# Impacts of Toxic Pollution on Life Expectancy and Cancer Rates for Local Communities

## Introduction to Machine Learning, Final Project Report

## December 15th, 2019

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This preamble this formatted as requested in the "Template" section of the Project requires. Also where applicable, I've labelled the sections with indices from the Project Requirements as found in `doc/Project Requirements.pdf` for reference. Please do read the full document however as all sections are still relevant.

# Introduction

## Problem Overview (3.a)

Using publicly available data from the EPA and CDC, I would like to explore the potential links of toxic dumping to general life expectancy and cancer rates at the local level, throughout the United States. Specifically, I have the data to do so from 2000 to 2016. Initially, I will constrain this range to 2010 to 2016 to align with the most recent Census (needed for life expectancy).

It is well known that certain chemicals are a contributing cause to a decline in public health. However, the process of disposing or sequestering these toxics are not equal, and local ecological factors may mean one method is significantly more dangerous for a given region than other methods.

## Motivation (3.b)

Environmental Accountability has historically been lower than required for long term ecological stability. Over time, the lack of accountability compounds to a large implicit cost for communities (and countries as a whole) as soil, air, and water supplies become more saturated with dangerous materials. The ability to identify a correlation between toxic dumping and public health is an important first step in fixing affected communities.

Therefore, my goal is to identify counties within the United States which have an above-average amount of industrial waste processing, and assess that area's life expectancy or cancer rates against national averages.

# Related Work (4.)

## References: Data Overview

**Four datasets** are considered for this project from 2010 to 2016. For measures of **Air Quality**, I consider the EPA's **AirData AQI (Air quality index) data set**. For measures of **toxicity**, I consider the EPA's **Toxics Release Inventory (TRI)** data set, which consists of toxic dumping reports by all companies in a given area. All companies are required to report their toxic dumping to the EPA.

In [1]:
```
## Work in the root directory
%cd
```

```
/home/cole/Desktop/intro-to-ml-final-project
```

In [2]:
```
import json

import geocoder
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MaxAbsScaler
```

In [3]:
```
def make_lat_lon_map(inputs, output_json_file='data/latlon.json', load_from='data/
    """
    Queries OpenStreetMap for Lat/Lon pairs given a list
    of input queries. The results are incrementally written
    to an output file in `data` by default. Errors are logged
    to a separate file for manual lookup.

    :param inputs:              A list of UNIQUE values to query
    :param output_json_file:    Optional separate JSON output file
    :param load_from:           Resumes from another JSON file
                                entries in the file will not be
                                reprocessed
    :return: `None`
    """
    # {"query": [lat, lon]}
    json_acc = {}

    # Remove duplicates
    inputs = list(set(inputs))

    if load_from:
        with open(load_from, 'r') as json_file:
            json_acc = json.load(json_file)
        inputs = [i for i in inputs if i not in json_acc.keys()]

    def dump(j):
        with open(output_json_file, 'w') as fp:
            json.dump(j, fp, indent=4)

    def dump_errors(e):
        with open("data/nominatim_errors.txt", 'w') as fp:
            for err in e:
                fp.write(err + '\n')

    errors = []
    for query in inputs:
        query = str(query)
        if query not in json_acc:
            g = geocoder.osm(query)

            if not g.ok:
                print("[ WRN ]", query, "--", str(g))
                errors.append(query)
                dump_errors(errors)

            else:
                print("[ MAP ] Found", g.latlng, "for", query)
                json_acc[query] = g.latlng
                dump(json_acc)
```

## Common Loading (Originally in `src/etl/load.py`)

We will first define a common loading procedure that works for most of the datasets considered here.

In [4]:
```
import glob
import json
import os
import re

import pandas as pd
```

In [5]:
```
# Not required for Notebook, function copied in
# from src.etl.preprocess import make_lat_lon_map

RAW_DATA = 'data/raw/'
PREPARED_DATA = 'data/prepared'

# Load the Lat/Lon Informtion
with open('data/latlon.json', 'r') as fp:
    lat_lon_json = json.load(fp)


def _load(subpath):
    """
    Common loadining method for CSVs in data directory.

    :param subpath:     Subpath in `data`
    :return:            DataFrame
    """
    path = os.path.join(RAW_DATA, subpath, '*.csv')
    all_files = glob.glob(path)

    li = []
    for filename in all_files:
        df = pd.read_csv(filename, index_col=None)
        li.append(df)

    return pd.concat(li, axis=0, ignore_index=True)


def _get_lat_lon(q):
    """
    Returns latitude and longitude pair from generated
    JSON file.

    :param q:   String query
    :return:    Latitude Longitude Pair
    """
    if q in lat_lon_json:
        return lat_lon_json[q]
    else:
        return [None, None]


def _change_precision(a, prec=0):
    """
    Changes the precision of the Latitude
    or Longitude arrays while preserving
    sparsity.

    :param a:       Input array
    :param prec:    New Decimal Precision
    :return:        Rounded array
    """
    acc = []
    for e in a:
        if e is None:
            acc.append(None)
        else:
            acc.append(round(float(e), prec))
    return acc
```

## TRI

We will begin by preparing the TRI dataset. In order to get this into a common format, we will make the following transformations:

1. Clean the column names to remove spaces and capitals
2. Select relevant columns (as defined in function)
3. Pivot on `industry` since it is categorical
4. Fix the schema for the columns which will become the index (lat, lon, year)
5. Change precision of lat and lon
6. Regroup by year, lat, lon and aggregate by **sum**

The TRI dataset is fortunate enough to not require lat, lon conversion. It comes with lat lon already.

In [6]:
```
def load_tri():
    """
    Loads the TRI CSV files into one DataFame

    :return: DataFrame
    """
    # Remove NA columns
    combined = _load('tri')

    # Clean column names
    cols = combined.columns
    cols = [c.split(' - ')[-1] for c in cols]
    cols = [c.split('. ')[-1].lower() for c in cols]
    combined.columns = cols
    combined = combined.rename(columns={'production wste (8.1-8.7)': 'production w
                                        'latitude': 'lat', 'longitude': 'lon'})

    # Select Relevant
    sel = ['year', 'lat', 'lon', 'industry sector',
           'fugitive air', 'stack air', 'water', 'underground',
           'underground cl i', 'underground c ii-v', 'landfills',
           'rcra c landfill', 'other landfills', 'land treatment',
           'surface impndmnt', 'rcra surface im', 'other surface i',
           'on-site release total', 'trns rlse', 'trns trt',
           'total transfers', 'm10', 'm41', 'm62', 'm40 metal', 'm61 metal', 'm71'
           'm81', 'm82', 'm72', 'm63', 'm66', 'm67', 'm64', 'm65', 'm73', 'm79',
           'm90', 'm94', 'm99', 'off-site release total', 'm20', 'm24', 'm26',
           'm28', 'm93', 'off-site recycled total', 'm56', 'm92',
           'm40 non-metal', 'm50', 'm54',
           'm61 non-metal', 'm69', 'm95', 'off-site treated total',
           'total transfer', 'total releases', 'releases', 'on-site contained',
           'off-site contain', 'production waste']

    combined = combined[sel].dropna(axis=1)
    combined.columns = [c.replace(' ', '_') for c in combined.columns]

    # Pivot industry
    d = pd.get_dummies(combined['industry_sector'], prefix='sector')
    df = pd.concat([combined, d], axis=1).drop(['industry_sector'], axis=1)

    # Fix schema
    df = df.dropna()
    df.year = df.year.astype(int)
    df.lat = df.lat.astype(int)
    df.lon = df.lon.astype(int)

    # Shift Precision
    df.lat = _change_precision(df.lat)
    df.lon = _change_precision(df.lon)

    # Group up
    df = df.dropna().groupby(by=['year', 'lat', 'lon'], as_index=False).sum()

    return df.dropna()
```

## AQI

We will begin by preparing the AQI dataset. In order to get this into a common format, we will make the following transformations:

1. Clean the column names to remove spaces and capitals
2. Select relevant columns (as defined in function)
3. Convert date to `year` by remove the month and day
4. Pivot on `defining_parameter` since it is categorical. This column denotes the worst factor for air quality that day
5. Regroup by `'year', 'state_name', 'county_name'`, aggregating by `mean`.
6. Convert `'state_name', 'county_name'` to `lat` and `lon` using the JSON file.
7. Fix the schema for the columns which will become the index (lat, lon, year)
8. Change precision of lat and lon
9. Regroup by year, lat, lon and aggregate by **sum**

In [7]:
```
def load_aqi():
    """
    Loads the AQI CSV files into one DataFame

    :return: DataFrame
    """
    # Remove NA columns
    combined = _load('aqi').dropna(axis=1)

    # Select relevant columns
    sel = ['State Name', 'county Name', 'Date', 'AQI', 'Defining Parameter']
    combined = combined[sel]

    # Clean column names
    combined.columns = [c.replace(" ", "_").lower() for c in combined.columns]

    # Convert date column to year only
    combined.date = combined.date.str.split('-').str[0]
    combined = combined.rename(columns={'date': 'year'})
    combined = combined.astype({'year': 'int64'})

    # Pivot defining_parameter column
    d = pd.get_dummies(combined['defining_parameter'], prefix='defining')
    df = pd.concat([combined, d], axis=1).drop(['defining_parameter'], axis=1)
    df = df.dropna().groupby(by=['year', 'state_name', 'county_name'], as_index=Fa

    # Convert to Lat/Lon
    loc = list(df.state_name + ", " + df.county_name)
    make_lat_lon_map(list(set(loc)))

    lat = [_get_lat_lon(i)[0] for i in loc]
    lon = [_get_lat_lon(i)[1] for i in loc]

    df['lat'] = _change_precision(lat)
    df['lon'] = _change_precision(lon)

    # Fix Schema
    df = df.dropna()
    df.year = df.year.astype(int)
    df.lat = df.lat.astype(int)
    df.lon = df.lon.astype(int)

    # Group up
    df = df.dropna().groupby(by=['year', 'lat', 'lon'], as_index=False).sum()

    return df.dropna()
```

## Cancer

We will begin by preparing the Cancer dataset. In order to get this into a common format, we will make the following transformations:

1. Clean the column names to remove spaces and capitals
2. Select relevant columns (as defined in function)
3. Pivot on `leading_cancer_sites` since it is categorical.
4. Fix the `MSA` column by defining a custom transformation policy for use in querying with **Nominatum**. This is required since the MSA regions sometimes include metropolitan area spanning across state lines for which Nominatim isn't able to handle.
5. Convert the cleaned `MSA` column to `lat` and `lon` .
6. Fix the schema for the columns which will become the index (lat, lon, year)
7. Change precision of lat and lon
8. Regroup by year, lat, lon and aggregate by **sum**

In [8]:
```
def load_cancer():
    path = os.path.join(RAW_DATA, "health/United States and Puerto Rico Cancer Sta
    cancer = pd.read_csv(path, delimiter='\t')

    # Select relevant columns
    sel = ['Year', 'Leading Cancer Sites', 'MSA', 'Count', 'Population', 'Age-Adju
    cancer = cancer[sel]
    cancer.columns = [c.replace(' ', '_').lower() for c in cancer.columns]

    # Pivot criteria
    d = pd.get_dummies(cancer['leading_cancer_sites'], prefix='cancer')
    d = d.multiply(cancer['count'], axis="index")
    cancer = pd.concat([cancer, d], axis=1).drop(['leading_cancer_sites', 'count']

    # Fix MSA
    tmp = cancer.msa
    ntmp = []

    # Also load manual map
    manual = {}
    with open('data/cancer_manual_map.txt', 'r') as fp:
        for l in fp:
            items = l.split('|')
            manual[items[0].strip()] = items[1].strip()

    # MSA Conversion Policy
    for t in tmp:
        t = str(t)
        t = t.replace('-', ' ')
        if len(re.split(',|,,', t)) == 1:
            ntmp.append(t)
            continue

        states = re.split(',|,,', t)[1]
        state = states.split()[0]

        areas = t.split()
        if len(areas) > 1:
            area = t.split()[0] + ' ' + t.split()[1]
        else:
            area = areas[0]

        tt = area + ", " + state

        if tt in manual:
            ntmp.append(manual[tt])
        else:
            ntmp.append(tt)

    cancer.msa = ntmp
    cancer = cancer.dropna()

    # Convert to Lat/Lon
    loc = list(cancer.msa)
    make_lat_lon_map(list(set(loc)))

    lat = [_get_lat_lon(i)[0] for i in loc]
    lon = [_get_lat_lon(i)[1] for i in loc]

    cancer['lat'] = _change_precision(lat, prec=0)
    cancer['lon'] = _change_precision(lon, prec=0)

    # Fix Schema
```

## Life Expectancy

We will begin by preparing the Life Expectancy dataset. In order to get this into a common format, we will make the following transformations:

1. Clean the column names to remove spaces and capitals
2. Select relevant columns (as defined in function)
3. Fix the Life Exp range to Min and Max values, which could potentially be good features.
4. Group by state and county, aggregate by mean to get the average life exp for that state and county
5. Convert state and county to `lat` and `lon` using the JSON file
6. Fix the schema for the columns which will become the index (lat, lon, year)
7. Change precision of lat and lon
8. Regroup by year, lat, lon and aggregate by **sum**

In [9]:
```
def load_life_exp():
    path = os.path.join(RAW_DATA, 'health', 'U.S._Life_Expectancy_at_Birth_by_Stat
    life = pd.read_csv(path)

    # Select Relevant
    sel = ['State', 'County', 'Life Expectancy',
           'Life Expectancy Range']
    life = life[sel].dropna()

    # Fix column names
    life.columns = [c.replace(' ', '_').lower() for c in life.columns]

    # Fix Life Exp Range to Min and Max
    rng = list(life.life_expectancy_range)
    rng_max = [float(str(r).split('-')[1].strip()) for r in rng]
    rng_min = [float(str(r).split('-')[0].strip()) for r in rng]

    life['life_expectancy_max'] = rng_max
    life['life_expectancy_min'] = rng_min
    life = life.rename(columns={'life_expectancy': 'life_expectancy_avg'})
    life = life.drop('life_expectancy_range', axis=1).dropna()

    life = life.groupby(['state', 'county'], as_index=False).mean()

    # Convert to Lat/Lon
    print("Getting lat lon list")
    loc = list(life.state + ", " + life.county)
    make_lat_lon_map(list(set(loc)))

    lat = [_get_lat_lon(i)[0] for i in loc]
    lon = [_get_lat_lon(i)[1] for i in loc]

    life['lat'] = _change_precision(lat, prec=0)
    life['lon'] = _change_precision(lon, prec=0)

    # Fix Schema
    life = life.dropna()
    life.lat = life.lat.astype(int)
    life.lon = life.lon.astype(int)

    # Group up
    life = life.dropna().groupby(by=['lat', 'lon'], as_index=False).sum()

    return life.dropna()
```

## Load All

Combine the datasets by **year, lat, and lon**. This is then written to a file that will constitute our **main dataset**.

In [10]:
```
def load_all(from_file=True):
    if from_file:
        return pd.read_csv('data/merged.csv')

    print("[ LOAD ] Loading AQI...")
    aqi = load_aqi()
    print(aqi)

    print("[ LOAD ] Loading TRI...")
    tri = load_tri()
    print(tri)

    print("[ LOAD ] Loading Life...")
    life = load_life_exp()
    print(life)

    print("[ LOAD ] Loading Cancer...")
    cancer = load_cancer()
    print(cancer)

    # Join
    j = aqi.merge(tri, on=['year', 'lat', 'lon'], how='inner')
    j = j.merge(cancer, on=['year', 'lat', 'lon'], how='inner')
    j = j.merge(life, on=['lat', 'lon'], how='left')
    j = j.dropna()

    # TODO: Fix weird behavior with duplicated rows in merge that make this line r
    j = j.groupby(by=['year', 'lat', 'lon'], as_index=False).mean()

    j.to_csv('data/merged.csv', index=False)
    return j
```

In [11]:
```
df = load_all(from_file=True)
df
```

Out[11]:

| | year | lat | lon | aqi | defining_CO | defining_NO2 | defining_Ozone | defining_PM10 | defining_PM2.5 | c |
|---|---|---|---|---|---|---|---|---|---|---|
| **0** | 2010 | 21 | -158 | 39.715068 | 0.000000 | 0.00274 | 0.230137 | 0.024658 | 0.742466 | |
| **1** | 2010 | 26 | -98 | 44.077348 | 0.000000 | 0.00000 | 0.406077 | 0.002762 | 0.591160 | |
| **2** | 2010 | 27 | -82 | 42.367123 | 0.000000 | 0.00000 | 0.695890 | 0.010959 | 0.293151 | |
| **3** | 2010 | 28 | -82 | 183.767123 | 0.000000 | 0.00000 | 3.038356 | 0.002740 | 0.821918 | |
| **4** | 2010 | 28 | -81 | 208.062127 | 0.000000 | 0.00000 | 3.714128 | 0.000000 | 1.285872 | |
| **...** | ... | ... | ... | ... | ... | ... | ... | ... | ... | |
| **581** | 2016 | 43 | -74 | 104.521436 | 0.000000 | 0.00000 | 1.748634 | 0.000000 | 1.251366 | |
| **582** | 2016 | 44 | -116 | 34.267218 | 0.000000 | 0.00000 | 0.000000 | 0.000000 | 1.000000 | |
| **583** | 2016 | 45 | -123 | 30.764543 | 0.000000 | 0.00000 | 0.407202 | 0.000000 | 0.592798 | |
| **584** | 2016 | 47 | -122 | 103.114754 | 0.000000 | 0.31694 | 0.989071 | 0.000000 | 1.693989 | |
| **585** | 2016 | 48 | -117 | 85.160502 | 0.002732 | 0.00000 | 0.352459 | 0.169399 | 2.475410 | |

586 rows × 125 columns

## Data Evaluation: High Level Statistics

Let us view some high level statistics about our dataset. Namely, we should look at the:

1. Number of Rows
2. Number of Columns
3. Columns with Highest Variance
4. Columns with Lowest Variance
5. Some basic correlations

In [12]:
```
print("Number of Rows:", len(df))
print("Number of Cols:", len(df.columns), '\n')

print("Highest Variance Cols:")
print(df.var().sort_values(ascending=False)[:10], '\n')

print("Lowest Variance Cols:")
print(df.var().sort_values()[:10], '\n')

print("Top 20 Correlations to Age-Adjusted Rate:")
print(df[[c for c in df.columns if 'cancer' not in c]]
      .corr()['age-adjusted_rate'].sort_values(ascending=False)[:20])
```

```
Number of Rows: 586
Number of Cols: 125

Highest Variance Cols:
population                 3.779196e+15
production_waste           2.542578e+11
total_releases             1.909209e+10
on-site_release_total      1.894071e+10
other_surface_i            5.614605e+09
total_transfer             1.802190e+09
off-site_recycled_total    1.550502e+09
m24                        1.442020e+09
water                      2.049389e+08
off-site_release_total     1.271601e+08
dtype: float64

Lowest Variance Cols:
releases              0.000000e+00
landfills             0.000000e+00
underground           0.000000e+00
m63                   0.000000e+00
m71                   0.000000e+00
surface_impndmnt      0.000000e+00
sector_Publishing     3.180443e-07
sector_Apparel        6.450643e-07
sector_Coal Mining    2.369974e-05
sector_Tobacco        5.922906e-05
dtype: float64

Top 20 Correlations to Age-Adjusted Rate:
age-adjusted_rate                      1.000000
population                             0.495891
defining_PM2.5                         0.422032
aqi                                    0.419695
defining_Ozone                         0.390418
defining_NO2                           0.371733
sector_Petroleum Bulk Terminals        0.357192
lon                                    0.314356
life_expectancy_min                    0.314105
life_expectancy_max                    0.305783
life_expectancy_avg                    0.291387
sector_Tobacco                         0.286238
sector_Textiles                        0.215277
sector_Miscellaneous Manufacturing     0.192700
m93                                    0.160954
m95                                    0.139101
defining_CO                            0.137515
underground_cl_i                       0.136676
m69                                    0.116186
sector_Electric Utilities              0.104435
Name: age-adjusted_rate, dtype: float64
```

## Interpretation

From above, we can see that there are no columns in our design matrix that are immediately strongly correlated with the Age-Adjusted Rate of cancer levels for a given year and area.

This was expected however. Efforts to relate toxic dumping with cancer rates has been historically inconclusive as evidenced by the following paper survey.

---

### Hazardous waste and health impact: a systematic review of the scientific literature

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5637250/ (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5637250/)

In this survey study, the authors assessed 57 papers on the health impacts of toxic waste. The overall results from many studies were inconclusive – There are many confounding factors which contribute to cancer rates among individuals. However, they found that oil industry waste to be the most hazardous of the types considered in the survey. This study is fairly recent, published in 2017, but again considers a traditional sample of selected communities, instead of a national survey.

---

# Experiment: Visualization (Originally `src/model/cluster.py`)

We can now view the prepared datasets individually and together to assess potential clusters, and to help select our model later on.

We will use a 2-component **PCA Decomposition** on the fully prepared dataset. Let us define a generalized visualization function.

In [13]:
```
from matplotlib import pyplot as plt
from sklearn.decomposition import PCA
```

In [14]:
```
def view_pca(df, emphasize_column=None, title=None, xlabel=None, ylabel=None):
    """
    Charts the 2-component PCA decomposition of
    the given DataFrame, with optional
    coloring upon a separate column. This
    column will NOT be part of the PCA decomposition.

    :param df:                  DataFrame to decompose
    :param emphasize_column:    Column for coloring PCA
    :param title:               Title of Plot
    :param xlabel:              X axis label
    :param ylabel:              Y axis label
    :return:                    `None`
    """
    c = None
    if emphasize_column:
        c = df[emphasize_column]
        df = df.drop(emphasize_column, 1)

    pca = PCA().fit_transform(df)
    plt.scatter(pca[:, 0], pca[:, 1], c=c)

    plt.title(title)
    plt.xlabel(xlabel)
    plt.ylabel(ylabel)
    plt.show()
```

## Defining our Y columns

In order to have a meaningful clustering example, we need to define our Y columns and remove them from the DataFrame before the PCA decomposition. The following function will **officially define the columns of our Y set**.

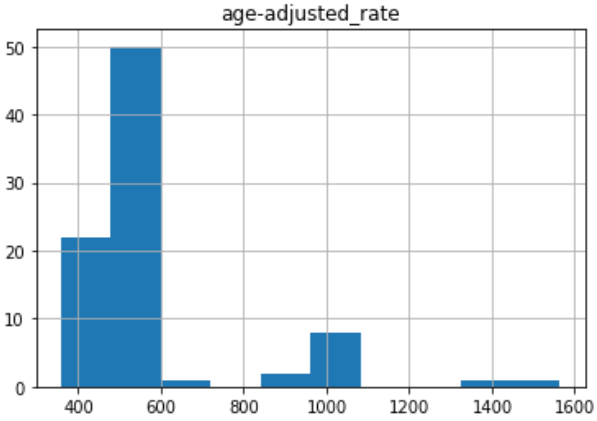
In [15]:
```
def _in_terms(t):
    y_terms = ['age-adjusted_rate', 'count', 'cancer', 'population', 'life_expecta
    for ty in y_terms:
        if ty in t:
            return True
    return False

y_cols = [c for c in df.columns if _in_terms(c)]
x_cols = [c for c in df.columns if c not in y_cols]
```

## Selected Distributions

Below, we visualize two major features in the X and Y set, to see how their values are distributed.

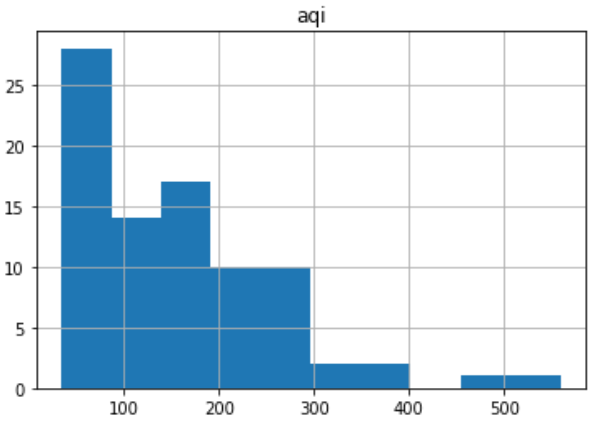
In [16]:
```
dfg = df[['lat', 'lon', 'age-adjusted_rate']].groupby(by=['lat', 'lon']).mean()
dfg.hist()
```

Out[16]:
```
array([[<matplotlib.axes._subplots.AxesSubplot object at 0x7f3a5bcc1fd0>]],
      dtype=object)
```




In [17]:
```
dfg = df[['lat', 'lon', 'aqi']].groupby(by=['lat', 'lon']).mean()
dfg.hist()
```

Out[17]:
```
array([[<matplotlib.axes._subplots.AxesSubplot object at 0x7f3a5999bc18>]],
      dtype=object)
```

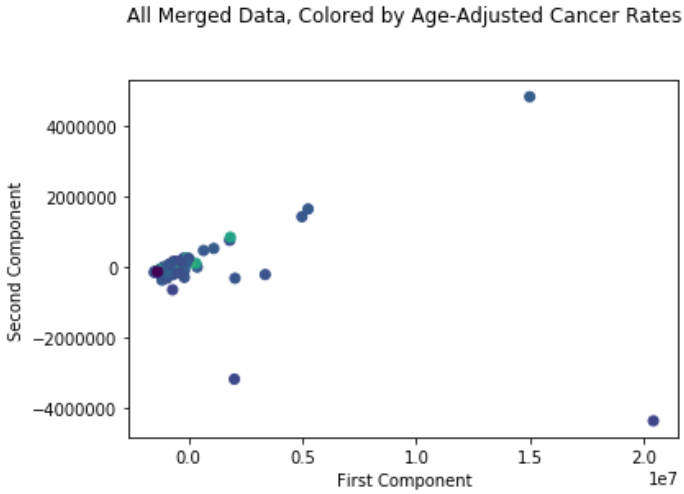



## All Merged Data w. EMA, Colored by Age-Adjusted Cancer Rates

Visualize the initial clusters of age-adjusted cancer rates for each area. We will group each area by adding up all the years observed.

In [18]:
```
# Sum over all years
grouped = df.groupby(by=['lat', 'lon']).sum()
drop_cols = [y for y in y_cols if y != 'age-adjusted_rate']
```

In [19]:
```
view_pca(grouped.drop(drop_cols, 1), 'age-adjusted_rate',
         title="All Merged Data, Colored by Age-Adjusted Cancer Rates\n\n",
         xlabel="First Component",
         ylabel="Second Component")
```

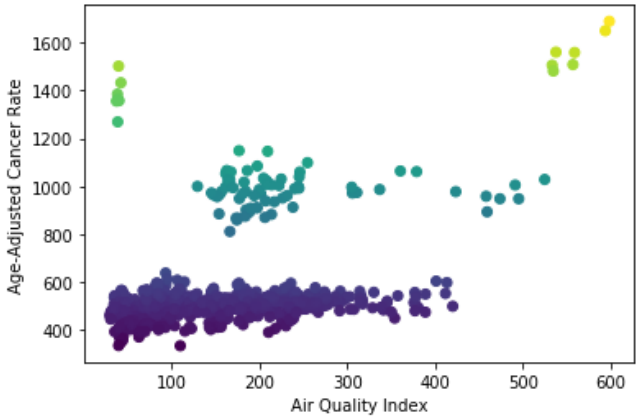



We can immediately see some outliers, but let's take a look at some specific features as they relate to the age adjusted rate

## Age Adjusted Rate vs AQI (Colored: Age Adjusted Rate)

In [20]:
```
plt.scatter(df['aqi'], df['age-adjusted_rate'], c=df['age-adjusted_rate'])
plt.xlabel("Air Quality Index")
plt.ylabel("Age-Adjusted Cancer Rate")
```

Out[20]:
```
Text(0, 0.5, 'Age-Adjusted Cancer Rate')
```

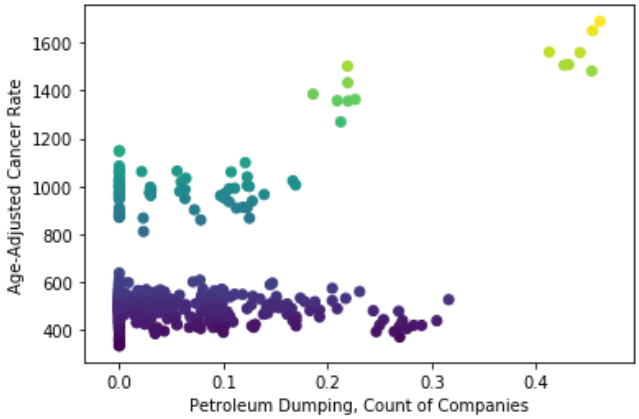



This looks really good. We can tell the relationship isn't linear, but there does exist defined clusters which pocket nicely with the age adjusted rate!

## Age Adjusted Rate vs Number of Dumpings by Petroleum Companies (Colored: Age Adjusted Rate)

In [21]:
```
plt.scatter(df['sector_Petroleum Bulk Terminals'], df['age-adjusted_rate'], c=df['
plt.xlabel("Petroleum Dumping, Count of Companies")
plt.ylabel("Age-Adjusted Cancer Rate")
```

Out[21]:
```
Text(0, 0.5, 'Age-Adjusted Cancer Rate')
```




This one is also pretty good. We notice again that there are clusters of high-count of dumping from Petroleum Companies, with high cancer rates as well.

---

# Algorithm: Feature Engineering (Originally `src/model/features.py`)

After our data is loaded into a single Pandas DataFrame, we now engineer some features that might be helpful. One such feature is the **exponential moving average** for each feature column. I do this to model the time-weighted importance of each factor which may contribute to life expectancy and cancer rates, with the assumption that **areas will consistently high levels of air pollution and toxic dumping exhibit higher rates and lower life expectancy than areas which have a higher recent spike in air pollution and toxic dumping**. The EMA will capture this sentiment using one, two, and three year lags.

Each feature will become a separate EMA column, denoted by `_emaX` where `X` is either `1, 2, or 3`.

In [22]:
```
def sma_featurizer(df, by=None, lags=None, ema=True):
    """
    Computes the SMA of each column, grouped by
    the `by` set. This follows for each `i` in
    `lags`. The default `by` is `[lat, lon]`. The
    default `lags` is `[1,2,3]`, which represent years
    in the merged dataset in this project. SMA
    columns will be appended with prefix smaN_.

    :param df:      DataFrame to featurize
    :param by:      Grouping columns (default: [lat, lon]
    :param lags:    SMA i periods (default: [1,2,3])
    :param ema:     Use exponential moving averages
    :return:        Featurized DataFrame
    """
    # Resolve defaults
    if by is None:
        by = ['lat', 'lon']
    if lags is None:
        lags = [1, 2, 3]

    # Re-index DataFrame to by columns plus year
    df = df.set_index(by + ['year'])

    # Group by without year to compute SMA/EMA
    g = df.groupby(by=by)

    # Define an inner convenience function
    def roll(i):

        # Apply the SMA/EMA to the inner groupings, which should
        # contain "year"
        if ema:
            r = g.apply(lambda x: x.sort_values(by='year').ewm(i).mean())
            r.columns = ["ema" + str(i) + "_" + c for c in r.columns]
        else:
            r = g.apply(lambda x: x.sort_values(by='year').expanding(i).mean())
            r.columns = ["sma" + str(i) + "_" + c for c in r.columns]
        return r

    # Compute for all lags
    features = roll(lags[0])
    for lag in lags[1:]:
        tmp = roll(lag)

        # Join on by plus year, since year is also still in index
        features = features.join(tmp, how='inner')

    # Join on the original DataFrame, sort, return
    return df.join(features, how='inner').sort_index()
```

## Featurize our DataFrame

In [23]:
```
df_ema = sma_featurizer(df, ema=True).dropna()
df_ema
```

Out[23]:

| | | | aqi | defining_CO | defining_NO2 | defining_Ozone | defining_PM10 | defining_PM2.5 | definin |
|---|---|---|---|---|---|---|---|---|---|
| **lat** | **lon** | **year** | | | | | | | |
| **21** | **-158** | **2010** | 39.715068 | 0.000000 | 0.002740 | 0.230137 | 0.024658 | 0.742466 | 0.0 |
| | | **2011** | 39.260274 | 0.000000 | 0.000000 | 0.356164 | 0.016438 | 0.624658 | 0.0 |
| | | **2012** | 34.628415 | 0.000000 | 0.000000 | 0.352459 | 0.013661 | 0.628415 | 0.0 |
| | | **2013** | 32.632877 | 0.000000 | 0.000000 | 0.386301 | 0.008219 | 0.605479 | 0.0 |
| | | **2014** | 29.901961 | 0.000000 | 0.002801 | 0.641457 | 0.044818 | 0.299720 | 0.0 |
| **...** | **...** | **...** | ... | ... | ... | ... | ... | ... | |
| **48** | **-117** | **2012** | 51.567907 | 0.005464 | 0.000000 | 0.341530 | 1.010929 | 0.642077 | 0.0 |
| | | **2013** | 56.944754 | 0.008219 | 0.000000 | 0.372603 | 1.024658 | 0.594521 | 0.0 |
| | | **2014** | 49.402620 | 0.016438 | 0.000000 | 0.326027 | 1.147945 | 0.509589 | 0.0 |
| | | **2015** | 109.913899 | 0.000000 | 0.000000 | 0.349862 | 0.414061 | 2.236077 | 0.0 |
| | | **2016** | 85.160502 | 0.002732 | 0.000000 | 0.352459 | 0.169399 | 2.475410 | 0.0 |

586 rows × 488 columns

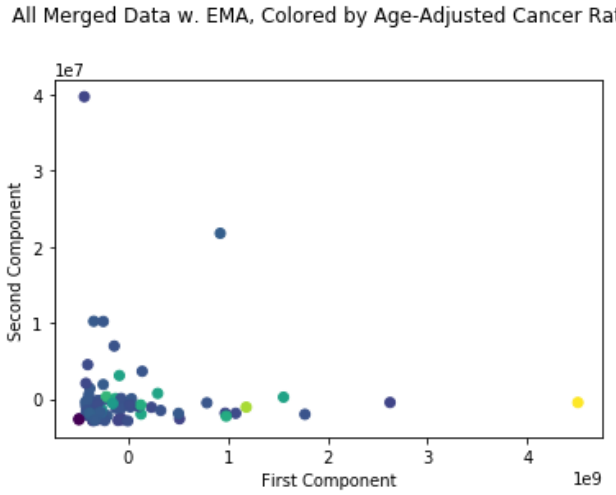
In [24]:
```
print("Number of Rows:", len(df_ema))
print("Number of Cols:", len(df_ema.columns), '\n')

print("Highest Variance Cols:")
print(df_ema.var().sort_values(ascending=False)[:10], '\n')

print("Lowest Variance Cols:")
print(df_ema.var().sort_values()[:10], '\n')

print("Top 20 Correlations to Age-Adjusted Rate:")
print(df_ema[[c for c in df_ema.columns if 'cancer' not in c]]
      .corr()['age-adjusted_rate'].sort_values(ascending=False)[:20])
```

```
Number of Rows: 586
Number of Cols: 488

Highest Variance Cols:
population               3.779196e+15
ema1_population          3.742045e+15
ema2_population          3.724200e+15
ema3_population          3.714826e+15
production_waste         2.542578e+11
ema1_production_waste    1.859462e+11
ema2_production_waste    1.587683e+11
ema3_production_waste    1.465370e+11
total_releases           1.909209e+10
on-site_release_total    1.894071e+10
dtype: float64

Lowest Variance Cols:
surface_impndmnt         0.0
ema3_surface_impndmnt    0.0
ema3_underground         0.0
releases                 0.0
ema3_m71                 0.0
m71                      0.0
m63                      0.0
ema1_releases            0.0
ema1_underground         0.0
ema2_releases            0.0
dtype: float64

Top 20 Correlations to Age-Adjusted Rate:
age-adjusted_rate         1.000000
ema1_age-adjusted_rate    0.998972
ema2_age-adjusted_rate    0.998260
ema3_age-adjusted_rate    0.997837
ema3_population           0.496632
ema2_population           0.496499
ema1_population           0.496255
population                0.495891
ema3_defining_PM2.5       0.443200
ema2_defining_PM2.5       0.441238
ema1_defining_PM2.5       0.436570
defining_PM2.5            0.422032
aqi                       0.419695
ema1_aqi                  0.417988
ema2_aqi                  0.416747
ema3_aqi                  0.416067
defining_Ozone            0.390418
ema1_defining_Ozone       0.385056
ema2_defining_NO2         0.384588
ema3_defining_NO2         0.384346
Name: age-adjusted_rate, dtype: float64
```

In [25]:
```
y_cols = [c for c in df.columns if _in_terms(c)]
x_cols = [c for c in df.columns if c not in y_cols]
```

In [26]:
```
# Sum over all years
grouped = df_ema.groupby(by=['lat', 'lon']).sum()
drop_cols = [y for y in y_cols if y != 'age-adjusted_rate']
```

In [27]:
```
view_pca(grouped.drop(drop_cols, 1), 'age-adjusted_rate',
         title="All Merged Data w. EMA, Colored by Age-Adjusted Cancer Rates\n\n",
         xlabel="First Component",
         ylabel="Second Component")
```



# Algorithm: Predictive Modelling

Now lets see about predicting our values in Y, **life exp, and cancer rates** using our design matrix, **TRI and AQI values**. Since we have multiple such Y columns, we will do so in a **One-vs-All** approach.

## Model Selection

I originally tried a linear model, **ElasticNet** but found that the approach gave very bad R2 values. This is likely because our feature space isn't linear, as we saw in the above scatter plots.

Moreover, we are now considering nearly **500 columns**, many of which will be completely irrelevant for our predictions. I originally tried to use **Backward Featrure Selection** by predicting the `age-adjusted_rate` values, but this proved computationally intractable since our feature space is so big, as we would have to do this **for every single Y column** when using One-vs-All.

Thus, I decided to use a model with **selects features implicitly**, **Gradient Boosting Regression**. It was the perfect choice since it's a tree method which allows for non-linear relationships, automatically uses only the most relevant features, and returns to me the most important features for each and every Y column I'm trying to predict.

## Splitting the Data (Originally `src/etl/preprocess.py`)

The data will need to split in a stratified way to prevent poisoning the test set. That is, our DataFrame is **not unique by latitude and longitude** since we are considering multiple years for each lat/lon pair. Also, our values are **not on the same scale**, so we will need to scale the values to a normalized range.

The function below will do all of the above, and stratify by latitude and longitude for us. It will also reform the index of the DataFrame to be `lat, lon, year` .

In [28]:
```
import json

import geocoder
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MaxAbsScaler
```

In [29]:
```
def split(df, y_cols=None, pct=0.20, shuffle=True, normalize=True):
    """
    Splits DataFrame into training and test sets. If `y_cols`
    is provided, also breaks out those columns as a separate
    Numpy Array. Will return either:
        x, y
        or
        x_train, y_train, x_test, y_test

    The split is stratified by Lat and Lon.

    :param df:          DataFrame to split
    :param y_cols:      Y columns of DataFrame
    :param pct:         Validation Percent
    :param shuffle:     Shuffle the rows before splitting
    :param normalize    Scale the data using MaxAbsScaler
    :return:            Numpy Arrays
    """

    remove_lat_lon_afterwords = False
    if 'lat' not in df or 'lon' not in df:
        df['lat'] = [d[0] for d in df.index]
        df['lon'] = [d[1] for d in df.index]
        remove_lat_lon_afterwords = True

    df['strat_col'] = df['lat'].astype(str) + " " + df['lon'].astype(str)

    if y_cols:
        y = df[y_cols]
        cols = [c for c in df.columns if c not in y_cols]
        x = df[cols]

        x_train, x_test, y_train, y_test = train_test_split(x, y, test_size=pct, s
                                                            stratify=df['strat_col
        x_train = x_train.drop('strat_col', 1)
        x_test = x_test.drop('strat_col', 1)

        if remove_lat_lon_afterwords:
            x_train = x_train.drop(['lat', 'lon'], 1)
            x_test = x_test.drop(['lat', 'lon'], 1)

        # Fit the scaler to training only
        if normalize:
            x_scaler = MaxAbsScaler()
            x_scaler.fit(x_train)
            y_scaler = MaxAbsScaler()
            y_scaler.fit(y_train)

            return x_scaler.transform(x_train), y_scaler.transform(y_train), \
                   x_scaler.transform(x_test), y_scaler.transform(y_test)
        else:
            return x_train, y_train, x_test, y_test
    else:
        # No Y columns provided, simply split the data
        x_train, x_test = train_test_split(df, test_size=pct, shuffle=shuffle,
                                           stratify=df['strat_col'])
        x_train = x_train.drop('strat_col', 1)
        x_test = x_test.drop('strat_col', 1)

        if remove_lat_lon_afterwords:
            x_train = x_train.drop(['lat', 'lon'], 1)
            x_test = x_test.drop(['lat', 'lon'], 1)
```

## Fitting the Model

We will define the function below to fit a One-vs-All Classifier. We will use this function in a loop to fit for every column in Y (Ignoring EMA columns in Y)

In [30]:
```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.metrics import mean_squared_error, r2_score
```

In [31]:
```
def fit_predict(x_tr, y_tr, x_te, y_te, label):
    """
    Fits a prediction model in a One-vs-All fashion. Prints
    the results to the console, and returns the classifier object.

    :param x_tr:    X train
    :param y_tr:    Y train (1D)
    :param x_te:    X test
    :param y_te:    Y test (1D)
    :param label:   Label for Y column value
    :return:        GBM regressor instance
    """
    gbm = GradientBoostingRegressor(n_estimators=200)
    gbm.fit(x_tr, y_tr)

    print('---', label, '-----------------------')

    for i in sorted(zip(gbm.feature_importances_, x_cols))[-5:]:
        print(i)

    print("MSE", mean_squared_error(y_te, gbm.predict(x_te)))
    print("R2 ", r2_score(y_te, gbm.predict(x_te)))

    return gbm
```

## Results

Below are the classification results for **every column in Y** using a **Vanilla GBM with 200 estimators**.

In [32]:
```
# Split train and test
x_train, y_train, x_test, y_test = split(df, y_cols=y_cols)

# Loop over all Y, ignore EMA columns
for i in range(len(y_cols)):
    if 'ema' in y_cols[i] or 'sma' in y_cols[i]:
        continue

    fit_predict(x_train, y_train[:, i], x_test, y_test[:, i], y_cols[i])
```

```
--- population ----------------------
(0.043911285559348326, 'sector_Miscellaneous Manufacturing')
(0.05164019940200082, 'defining_NO2')
(0.07323452159634752, 'defining_PM2.5')
(0.0969742692054744, 'total_releases')
(0.3632588940674711, 'aqi')
MSE 0.0010837653253395608
R2  0.9554514060331794
--- age-adjusted_rate ----------------------
(0.0655782094166896, 'sector_Textiles')
(0.08457586036963097, 'lat')
(0.10128515710086505, 'sector_Petroleum Bulk Terminals')
(0.16841495839644285, 'aqi')
(0.17430952413402928, 'lon')
MSE 0.0013752791529830215
R2  0.9310211221993245
--- cancer_Brain and Other Nervous System ----------------------
(0.04251661858094999, 'sector_Miscellaneous Manufacturing')
(0.09311603311314771, 'total_releases')
```

## Explanation of Results, Interpretation

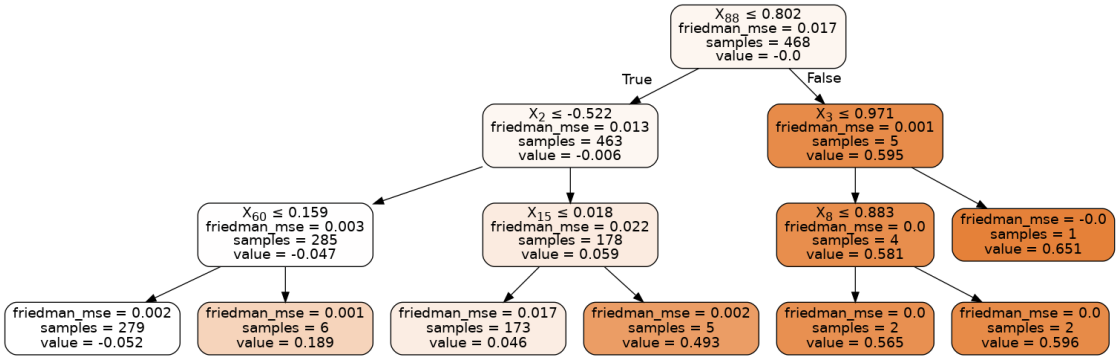
The results are overall quite good! The R2 value is consistently high, but I think it would be interesting to introduce some **value jitter to the X training set** in order to see how robust our findings really are. We can't have a model that only works in delicate circumstances.

## Tree Visualization for first three levels of Age-Adjusted Rate GBM (first tree)

In [37]:
```
import io

import pydotplus
from PIL import Image
from matplotlib import pyplot as plt
from sklearn.externals.six import StringIO
from sklearn.tree import DecisionTreeRegressor
from sklearn.tree import export_graphviz
```

In [40]:
```
def visualize_best_tree(x, y, levels=3):
    t = GradientBoostingRegressor(max_depth=levels, n_estimators=200)
    t.fit(x, y)

    t = t.estimators_[0, 0]

    dot_data = StringIO()
    export_graphviz(t, out_file=dot_data,
                    filled=True, rounded=True,
                    special_characters=True)
    graph = pydotplus.graph_from_dot_data(dot_data.getvalue())

    img = Image.open(io.BytesIO(graph.create_png()))
    img.save('doc/plots/age-adjusted_rate-tree-viz.png')
    display(img)
```

In [41]:
```
visualize_best_tree(x_train, y_train[:, 1])
```




In [42]:
```
print("Legend:")
print("X8:", x_cols[8])
print("X2:", x_cols[2])
print("X66:", x_cols[66])
print("X40:", x_cols[40])
print("X1:", x_cols[1])
print("X70:", x_cols[70])
print("X61:", x_cols[61])
```

```
Legend:
X8: defining_PM2.5
X2: lon
X66: off-site_contain
X40: m65
X1: lat
X70: sector_Chemical Wholesalers
X61: off-site_treated_total
```

## Adding Noise to Training Data

In [43]:
```
import numpy as np
```

In [44]:
```
noise = np.random.normal(0,1, x_train.shape) * 0.01
x_train += noise
```

In [45]:
```
# Loop over all Y, ignore EMA columns
for i in range(len(y_cols)):
    if 'ema' in y_cols[i] or 'sma' in y_cols[i]:
        continue

    fit_predict(x_train, y_train[:, i], x_test, y_test[:, i], y_cols[i])
```

```
--- population ----------------------
(0.05434242243238677, 'sector_Computers and Electronic Products')
(0.06671474146090242, 'defining_NO2')
(0.11538740948037528, 'sector_Petroleum Bulk Terminals')
(0.14344653315495692, 'defining_PM2.5')
(0.2234780731943129, 'aqi')
MSE 0.0012358270716577278
R2  0.9492008489833943
--- age-adjusted_rate ----------------------
(0.06285623799948302, 'sector_Textiles')
(0.0673274924056882, 'sector_Tobacco')
(0.11054140237138206, 'lon')
(0.12639806472316525, 'lat')
(0.18136236406146614, 'aqi')
MSE 0.0021832009625672843
R2  0.8904987746781435
--- cancer_Brain and Other Nervous System ----------------------
(0.046961163347359614, 'sector_Electrical Equipment')
(0.05639569996896978, 'defining_NO2')
```

## Evaluation: Goodness of Analytic

We can see that adding noise may not help our prediction, but it doesn't destroy it either. This leads me to believe that the predictions we originally have are reasonably accurate at least on the surface.

If the model were simply fitting to, and memorizing the input data, then the noise would have destroyed the predictive accuracy (R2 value) of our model more than it did.

Also in-line with our earlier correlation analysis, no one feature is important alone in predicting cancer rates and life expectancy. They all contribute a fair amount, without over-fitting to one given feature. We see that in our GBM `feature_importances` values, no one column really exceeds about `0.35` for any analysis. (This value ranges from 0.0 to 1.0, and all values add up to 1.0)

## Evaluation: Findings

More often than not, the most defining characteristics for different cancer rates were the number of **Petroleum Bulk Terminals** dumpings, and the **Air Quality Index** for a given area.

Surprisingly, the defining characteristic for the AQI that was most important in determining cancer rates was **PM2.5**. From previous experience in Air Quality research, PM2.5 is often **not** the defining characteristic. Normally it is Ozone, which has been clinically proven to have an adverse affect on sensitive groups.

I also intentionally left **lat** and **lon** as features of the data set to see if cancer rates were simply concentrated to parts of the United States, rather than factors *within* those areas. In this way, these features model the **spurious correlation** of our other features, since latitude and longitude were part of our grouping index.

In `age-adjusted_rate` we see that `lat` and `lon` are both in the top 5 most important features for the GBM regressor which probably indicates some of these relationships are spurious.

# Evaluation: Future Work

Future work would need to be conducted in determining the causal relationships between these features and actual cancer rates. It is not enough to say that these correlations are linked. However, these studies are often expensive and **the novelty of this application is to show which factors are worth exploring**. For that, I believe **Air Quality** and **Tobacco / Petroleum Dumping** should be explored in greater detail to assess the health risk as it relates to life expectancy and cancers.

Moreover, more work can be done to this application to better relate the features in the design matrix. For instance, not all types of dumping may be equally harmful, and this model does not currently have a way to determine that as it sees the *kind of* dumping as an independent feature to the *industry* that is dumping. This however requires an intuitive understanding and industry knowledge of toxic dumping.

In [ ]: