Guidehouse

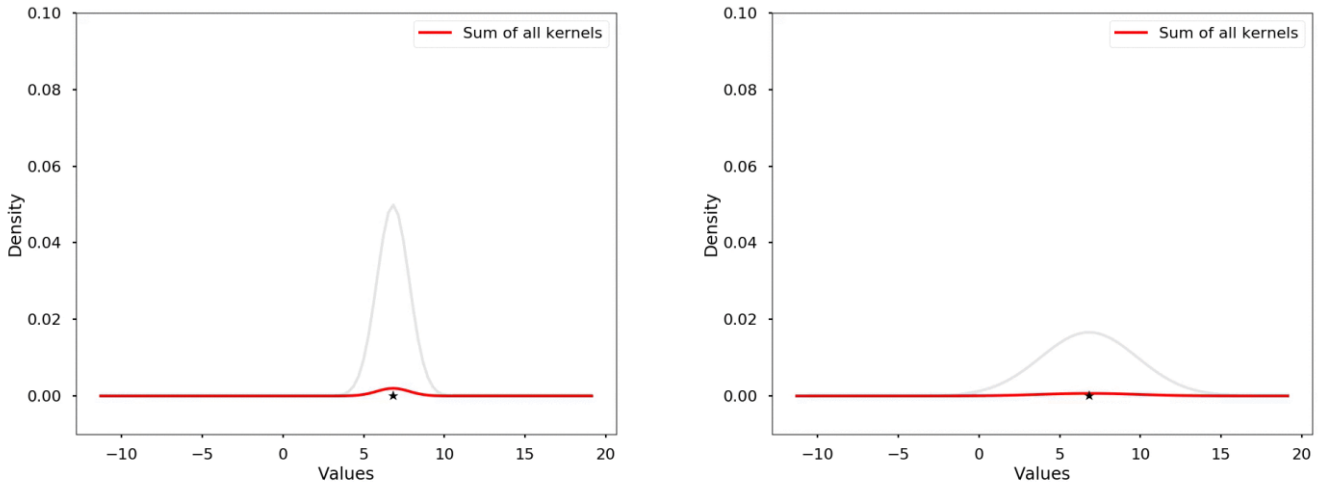
Popping the Kernel

Using Constrained Optimization to Estimate the Values behind a Kernel Estimation

June 14, 2022

What is Kernel Estimation?

- Kernel Estimation is a transformation of a dataset through the application of a distribution, the kernel
- Kernels are defined by their shape and determines the properties of the resulting transform
- A kernel's width is its most important attribute
- Kernels can be useful tools to:
  - investigate spatial or cyclic patterns
  - remove noise
  - develop a probability density function



http://qingkaikong.blogspot.com/2018/05/kernel-density-estimation-animation.html

Why would we want to undo a Kernel Estimation?

- The kernel obfuscates the data
- The kernel applied to the data can constrain your analysis
- There is almost no way to apply a different kernel to the data without the raw data itself
  – Only if the new kernel's size is a multiple of the kernel already applied to the data, this can be very limiting

How would we undo a Kernel Estimation?

- Each output of a Kernel Estimation can be viewed as its own linear equation
- And with many of the linear equations sharing variables, the entire transformation can then be viewed as the following system of linear equations

$$\boldsymbol{A} \times \boldsymbol{x} = \boldsymbol{b}$$

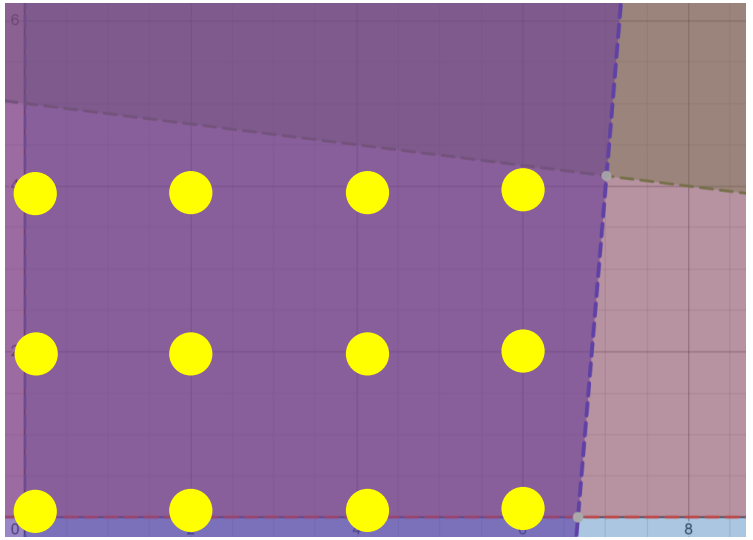
The coefficient matrix constructed from the kernel

Each underlying data point

Every output from the kernel estimation

How would we undo a Kernel Estimation? Cont.

- Due to the nature of kernel density estimations, the system will have more variables than constraining equations, this means there are infinitely many solutions to the system
- This solution space can be reigned in by further constraining the system
- These constraints can take the form of inequalities, setting upper and lower bounds on the variables, or number classification, either continuous, integer, or binary



Where Do These Fit into the Data Engineer's Toolbox?

Data Transformation	Action	Reaction
Row Wise	Union	Filter
Column Wise	Join	Subset
Reshaping	Pivot	Melt
Accumulation	Cumulative Sum	Lag
Rolling Aggregations	**Kernel Estimation**	**Constrained Optimization**

One-Dimensional Example:

Time Series Data

Vital Statistics Rapid Release Drug Overdose Data

- The VSRR data tracks the mortality statistics indexed by region, month and drug
- The mortality statistics are recorded as the sum of the current month's death count and the death count of the preceding 11 months
- This hides some of the month-to-month variation and makes it easier to identify a general trend but obfuscates the underlying data and constrains the analysis through a 12-month window
- Each month's exact death count can't be determined, they can be estimated through constrained optimization

Developing the System

- A 12-month rolling sum is simply a uniform kernel with a width of 12 and a height of 1
- Developing the system starts by representing a given month as i, its 12-month rolling death tally as Σ_i, the death tally for that month as x_i, and the the death tally for the preceding 11 months as x_{i-1} ... x_{i-11} will yield the following constraining equation

$$x_{i-11} + x_{i-10} + x_{i-9} + x_{i-8} + x_{i-7} + x_{i-6} + x_{i-5} + x_{i-4} + x_{i-3} + x_{i-2} + x_{i-1} + x_i = \Sigma_i$$

- The next month can be represented as $i + 1$, its 12-month rolling death tally as Σ_{i+1}, the death tally for that month as x_{i+1}, and will yield the following constraining equation

$$x_{i-10} + x_{i-9} + x_{i-8} + x_{i-7} + x_{i-6} + x_{i-5} + x_{i-4} + x_{i-3} + x_{i-2} + x_{i-1} + x_i + x_{i+1} = \Sigma_{i+1}$$

Constraining the System

- The system has 11 more variables than constraining equations.
- Knowing the variables represent overdose deaths, the solution space can be constrained to a finite set
- These additional constraints can be implemented by first confining the solution space to integers
- Followed by applying a constraining inequality where none of the elements in the variable matrix can be less than 0

Initial Python Implementation

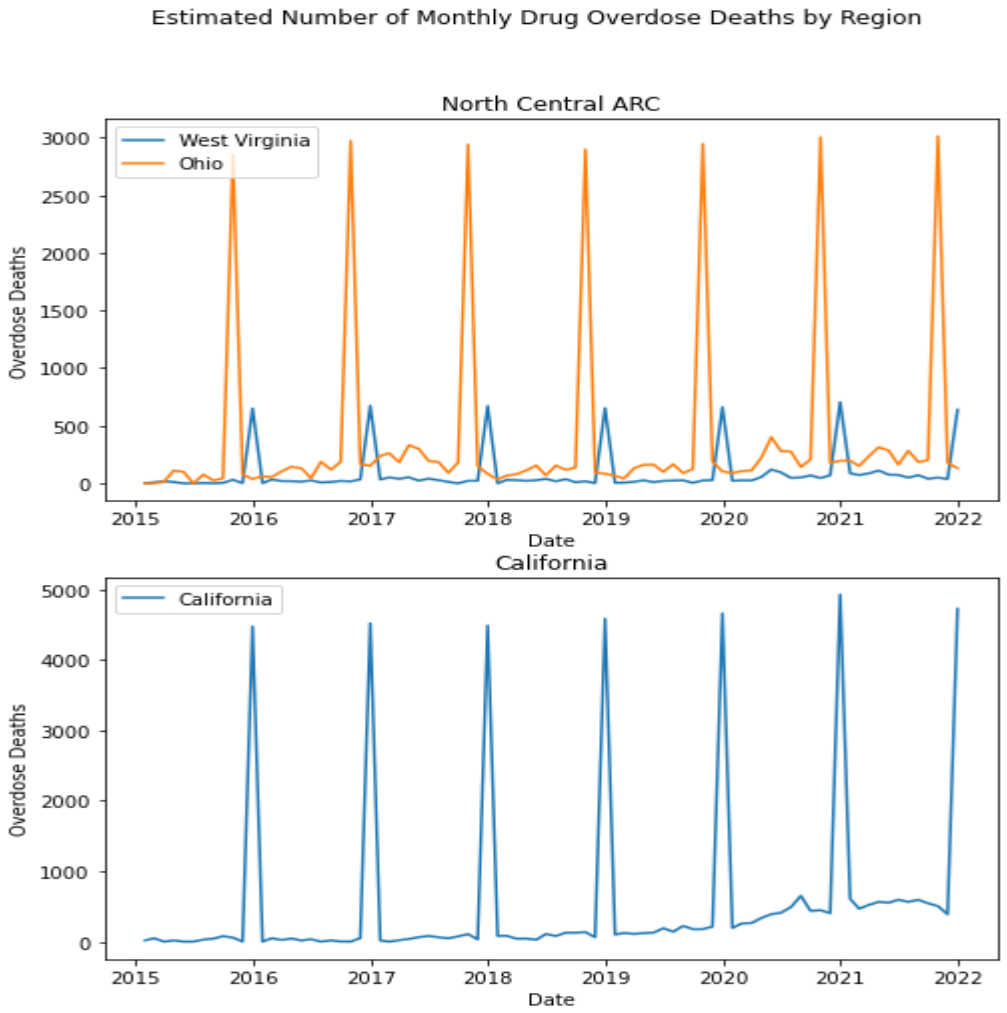
```
# import requisite packages
import pandas as pd
import numpy as np
import pulp

# import and clean data
…

# function to create coefficients matrix
def sliding_windows(kernel, num_constraining_eqs):
    kernel = np.asarray(kernel)
    p = np.zeros(num_constraining_eqs -1,dtype= kernel.dtype)
    b = np.concatenate((p, kernel,p))
    s = b.strides[0]
    strided = np.lib.stride_tricks.as_strided
    return strided(b[num_constraining_eqs -1:], shape=(num_constraining_eqs,len(kernel)+ num_constraining_eqs -1), strides=(-s,s))
```

Initial Python Implementation Cont.

```
# driver
period = 12
regions = death_df["Region"].unique()

monthly_deaths_df = pd.DataFrame()
for region in regions:
    series = death_df[death_df["Region"] == region].sort_values(by='End Date’)
    sol = series["Reported Number of Drug Overdose Deaths"].dropna().to_numpy()
    if (len(sol) < 2):
        marginal_values = np.empty(len(series.index))
        marginal_values[:] = np.nan
        series["Estimated Monthly Marginal Reported Number of Drug Overdose Deaths"] = marginal_values
        continue
    coef = sliding_windows(np.ones(period), len(sol))

    #pulp Linear Algebra Solver yeilds a solution not guaranteed to be the correct solution but all the values
    #it produces will be non-negative, discrete and yeild the values in the dataset when summed across a 12 month window
    mod = pulp.LpProblem(region.replace(" ", "_"))
    #constrain monthly death tally values to integers greater than or equal to 0
    vars = pulp.LpVariable.dicts('x', range(len(coef[0])), lowBound=0, cat='Integer')
    #set up constraining equations
    for row, rhs in zip(coef, sol):
        mod += sum([row[i]*vars[i] for i in range(len(row))]) == rhs
    mod.solve()

    #discarding the leading 11 values which dont have corresponding 12 month rolling sums
    marginal_values = [vars[i].value() for i in range(len(coef[0]))][(period -1):]
    series["Estimated Monthly Marginal Reported Number of Drug Overdose Deaths"] = np.pad(marginal_values, (len(series.index)-
len(marginal_values),0), 'constant', constant_values=(np.nan))
    monthly_deaths_df = pd.concat([monthly_deaths_df, series])
```

Initial Solution

- Solving this system via optimization yields the least entropic, most volatile solution with an overwhelming majority of deaths occurring one month a year.
- In all likelihood, the system does not behave this way



Further Constraining the System

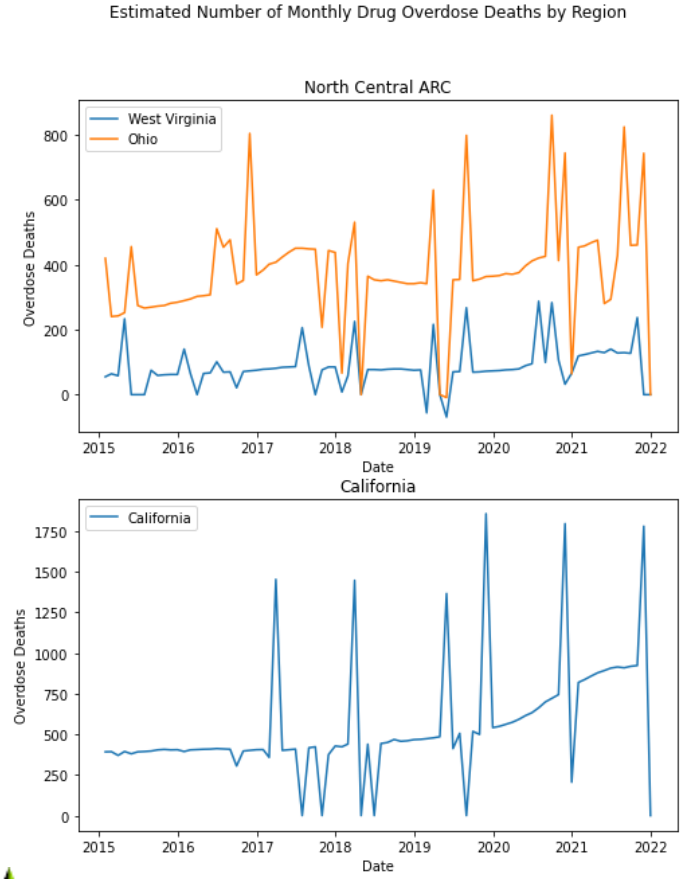
- To get a less volatile solution, the system can be further constrained by applying another constraining inequality where none of the elements in the variable matrix can be exceed a given value
- There can be many implementations of this, but here it is implemented as a maximum percentage deviation **above** the 12-month moving average, also referred to as a smoothing factor or volatility factor
- If the smoothing factor is too low, tightly tying the monthly values to the moving average, the system will be overly constrained, and no solution can satisfy all the constraints put on the system
- If the smoothing factor is too high the resulting solution will be artificially cyclical and very volatile, as was seen previously
- Selecting the right smoothing factor depends on the ratio of unknown values to constraining equations, the magnitude of the values in the series and can only be identified via trial and error.

Python Implementation of More Constraints

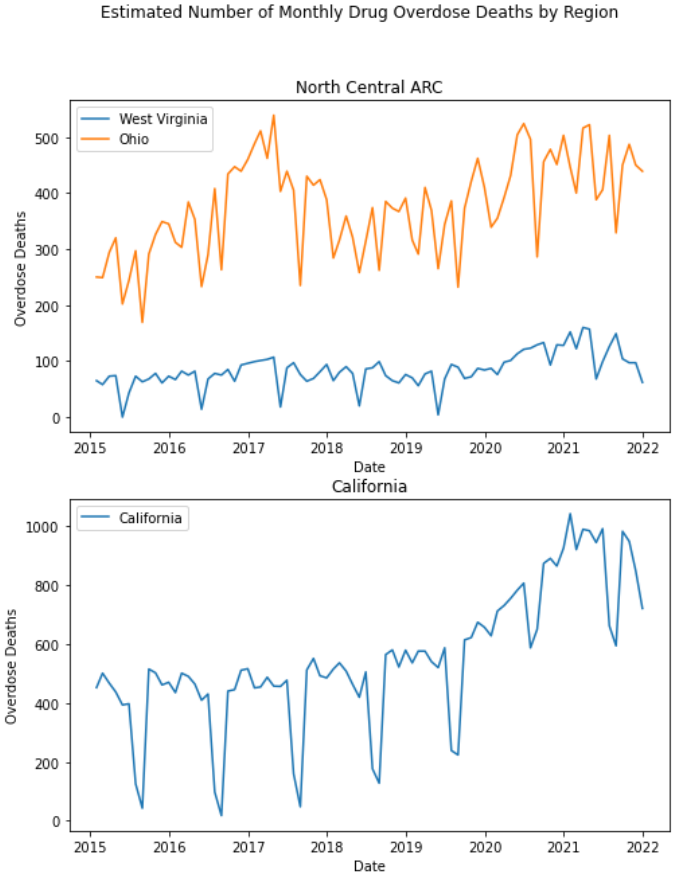
```
period = 12
volatility_factor = 1.3 # must be between 1 and period
regions = death_df["Region"].unique()
monthly_deaths_df = pd.DataFrame()
for region in regions:
    series = death_df[death_df["Region"] == region].sort_values(by='End Date’)
            sol = series["Reported Number of Drug Overdose Deaths"].dropna().to_numpy()
            if (len(sol) < 2):
                        marginal_values = np.empty(len(series.index))
                        marginal_values[:] = np.nan
                        series["Estimated Monthly Marginal Reported Number of Drug Overdose Deaths"] = marginal_values
                        continue
    coef = sliding_windows(np.ones(period), len(sol))
    #pulp Linear Algebra Solver yeilds a solution not guaranteed to be the correct solution but all the values
    #it produces will be non-negative, discrete and yeild the values in the dataset when summed across a 12 month window
    mod = pulp.LpProblem(region.replace(" ", "_"))
    #set up contraining inequalities
    #constrain monthly death tally values to integers greater than or equal to 0
    vars = pulp.LpVariable.dicts('x', range(len(coef[0])), lowBound=0, cat='Integer’)
    #constrain monthly death tally values to be less than n% greater than the moving average
    upBound_vector = np.around(((volatility_factor/period)*np.pad(sol, (period-1,0), 'constant', constant_values=sol[0]) + .5), 0)
    for pointer in vars.keys():
        vars[pointer].upBound = upBound_vector[pointer]
    #set up constraining equations
    for row, rhs in zip(coef, sol):
        mod += sum([row[i]*vars[i] for i in range(len(row))]) == rhs
    mod.solve()
    #currently discarding the leading 11 values which dont have corresponding 12 month rolling sums
    marginal_values = [vars[i].value() for i in range(len(coef[0]))][(period -1):]
    series["Estimated Monthly Marginal Reported Number of Drug Overdose Deaths"] = np.pad(marginal_values, (len(series.index)-
len(marginal_values),0), 'constant', constant_values=(np.nan))
    monthly_deaths_df = pd.concat([monthly_deaths_df, series])
```

Comparison of Constraints

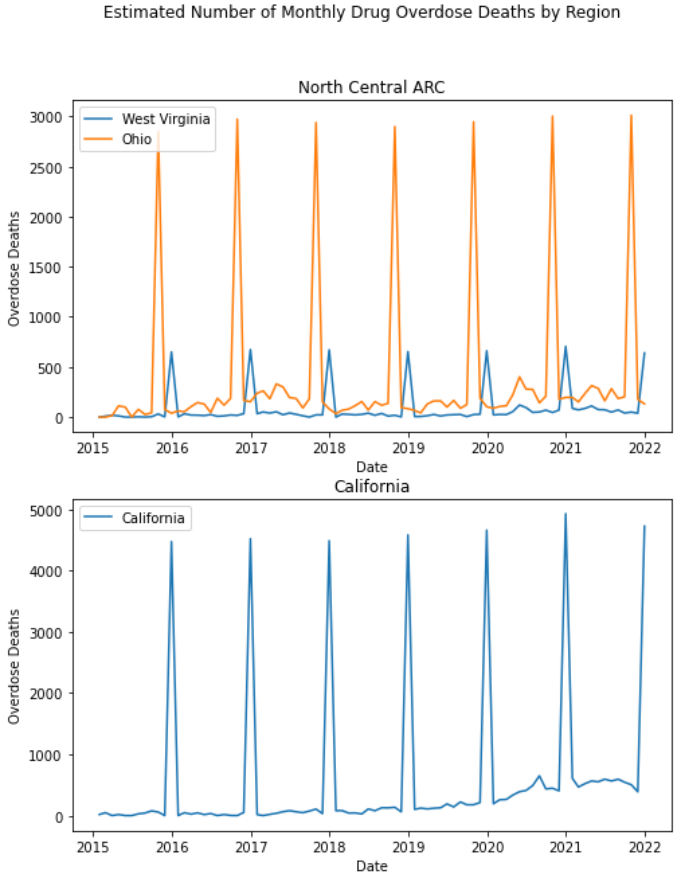
Overly Constrained



More Optimally Constrained



Unconstrained



Refining the Systems Constraints

- Applying a dynamic upper bound to the variables results in a system that behaves a lot more realistic, but there are still drastic sharp rises and drops that appear at almost the same time every year
- Instead of applying a static lower bound of 0 to all the variables, the lower bound can be made dynamic as well
- Using the same volatility factor as the upper bound, the variables can have a maximum percentage deviation **below** the 12-month moving average

Python Implementation of More Refined Constraints

```
period = 12
volatility_factor = 1.3 # must be between 1 and period
regions = death_df["Region"].unique()
monthly_deaths_df = pd.DataFrame()
for region in regions:
    series = death_df[death_df["Region"] == region].sort_values(by='End Date’)
            sol = series["Reported Number of Drug Overdose Deaths"].dropna().to_numpy()
            if (len(sol) < 2):
                        marginal_values = np.empty(len(series.index))
                        marginal_values[:] = np.nan
                        series["Estimated Monthly Marginal Reported Number of Drug Overdose Deaths"] = marginal_values
                        continue
    coef = sliding_windows(np.ones(period), len(sol))
    #pulp Linear Algebra Solver yeilds a solution not guaranteed to be the correct solution but all the values
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    #constrain monthly death tally values to integers greater than or equal to 0
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    #constrain monthly death tally values to be less than n% greater than the moving average
    lowBound_vector = np.around(((1/(volatility_factor*period))*np.pad(sol, (period-1,0), 'constant', constant_values=sol[0]) + .5), 0)
    upBound_vector = np.around(((volatility_factor/period)*np.pad(sol, (period-1,0), 'constant', constant_values=sol[0]) + .5), 0)
    for pointer in vars.keys():
         vars[pointer].lowBound = lowBound_vector[pointer]
        vars[pointer].upBound = upBound_vector[pointer]
    #set up constraining equations
    for row, rhs in zip(coef, sol):
        mod += sum([row[i]*vars[i] for i in range(len(row))]) == rhs
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    series["Estimated Monthly Marginal Reported Number of Drug Overdose Deaths"] = np.pad(marginal_values, (len(series.index)-
len(marginal_values),0), 'constant', constant_values=(np.nan))
    monthly_deaths_df = pd.concat([monthly_deaths_df, series])
```
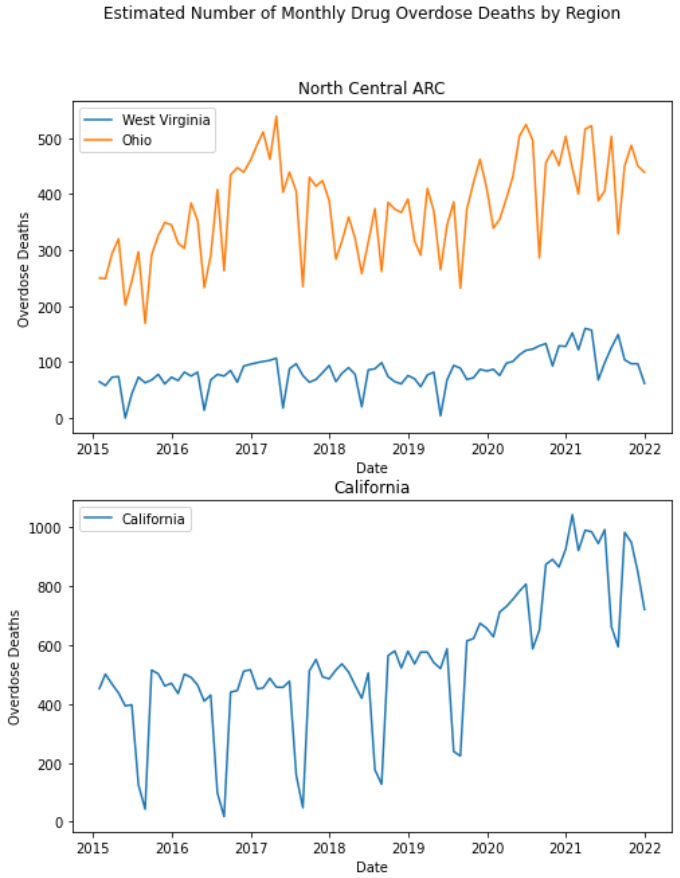

Comparison of Constraints

Non-Negative Lower Bound



Dynamically Constrained Lower Bound