Callum Weinberg: PSTAT 262 FE Final Project

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Abstract

Introduction

Accessing this Report

This report was completed for final exam credit for "PSTAT 262 FE" at University of California Santa Barbara in the spring quarter of 2022. The [] project on my Github page [] contains this report, a PDF with slides corresponding to the presentation of this report, and an interactive R-Markdown file that contains the relative statistical programming for this report. The R-Markdown file can be accessed here []. The Github project folder also contains the data used in the report and other files related to running the code and processing the data in the report.

Background

Greenhouse gas emissions from human activity are known to significantly contribute to global warming and climate change. Carbon dioxide emissions are the most prevalent greenhouse gas emissions in the United States currently.[7] Carbon dioxide is known to diffuse through the global atmosphere easily,[18][14, p. 2497] and therefore carbon dioxide levels in the atmosphere are generally similar throughout the globe.[16] However, local concentrations of carbon dioxide can be higher, especially close to emission sources.[16][14, p. 2497]

As of 2010, the impact of CO2 concentrations on local outcomes has not been studied extensively. In a 2010 paper, Mark Jacobson researches the effects of "domes" of CO2 over cities. The results of the paper suggest that CO2 levels may increase ozone and particulate matter and also may be associated with higher premature mortality.[14, p. 2497] Heightened ground-level ozone concentrations are associated with negative health outcomes.[6]. Therefore it is important to understand any relationship between local CO2 emissions and local ozone concentration.

Geospatial data and time series data are often high dimensional. [1] Therefore applying feature extraction methods is often advantageous for statistical learning tasks. Principal Component Analysis (PCA) is a fundamental feature extraction methods. PCA is a method of performing a linear projection of a data set onto a subspace in which the variance of the data is maximized.[21, Part II Section 3.1] The resulting principal components have the useful properties that each is orthogonal to each other, and the maximum variance is captured by the first component and then each component has less of the variance. Therefore PCA is useful when variables are correlated with each other, as an orthogonal projection of the data can be extracted. Additionally, since principal components capture subsequently less variance of the data, PCA can be used as a dimensionality reduction technique, as a subset of the principal components may capture a large amount of the variation in the data.

PCA relies on linear basis projections of the original data.[21, Part II Section 4] An generalization of PCA is kernel principal component analysis (KPCA). The motivation for KPCA is that a linear basis may not be optimal for describing the data. KPCA allows for non-linear projections of the data by implementing a feature map. The data is mapped into a higher dimensional space that allows for non-linear representations of the projected data to be found. This is described more in the methods

[1] high dimensional data refers to data sets in which the number of variables is large, especially if the number of variables is close to or greater than the number of observations.

section.

[PARAGRAPH TYING THESE TOGETHER - WHY KERNEL METHODS ARE USEFUL FOR TIME SERIES OR SPATIAL DATA]

Purpose

The purpose of this report is twofold. The first objective is to explore the relationship between ozone levels and carbon emissions at a localized level. The data in this report (see Data section) is limited to a time series for a single location (Los Angeles), for a number of covariates representing different sector-sources of carbon emissions. Although this objective was inspired by Jacobson's 2010 paper,[14] this report does not attempt to replicate the analysis of the paper.

The second objective is to complete the first objective via PCA and kernel PCA methods. Specifically, PCA and KPCA are explored in detail through the CO2 data. Then Principal Component regression and kernel principal component regression models are fit to relate the CO2 data and the ozone data. PCA and kernel PCA

It need be stressed the results of this report should not in any way be construed as evidence for a causal relationship between localized carbon emissions and ozone levels. While such a relationship is a driving interest of this report, the scope of the report falls far short of the level of work that would be required to prove or disprove a causal relationship. Specifically, this work would likely need to be expanded to a geospatial-time model that controlled for confounding variables, would likely require a understanding of potential mechanisms that would cause such a relationship, and would require input of domain expertise.

Methodology

PCA

The key idea of PCA is to reduce the number of dimensions of a data set, and in doing so, create orthogonal principal components. PCA is accomplished by finding a linear subspace that maximizes the variance of the data, when the data is projected onto the subspace.[21, Part II Section 3.1] The following illustrates this concept:

$$X_{N\times p}W_{p\times p} = Z_{N\times d}$$

Where N is the number of observations in the data, p is the number of variables in the data. X is the original matrix of the data, W is the projection matrix, and Z is the transformed data. The columns of Z are referred to as the principal components. The are orthogonal to each other. The first principal component is effectively a new variable that explains the most variation in the data as is formed from a linear combination of the variables (as is seen in $X_{N\times p}W_{p\times p}$). The variance explained by the first principal component is then "subtracted out", and each additional principal component explains less of the data. In PCA, there can be up to p principal components. However for high dimensional data, it may only be necessary to keep a small subset of the principal components.

The columns of data matrix X should be centered before performing PCA, so that the projection captures the direction of the variance and not the mean.[9] Additionally, the columns of X should be scaled to a variance of one if the variances for each column (variable) are not roughly the same. Otherwise, the magnitude of the variance will be captured in earlier principal components.

PCA can be more generally formulated as special case of the eigenvalue problem:[21, Part IV Section 2]

$$C_X W_X = \lambda W_X$$

Where C_X is the covariance Matrix of X: $X'X$.

Methods For Performing PCA

One method to perform PCA is eigenvalue decomposition of C_X. The eigenvectors comprise W_X. The vectors should be sorted descending on the eigenvalues, as the vectors with largest corresponding eigenvalues have the maximum variance (the eigenvalues correspond to the diagonal of C_X, and therefore are the percent of the variance of each component).

Another method for performing PCA is Singular Value Decomposition (SVD). SVD of a matrix takes the following form:

$$X = U\Sigma V^T$$

Where X is the centered (and often scaled) data. Then $U\Sigma$ results in the principal components (and Σ are the singular values, which are the square root of the eigenvalues[21, Part II Section 3.7] . The projection matrix is given by V. SVD results in the columns of U being sorted descending on eigenvalues, providing a small benefit over eigenvalue decomposition.[5]

Both eigenvalue decomposition and SVD require the computation of all principal components. The NIPALS algorithm (Nonlinear Iterative Partial Least Squares) is a method for finding principal components that allows for only the first q components to be found. This can be useful if the number of variables p is larger, or if the Kernel Matrix K (see below) is large. One implementation of the NIPALS algorithm is as follows:

1. Center (and scale) $X_{N\times p}$
2. Initialize a vector $t_{N\times 1}$ to some random value (can use a column of X
3. Calculate vector v (called a loading vector) $v = \frac{t^T X}{t^T t}$
4. Normalize v, such that $v = \frac{v}{\sqrt{v^T v}}$
5. Calculate t by regressing X onto p: $t_{new} = \frac{Xv}{v^T v}$
6. Check the sum of squared difference between t_{new} and t. If it is less than some threshold, say 10^{-9}, stop iteration of this loop.[5]
7. Set the pth vector of the principal component matrix equal to t and the pth vector of the projection matrix equal to v
8. Deflate the matrix X such that $X = t_{new} v^T$
9. iterate for i principal components, up to the number of columns of X

[5][21, Part II Section 3.8]

An advantage for the NIPALS algorithm over SVD and eigen decomposition is not all of the principal components have to be calculated: some subset $i < p$ could be calculated. As will be discussed in the analysis section, NIPALS is likely slower if all of the principal components are being calculated.

Note that the prcomp() function from the stats package in R uses SVD to perform PCA [23].

Kernel PCA

PCA involves creating principal components from a linear projection of the data. It may be that the principal components are better represented by a non-linear projection of the original data. The general idea of KPCA is to transform the data via a kernel (called the Gram matrix) into a higher dimensional space. In this higher dimensional space, a linear projection may be suitable and PCA can be performed. A non-linear combination of features is chosen (called a feature mapping), represented by $\phi()$. Then the Kernel matrix is defined as $K = \phi(X)\phi^T(X)$. $\phi(X)$ is often unknown (as it is in this

report). However K can be calculated from variable X, which results in a matrix representing a set of points in the feature space. K is sufficient to perform PCA, and is similar to the Covariance Matrix C_x in linear PCA. Using K instead of $\phi(X)\phi^T(X)$ is called the "Kernel Trick."[21, Part II Section 4.1][20]

So KPCA can also be generally formulated as special case of the eigenvalue problem:[21, Part IV Section 2]

$$KW_X = \lambda W_X$$

.

Therefore, the KPCA principal components and projection vectors can be obtained using the same methodologies as PCA once the Kernel Matrix is determined. However if the feature mapping is unknown (as it is in this project), it is very challenging to find the point in the original space of X that the feature space maps to. This is called the "Pre-Image" problem,[21, Part II Section 4.5] and is outside the scope of this project (this report will only work with the principal components in the feature space).

Kernels

In order to apply the kernel trick, a kernel must be chosen. The kernel is applied to the feature space using some kernel function.[21, Part I Section 4] Many kernels are possible. PCA is a special case of KPCA when the linear kernel.

A very common kernel is the Radial Basis Function kernel, also called the Isotropic Stationary Kernel and the Squared Exponential Kernel. It takes the following form:[21, Part II Section 4.3]

$$k(x, x') = \sigma^2 exp\left(\frac{-(x - x')^2}{2l^2}\right)$$

$sigma^2$ is often ignored when applying this kernel. l^2 must be selected carefully, and its choice will affect the nature of the principal components.

Another kernel is the rational quadratic kernel, of the form: [21, Part II Section 4.3]

$$k(x, x') = \sigma^2\left(1 + \frac{-(x - x')^2}{2\alpha l^2}\right)^{-\alpha}$$

.

This kernel has two hyperparameters (not including σ^2). It is often a good choice for time series data.[2]. Both of these kernels are explored in the KPCA section of this report.

Statistical Code and Software

All of the statistical programming in this report is completed in R. R version 4.2.0 was used at the time this report was written.[10] The R-Markdown file related to this report can be found on the author's Github page (see Introduction). The following packages were implemented in addition to the functions available in 'base' R: [22], [27], [26], [29], [28], [11], [24], [19], [3], [17], [15], [31], [32], [25].

Data

The primary data sets used in this report are 1) ozone data from the U.S. Environmental Protection Agency (EPA)[4] and 2) CO2 emissions data from the Vulcan High-Resolution Hourly Fossil Fuel data set repository provided by the Oak Ridge National Laboratory Distributed Active Archive Center

[2]Author lacks an explicit citation for this, but wrote it down in a conversation with the professor in class

(ORNL DAAC). [12] CO2 emissions are estimated for the following sectors: residential, commercial, industrial, electricity production, onroad, nonroad, commercial marine vessel, airport, rail, and cement.[12] Seven of these ten CO2 variables will be used as the covariates (X matrix of data) in this report.

Additionally, a county boundary shapefile from the California Open Data Portal[2] was used for the map in figure 1 below and is available in the "Raw" folder on the Github page.

Data Access

Ozone data is available from the EPA at the hourly timescale for sensors throughout the United States.[4] It is made publicly available as part of the EPA's air quality monitoring program. The unit of measurement is "parts per million." The specific file chosen for the report is "hourly_44201_2014", which is available on the EPA's cite as a Zip File. Only the zip file was loaded to the Github repository: to fully rerun the analysis, extract the file in the folder "Raw/EPA_Air_Data/". For analysis in this report, the following variables are relevant: State.Name, County.Name, Date.Local, Datum, Longitude, Latitude, Site.Num, Sample.Measurement, and Units.of.Measurement. Only "Sample.Measurement" and "Units.of.Measurement", i.e. the ozone concentration (in parts per million) and the date information (in Date.Local) is relevant to the modeling of the report. The other variables are used to limit the data to the desired scope.

CO2 emissions data is provided in metric tons for each kilometer by kilometer grid in the continental United states.[12] [3] The data is made available by date by emission sector on the daac.ornl.gov website. For example, hourly airport emission data for the continental U.S. for March 10th, 2014 can be found in the file "Vulcan.v3.AK.hourly.1km.airport.mn.2014.d069.nc4" The data is stored in the .nc4 file format. Users are required to create an account to download the data, but the data is free and "openly share, without restriction."[12] The CO2 data was too large and did not compress well to load to the the Github page for this project (see introduction). Therefore the file "CO2_Long_v1.Rdata" (available in the "Intermediate" folder on the Github page) can be accessed as a starting point for rerunning the analyses in this report or extending them. Alternatively, a user can download a list of the files (see "Raw/Vulcan_CO2/March2014/List_of_Files.txt" and download them and place them in the "Raw/Vulcan_CO2/March2014/" folder to fully rerun the analysis.

Data Scope

The raw data files for both the ozone data and the CO2 data are large. Therefore a limited timescale was chosen to analyze the data. Specifically, the data is limited to 4PM on March 9th, 2014 until 3 PM on March 17th, 2014. [4] This results in slightly more than a week of data. The Vulcan data is available from 2010 until 2015. March 9th was chosen as a starting date since it is after daylight savings time of that year (2 AM of that data), in order to avoid any data-processing issues.[5]

Both data sets are limited to the Los Angeles area. For the ozone data, fourteen sensor sites measured ozone data during this time frame. Sites 9033 and 6012 were excluded from this analysis as they are in Lancaster, CA and Santa Clarita, CA. See Figure 1 below. Both sensors are North of mountain ranges and not near the center of the county. The data is available in the WG S84 reference coordinate system[30], with latitude and longitude of sensor-sites provided.

[3] Note that Alaska data is available as well, but is in a separate files.

[4] The data is provided in UTC, and this date-range is the data after converting to Pacific Timezone.

[5] 2014 was chosen as it was towards the end of of the time frame that the CO2 data is available. The month of March was chosen somewhat arbitrarily, although the author enjoyed choosing a week that contained March 16th as on that day in 2014, the University of Virginia beat Duke University in the ACC basketball championship 72 to 63 [8].

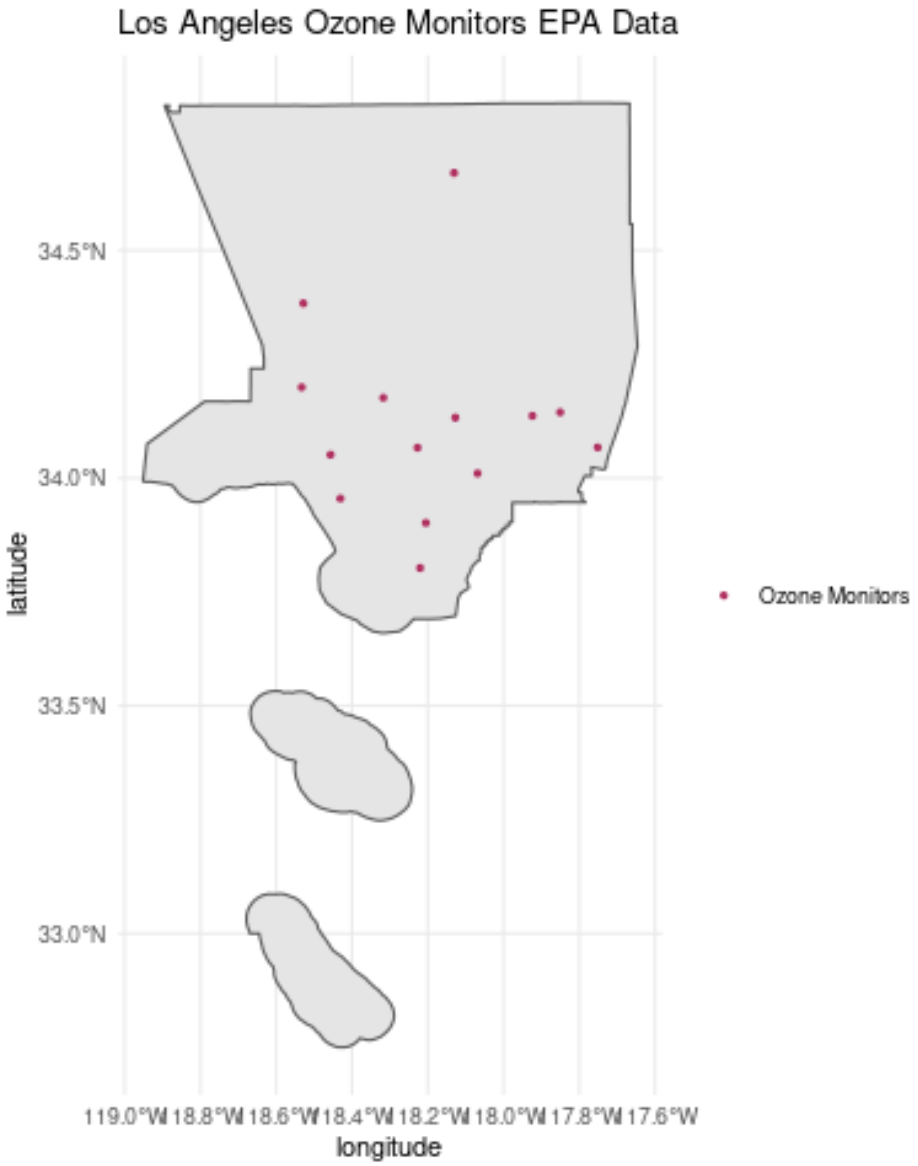

Figure 1: Ozone Monitors from EPA data, reporting ozone concentrations between PM on March 9th, 2014 until 3 PM on March 17th, 2014. L.A. County Site Numbers 9033 and 6012 are the two most northern points on the map.

The CO2 data is also limited to the Los Angeles area. The bounds are set to be the maximum and minimum latitude and longitudes of the ozone data, since the ozone data is more restricted. The Vulcan CO2 .nc4 data sets provide the data referenced in meters instead of longitude and latitude, and in the Lambert Conformal Conic reference system. See the R-markdown file (see Introduction) for a description of how the measurements were converted to align the geospatial references of both data sets.

Data Processing

The ozone and CO2 raw data sets were processed in the following steps to get data sets that are used for Explanatory Data Analysis (EDA), PCA, and KPCA. For the CO2 data, the .nc4 files are read into R using the ncdf4 package.[22] .nc4 file types are a bit challenging to work with in R: the author found the following resource very helpful for extracting information from .nc4 files for storage in data frames.[1] Specifically, the latitude and longitude equivalents (in meters, for Lambert Conformal Conic

reference system) were extracted from the "y" and "x" objects for the nc4 R-object (as created by the ncd4 package). The CO2 data is extracted using the ncvar_get() function for the "carbon_emissions" variable. This is done for all of the .nc4 files for all ten of the co2 emission types. The data is limited to: $y >= -401193.688560163, y <= -353976.762435499$, $x >= -1942544.51850291, x <= -1880037.22186271$. These bounds were found to be the equivalent for the maximum longitude and latitude bounds for the ozone sensors. The date-data was provided in "hours since 2010-01-01." This was converted to a date-time variable.

The ozone data was limited to Los Angeles county, California from the original data file (and WGS 84 reference system observations).

For both ozone and CO2 data (for each emissions source), the average across sensors for a given hour was calculated for use in the EDA and Analysis sections. For ozone concentration, this is likely the appropriate metric given the data is being aggregated over a region. For the CO2 data this decision is more circumspect. Arguably, total CO2 emissions by sector for a given hour may be more interesting for studying the relationship between ozone and localized CO2 emissions. However, the complicated nature and large size of the .nc4 data made studying the sensor sites a challenging problem. An average over the region was taken primarily because the author could not determine how often sensors may be missing data for the time frame. Finally the data sets were merged on the date and hour.

For the CO2 sector variables, cement and commercial marine vessel were not found to have any emission data for the time frame. Rail emissions were reported as constant for the time frame. As the rail emissions had no variability, they would not be useful in PCA, KPCA, or a regression problem, and are excluded from the analysis.

See the R Markdown file (see Introduction) for a complete description of the data processing.

Exploratory Data Analysis

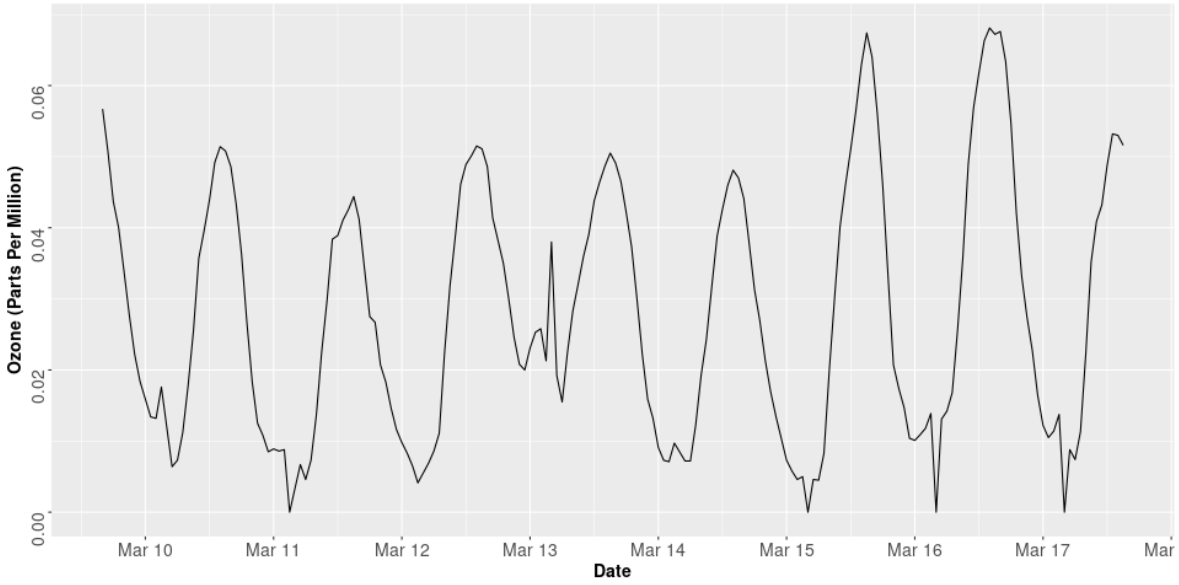

Figure 2: Average Ozone Concentration (Parts Per Million) Across Los Angeles County Sensors. Hourly from 4 PM May 9th, 2014 until 3 PM May 16th, 2014 (PST). Ozone sensor data excludes L.A. County Site Numbers 9033 and 6012 for the time period.

Figure 2 above shows the hourly time series for the average ozone concentration data for the L.A. County area (excluding the two sites, as explained in the above section). There is some noise to the data, but the ozone data is fairly cyclical. It peaks around .05 to .07 parts per million around 1 or 2 PM local time, and reaches the minimum of less than .01 parts per million around 1 or 2 AM most nights. May 13th is an exception, with ozone concentration reaching minimum of just below .02 parts

per million.

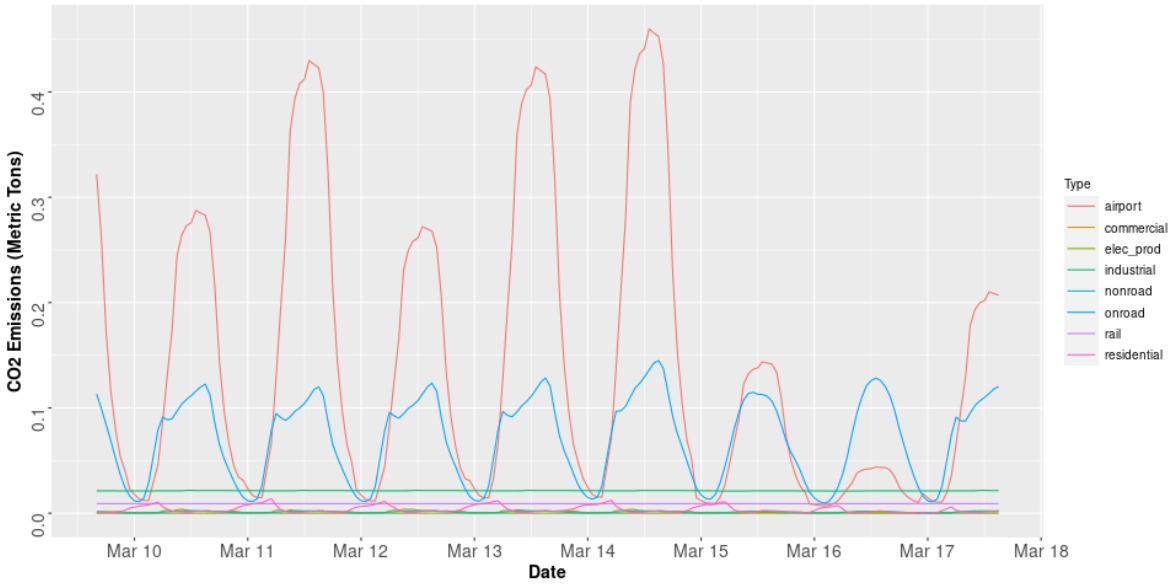

Figure 3: Average Metric Tons of CO2 Across Los Angeles County Sensors. Hourly from 4 PM May 9th, 2014 until 3 PM May 16th, 2014 (PST). Sensors Limited to bounds of Ozone Sensors, see Data Processing Section.

Figure 3 shows the hourly time series for average CO2 Emissions (Metric Tons). Airport emissions are by far the largest source of CO2 in the L.A. area for these dates. Peak airport emissions vary a lot of the course of the day and throughout the week, with lower peak emissions on May 15 and 16th (Saturday and Sunday). Onroad emissions are the next highest source of emissions, with peaks in the middle of the day and lows around midnight. Other emission sources are significantly lower, and cannot be discerned in the same graph. Note that rail emissions are estimated by Vulcan to be constant (but non-missing) over time.

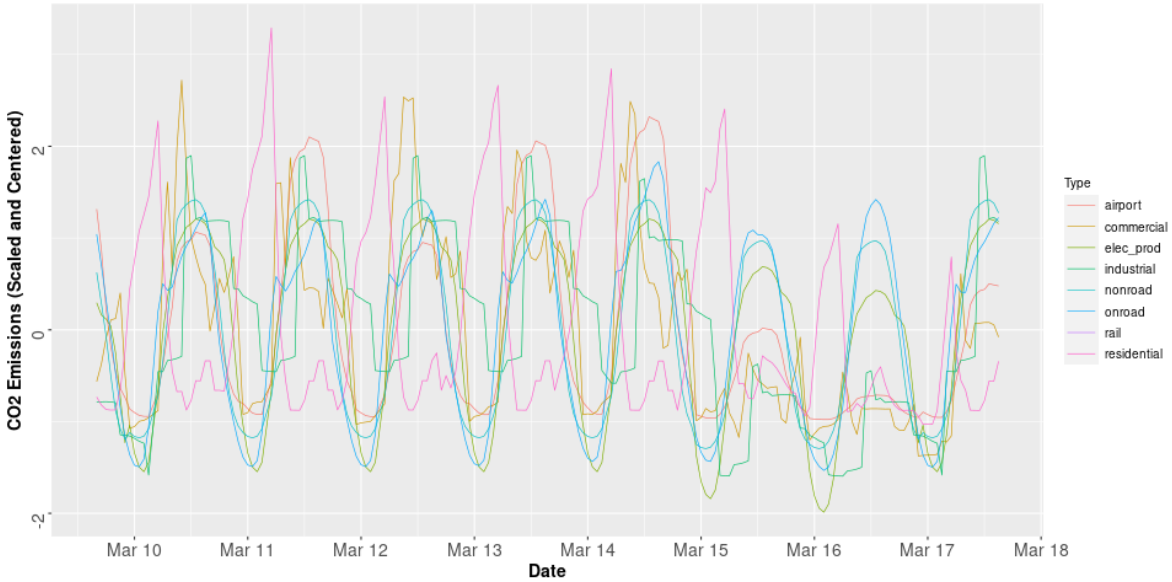

Figure 4: Average CO2 Scaled and Centered Across Los Angeles County Sensors. Hourly from 4 PM May 9th, 2014 until 3 PM May 16th, 2014 (PST). Rail emissions are not shown in this graph. Sensors Limited to bounds of Ozone Sensors, see Data Processing Section.

Figure 4 shows the sources of emissions scaled to a variance of 1 and centered to a mean of 0. This allows for visualizing the time series patterns of the sources with lower average emissions. Most emission source peak around midday and reach their minimum around midnight. The exception is residential emissions, which peak late evening to morning.

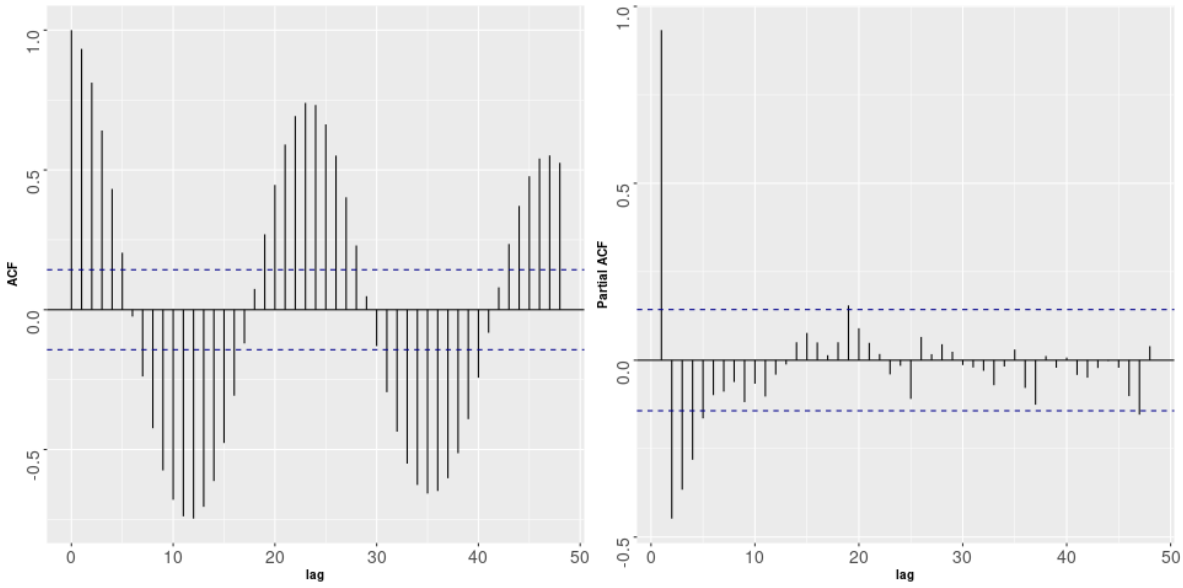

Figure 5: Autocorrelation function and partial autocorrelation function for ozone data over the time period, up to a lag of 48 hours. The blue lines indicate 95% confidence intervals for the ACF values.

The autocorrelation function (ACF) and partial autocorrelation function (PACF) for the ozone data is shown in Figure 5. In time series analysis, the ACF measures how correlated a observation at time t is to an observation at $t + lag$, for some $lag > 0$. The PACF is the correlation between the two lags while controlling for all other lags. These two graphs indicate that there is significant autocorrelation over time between the ozone concentrations. The ACF makes clear the cyclical nature of the ozone data, with observations near in hours positively correlated, and observations 12 hours apart negatively correlated. The PACF is used to inspect for some sort of "seasonal" trend, i.e. that observations a day apart are significantly correlated, after controlling for the other lags. The PACF indicates that the correlation is mainly happening at a lag of one hour, two hours or three hours. There does not appear to be daily season trend day-to-day (i.e. ozone concentration is not that correlated with ozone concentration 254 hours later). Note that this data set only spans one week. It is possible there would be weekly (and possibly annual) seasonal trends if more data were included in the report.

Figures 6 and 7 below show similar ACFs and PACFs for Airport CO2 and Residential CO2 emissions. However, the 24 lag (seen in the PACF) is significant in both cases. This suggests there is a predictable day-to-day relationship for CO2 emissions.

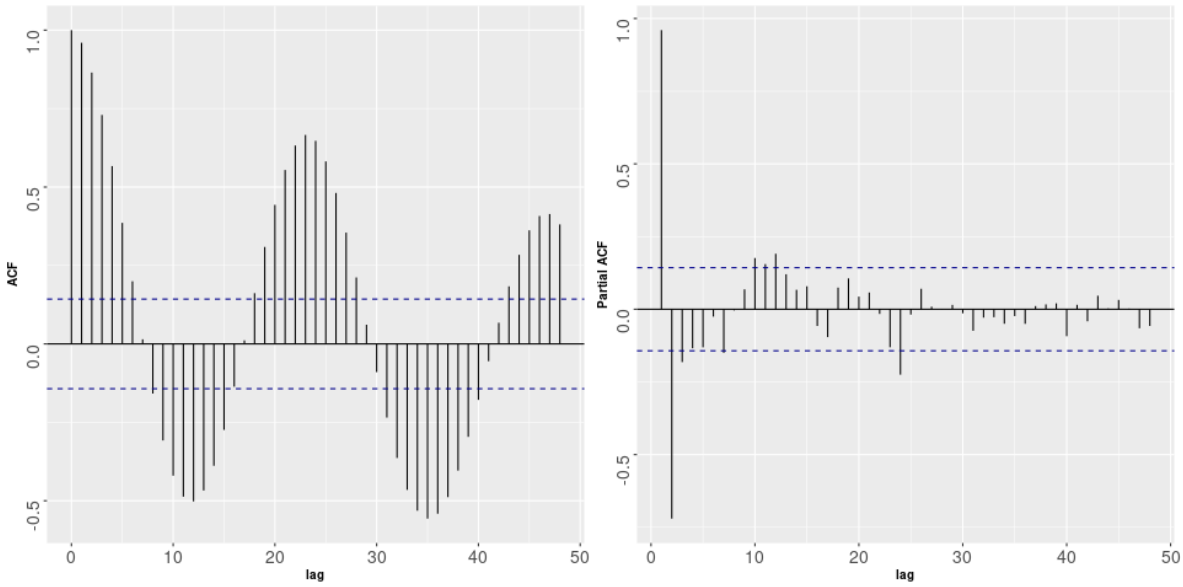

Figure 6: Autocorrelation function and partial autocorrelation function for Airport CO2 emissions data over the time period, up to a lag of 48 hours.

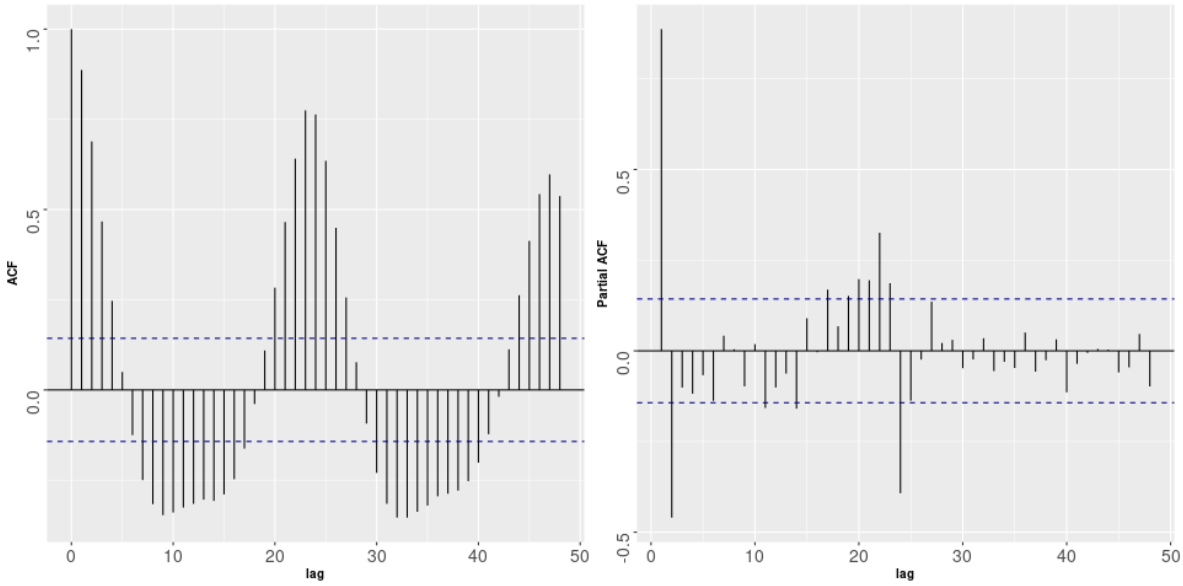

Figure 7: Autocorrelation function and partial autocorrelation function for Residential CO2 emissions data over the time period, up to a lag of 48 hours.

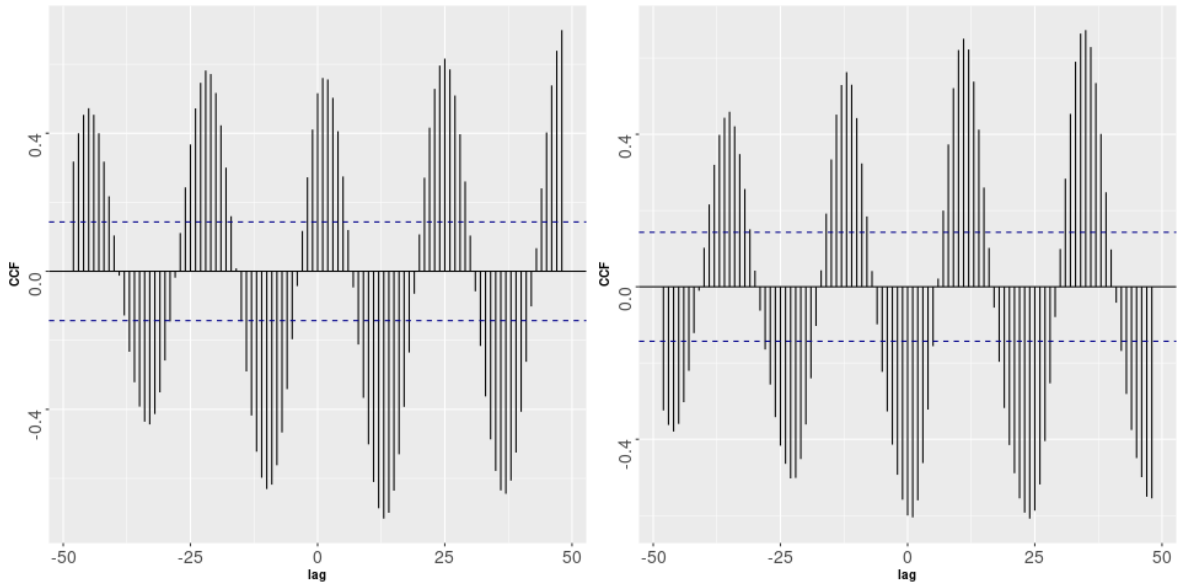

Figure 8: Cross-Correlation function functions Ozone vs. Airport CO2 (left) and Ozone vs. Residential CO2 (Right) over the time period, up to a lag of 48 hours.

Finally, figure 8 shows the cross-correlation functions between Ozone and Airport CO2 and Ozone and Residential CO2. Both show significant patterns of correlation between ozone and each variable.

All eight variables considered for the analysis portion of this report exhibit wave-like time series over the period. There is clear correlation between the variables, likely being driven by hour-of-the-day phenomena (e.g. there are not a lot of flights at the airport at midnight, and residential activities take place in the mornings and evenings while individuals are home). This correlation structure suggests a kernel method may be useful in capturing the relationships between these variables.

Analysis and Results

For the analysis section, X_c refers to the centered and scaled CO2 data, which is limited to the seven sectors: airport, commercial, electricity production, industrial, non-road, on-road, and residential. It contains 188 observations. Y refers to the Ozone data, which is one variable and 188 observations.

PCA Computation

As mentioned in the methodology section, a number of algorithms can be used to run PCA. Figure 9 illustrates the computational time taken to perform PCA using five different approaches.

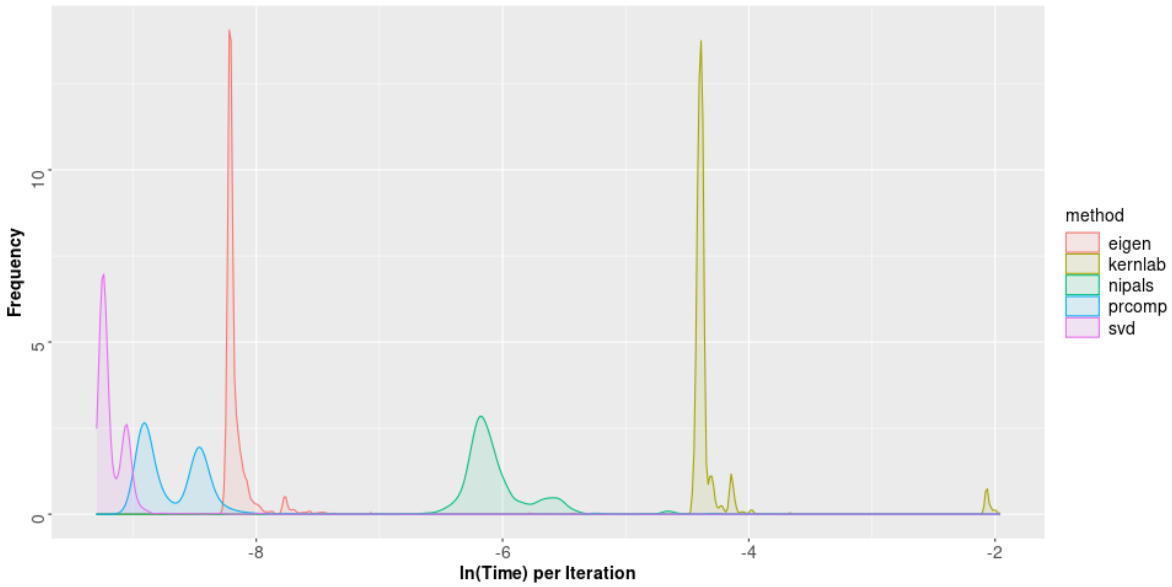

Figure 9: Log of time reported for visual clarity. 1000 iterations of performing PCA for five different methods. The data $X_{188\times 7}$ is the matrix of centered and scaled CO2 data.

The natural log of time is shown to reduce the impact of outliers on the graph. The log of times farther to the left correspond to shorter times to perform PCA. 1000 iterations were performed as there is some randomness to how long any given machine will perform this task, even while using the same data X_c.

Performing PCA via R's svd() function (part of the 'base' R functions) performs the best, while the kernlab package[15] (using the "vanilladot" kernel, kernlab's term for the linear kernel). NIPALS performs better than kernlab. Both have higher variance than the other three methods.

It is interesting that SVD performs slightly better than the prcomp function, since prcomp reportedly uses svd[23]. It is possible that prcomp involves some extra computation that is not necessary to just extract the principal components. SVD will be used for PCA as it performed most efficiently for X_c. In the KPCA section NIPALS will be reconsidered for its useful property of being able to compute a subset of principal components.

PCA Analysis

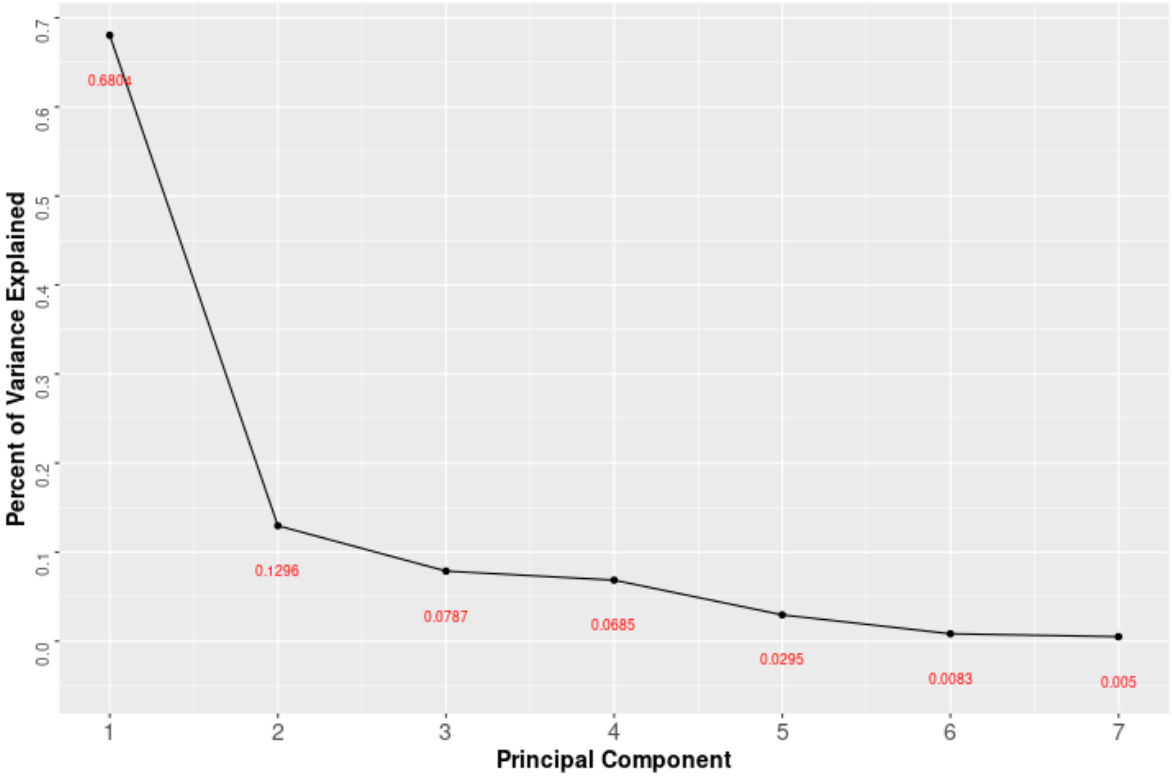

Figure 10: The percent of variation explained by each principal component for the CO2 data.

Figure 10 shows the scree plot for the PCA of X_c. The percent variance explained for each principal component can be found in a number of ways. For SVD, the eigenvalues are equal to the squared singular values (diagonal of matrix Σ), and the normalized eigenvalues (in descending order, as is constructed in SVD) represent the percentage of variation explained by each principal component. Here, 68% of the variation in the data can be explained by the principal component. The second principal component explains the next 13% of the variation. So with just 2 of 7 principal components, 81% of the total variance can be explained.

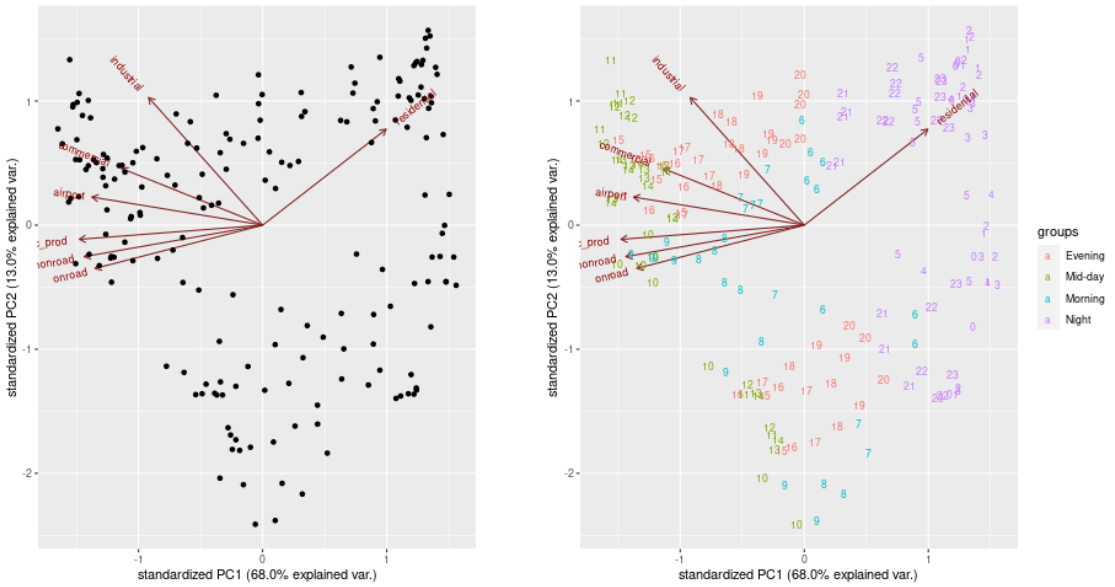

Figure 11: First and Second Principal Components Compared.

Above are the bi-plots of the first and second principal components.[6] The loading vectors (columns of the projection matrix) are shown by the arrows. The points represent the values of the first and second principal components for each observation. The bi-plot on the right groups the data based on time of day. Figure 12 shows normal ellipses drawn around the groupings. The following grouping was assigned by inspection:

- Hours 21, 22, 23, 0, 1, 2, 3, 4, 5 grouped as "Night"
- Hours 15, 16, 17, 18, 19, 20 grouped as "Evening"
- Hours 6, 7, 8, 9 grouped as "Morning"
- Hours 10, 11, 12, 13, 14 grouped as "Mid-day"

All of the seven CO2 variables are contributing significantly to the first component. Residential and industrial contribute the most to the second component. Three is a pretty clear distinction between the group defined as "night" and the rest of the day. This also corresponds to the residential loading vector, indicating the variation in residential CO2 emissions is distinct from the other emissions sources. This is expected given the breakdown shown in Figure 4 of the time series by group. Careful inspection of industrial emissions in figure 4 suggests a somewhat irregular pattern, possibly explaining its high contribution to components one and two. Although less distinct than night-emissions, it does seem that mid-day emission levels correspond to the non-residential emission sources.

[6]The following resource proved useful in implementing the ggbiplot[25] package. [13]

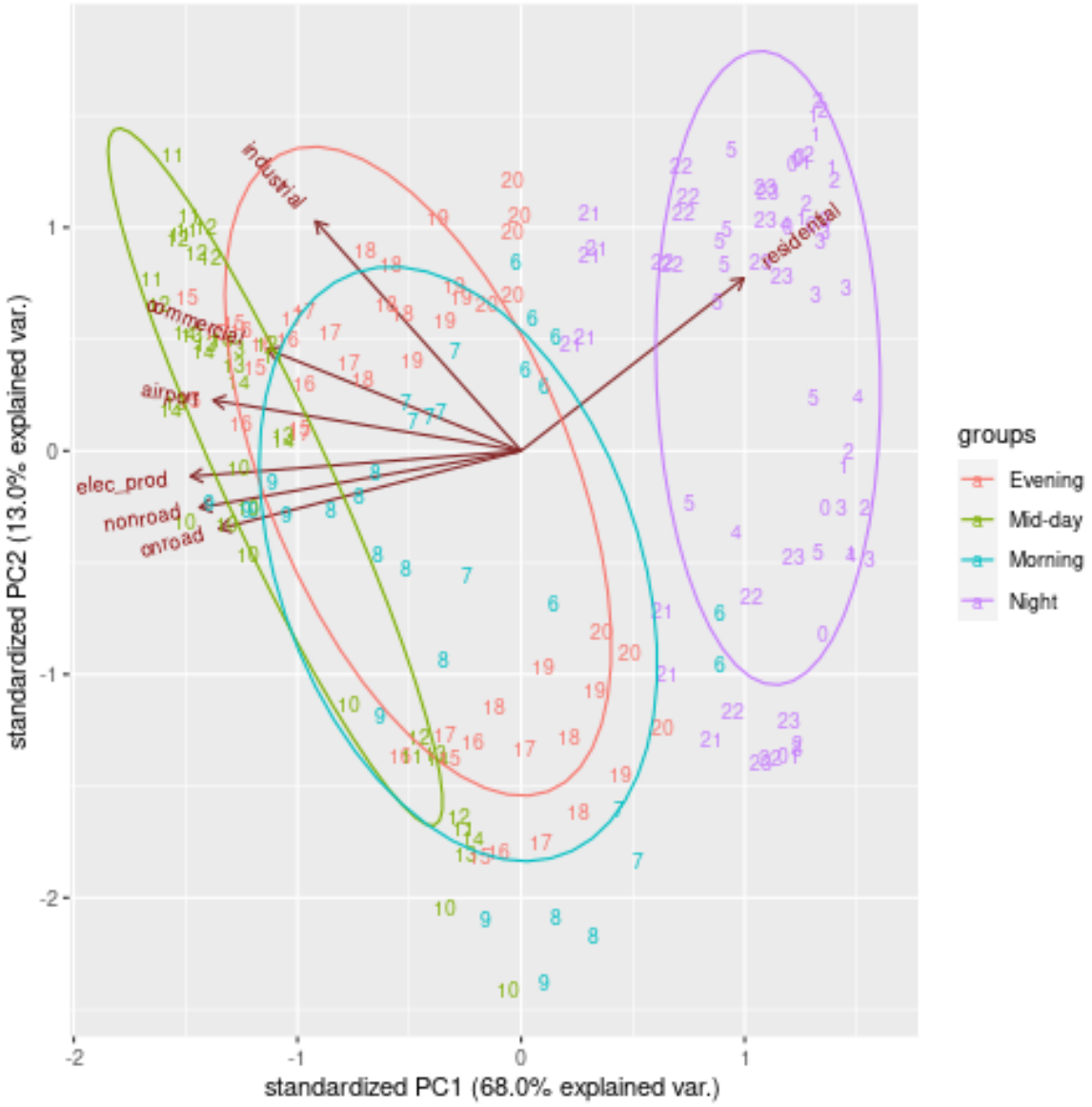

Figure 12: First and Second Principal Components Compared, with normal ellipse for groups.

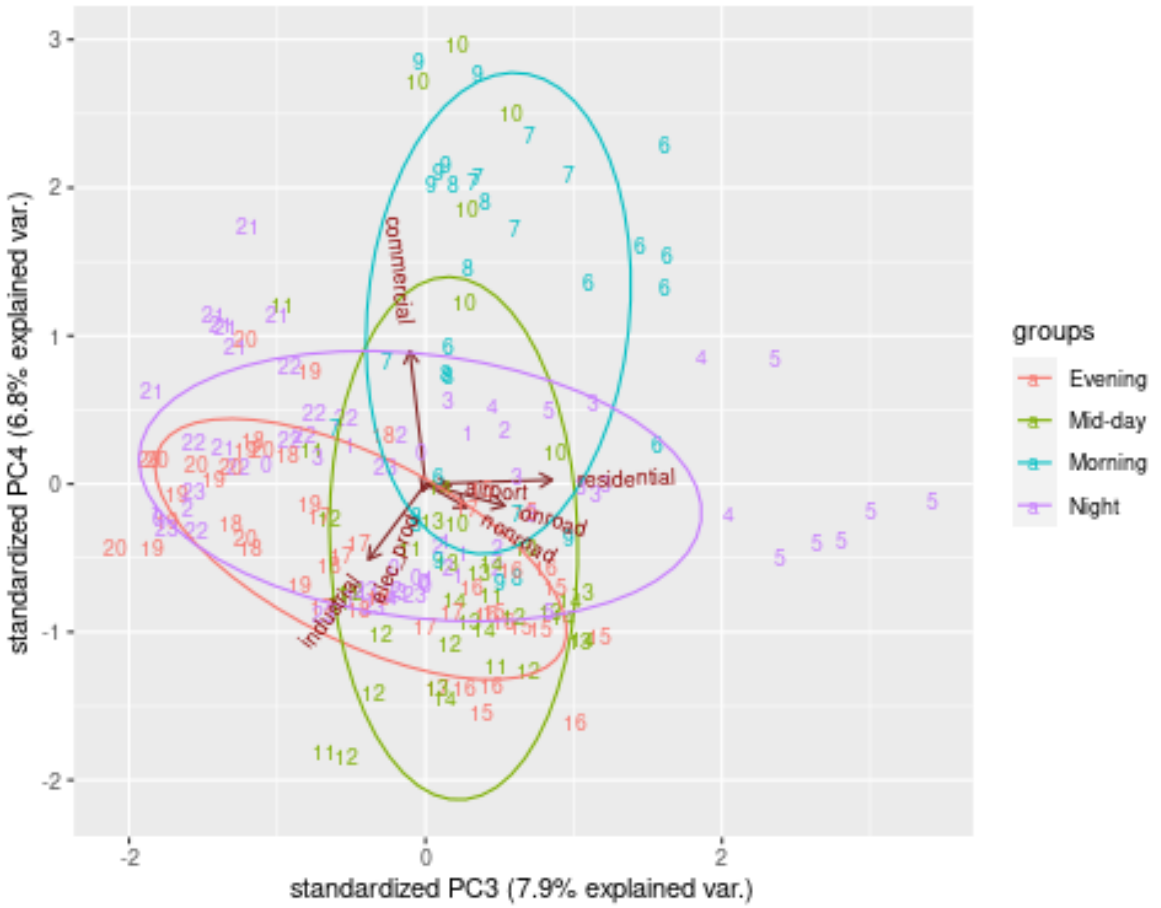

Figure 13: Third and fourth Principal Components Compared, with normal ellipse for groups.

Figure 13 shows the third and fourth principal components. The groupings are less distinct here. Residential CO2 emission variance appears completely deflated by principal component four, whereas commercial and industrial are still contributing (commercial just to principal component four).

In summary, these graphs suggest only one or two principal components are necessary to explain significant amounts of variation in the data. The first principal component is well defined by the time of day, whereas the second, third, and fourth are less so. One or two principal components may be sufficient to connect the CO2 emissions data to the Ozone data, as is explored in the next section.

Principal Component Regression

There are many reasons why principal component regression would be useful for modeling Ozone and CO2 data in this problem. One motivation is that the CO2 variables are highly collinearity. This results in an unstable model. For example, the variance inflation factor (VIF) for three of the seven CO2 variables when a model is fit is above 10 (a VIF of 5 is conventionally considered large and indicates multicollineary problems for a model). The principal components will all have a VIF of one since each vector is orthogonal to each other by design. Se the R Markdown file for an illustration of

this phenomena.

Instead, principal component regression is performed (PCR). For modeling ozone as a function of CO2 the main question is how many principal components to include. A model fit with all principal components results in high significance for the first, second, and fourth principal componentes and an adjusted R^2 of .1753. It seems unecessary to include all seven principal components here though, as the previous section illustrated that most of the variation was captured by the first few principal components.

Instead, if four components are selected, the significance of the one, two and four, and the value of their coefficients barely changes. The adjusted R^2 increases to .181. So the ozone data can be equally well modeled by the first four principal components of the CO2 data.[7]

The final model is shown below:

PC	Coefficient	Standard Error	P-Value
PC1	-0.0055698	0.0010155	$1.35x10^-7$
PC2	-0.0057490	0.0023270	0.01440
PC3	0.0001153	0.0029865	0.96924
PC4	-0.0097947	0.0032011	0.00255

Table 1: Principal Component Regression between Ozone and the Principal Components of CO2 Data. 184 df, Adjusted $R^2 = .181$

KPCA

Conclusion

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[7] Ideally some sort of cross-validation would be done to more robustly determine this result, but the author was running out of time on the project and did not extend the regression sections to prediction.

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