predicted to be negative and is positive, it's a false negative. If an example was predicted to be positive and is negative, it's a false positive.

Screenshot%202023-04-16%20at%204.04.32%20PM.png

```
In [154]: from sklearn.metrics import confusion_matrix
conf_matrix = confusion_matrix(expected,predicted)
print(conf_matrix)
```

```
[[ 729 460]
 [ 560 574]]
```

Accuracy

Accuracy is the ratio of the correct predictions (both positive and negative) to all predictions.

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

```
In [155]: # generate an accuracy score by comparing expected to predicted.
from sklearn.metrics import accuracy_score
accuracy = accuracy_score(expected, predicted)
print( "Accuracy = " + str( accuracy ) )
```

Accuracy = 0.5609126130004305

Precision and Recall.

Two additional metrics that are often used are **precision** and **recall**.

Precision measures the accuracy of the classifier when it predicts an example to be positive. It is the ratio of correctly predicted positive examples to examples predicted to be positive.

$$Precision = \frac{TP}{TP + FP}$$

Recall measures the accuracy of the classifier to find positive examples in the data.

$$Recall = \frac{TP}{TP + FN}$$

By selecting different thresholds we can vary and tune the precision and recall of a given classifier. A conservative classifier (threshold 0.99) will classify a case as 1 only when it is *very sure*, leading to high precision. On the other end of the spectrum, a low threshold (e.g. 0.01) will lead to higher recall.

```
In [156]: from sklearn.metrics import precision_score, recall_score
precision = precision_score(expected, predicted)
recall = recall_score(expected, predicted)
print( "Precision = " + str( precision ) )
print( "Recall= " + str(recall))
```

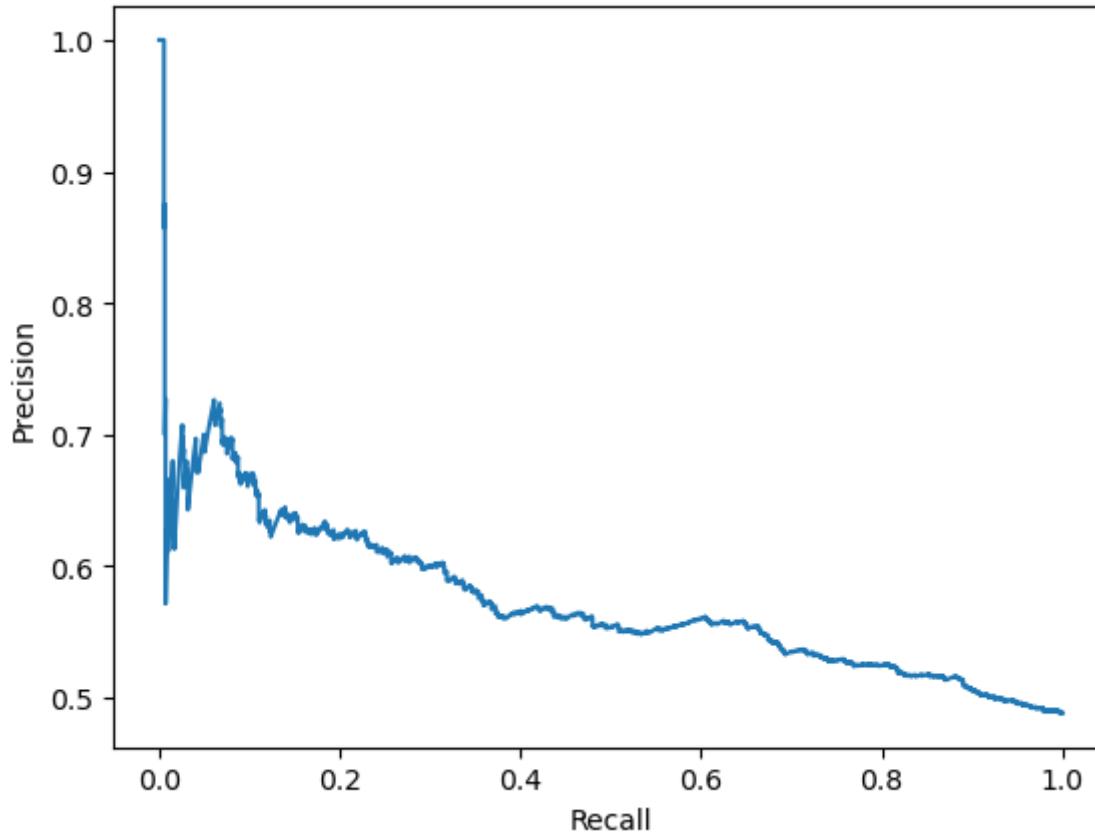
Precision = 0.5551257253384912
 Recall= 0.5061728395061729

```
In [157]: def plot_precision_recall(y_true,y_score):
    """
        Plot a precision recall curve

    Parameters
    -----
    y_true: ls
        ground truth labels
    y_score: ls
        score output from model
    """
    precision_curve, recall_curve, pr_thresholds = precision_recall_curve(y_true,y_score)
    plt.plot(recall_curve, precision_curve)
    plt.xlabel('Recall')
    plt.ylabel('Precision')
    auc_val = auc(recall_curve,precision_curve)
    print('AUC-PR: {0:1f}'.format(auc_val))
    plt.show()
    plt.clf()
```

```
In [158]: plot_precision_recall(expected, y_scores)
```

AUC-PR: 0.573307



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Precision and Recall at k%

If we only care about a specific part of the precision-recall curve we can focus on more fine-grained metrics. For instance, say NIH wants to host a workshop for people they think are likely to do brain cancer research in the future. The workshop is expensive so they only want to select the top 1% of people who are likely to do HPV research in the future. In that case, we would want to prioritize the 1% of applicants who are *most likely* to have future HPV cancer research, and it doesn't matter too much how accurate we are on the ones who aren't very likely to have HPV cancer research in the future. We can then focus on optimizing our **precision at 1%**.

```
In [159]: def plot_precision_recall_n(y_true, y_prob, model_name):
    """
    y_true: ls
        ls of ground truth labels
    y_prob: ls
        ls of predic proba from model
    model_name: str
        str of model name (e.g, LR_123)
    """
    from sklearn.metrics import precision_recall_curve
    y_score = y_prob
    precision_curve, recall_curve, pr_thresholds = precision_recall_curve(y_true, y_prob)
    precision_curve = precision_curve[:-1]
    recall_curve = recall_curve[:-1]
    pct_above_per_thresh = []
    number_scored = len(y_score)
    for value in pr_thresholds:
        num_above_thresh = len(y_score[y_score >= value])
        pct_above_thresh = num_above_thresh / float(number_scored)
        pct_above_per_thresh.append(pct_above_thresh)
    pct_above_per_thresh = np.array(pct_above_per_thresh)
    plt.clf()
    fig, ax1 = plt.subplots()
    ax1.plot(pct_above_per_thresh, precision_curve, 'b')
    ax1.set_xlabel('percent of population')
    ax1.set_ylabel('precision', color='b')
    ax1.set_ylim(0, 1.05)
    ax2 = ax1.twinx()
    ax2.plot(pct_above_per_thresh, recall_curve, 'r')
    ax2.set_ylabel('recall', color='r')
    ax2.set_ylim(0, 1.05)

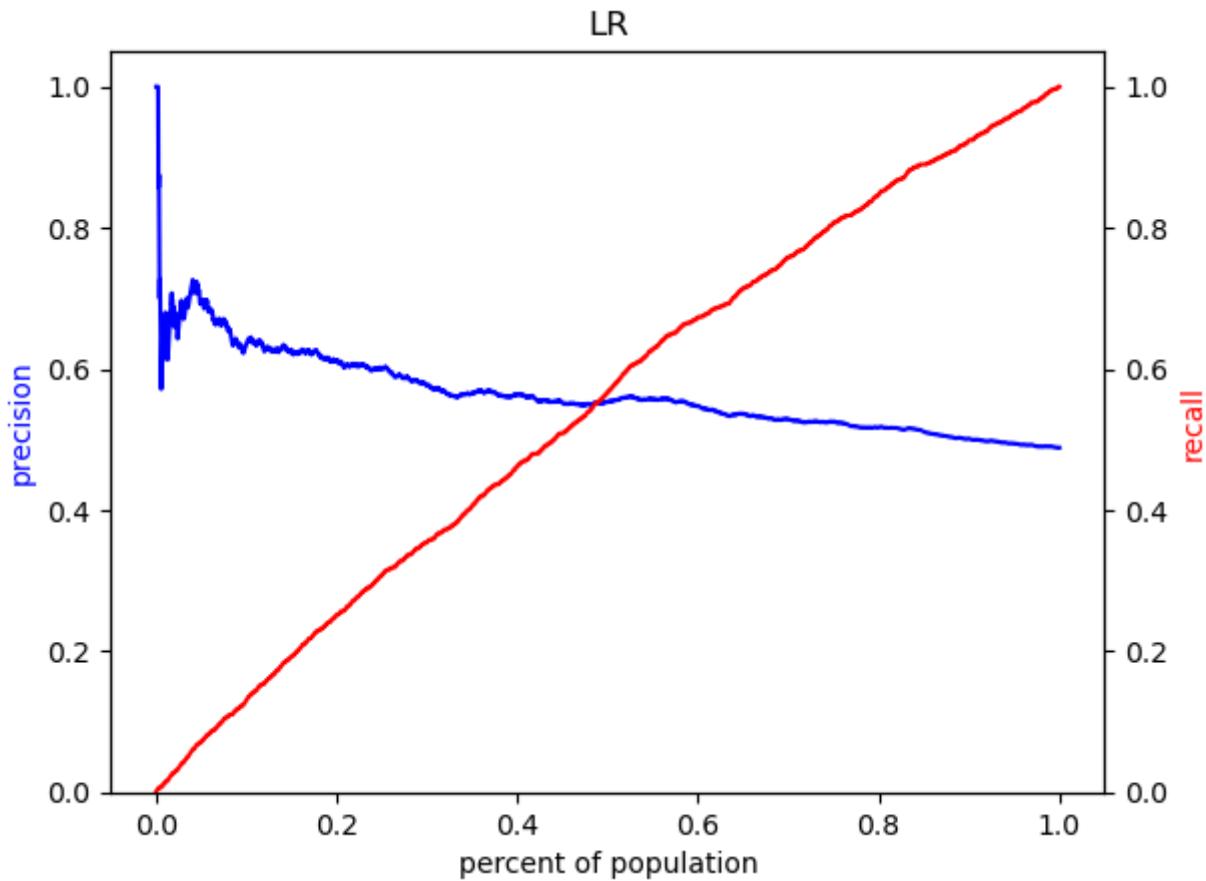
    name = model_name
    plt.title(name)
    plt.show()
    plt.clf()
```

```
In [160]: def precision_at_k(y_true, y_scores,k):

    threshold = np.sort(y_scores)[::-1][int(k*len(y_scores))]
    y_pred = np.asarray([1 if i >= threshold else 0 for i in y_scores ])
    return precision_score(y_true, y_pred)
```

```
In [161]: plot_precision_recall_n(expected,y_scores, 'LR')
```

<Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

```
In [162]: p_at_1 = precision_at_k(expected,y_scores, 0.01)
print('Precision at 1%: {:.2f}'.format(p_at_1))
```

Precision at 1%: 0.67

Assess Model Against Baselines

It is important to check our model against a reasonable **baseline** to know how well our model is doing. Without any context, .57% accuracy does not sound great... but that really depends on how well you would do by declaring everyone will not no Cancer researcher in the future, which would be stupid (not to mention useless) model.

A good place to start is checking against a *random* baseline, assigning every example a label (positive or negative) completely at random.

```
In [163]: random_score = [random.uniform(0,1) for i in enumerate(y_test)]
random_predicted = np.array([calc_threshold(score,0.5) for score in random_score])
random_p_at_5 = precision_at_k(expected[random_predicted], 0.01)
print('Precision at 1% (random): {:.2f}'.format(random_p_at_5))
```

```
Precision at 1% (random): 0.50
```

6) Adjust the parameters of your model (and/or create more features) until you are able to produce a model that does an ok job (it does not have to be great) at predicting your label in your test data. Report the accuracy, precision, and recall.(3 points)

Plots and values are few lines above:

When I ran the last time before submission,

Accuracy = 0.56

Precision = 0.56

Recall= 0.51

```
In [ ]:
```