CHAPTER I

INTRODUCTION

Historical analysis of atmospheric chemistry shows global ozone (O₃) concentrations are heavily influenced by multiple catalytic cycles involving halogen, nitrogen, hydrogen, and oxygen species (Caffrey et al. 2001; Dobson 1923; He and Carmichael 1999; Lyons, Reinhard, and Planavsky 2014; WMO 2022). The global movement of carbon among the atmosphere, biosphere, oceans, and geosphere, indirectly yet significantly influence O3 concentrations, in the troposphere through greenhouse gas effects and atmospheric chemistry interactions (Danyang Ma et al. 2023; Hata et al. 2023; Q. Liu et al. 2022). Continued regulation, monitoring, and development of air pollution control initiatives are essential for continued maintenance of ozone depleting substances (US EPA 2015a; WMO 2022) which can impact the evolutionary potential of biological mechanisms on Earth (Grenfell et al. 2010; Kasting and Siefert 2002). The source of atmospheric cycles seems to be this highly reactive, unstable, triatomic molecule; providing a canvas for dioxide cycles necessary for organic systems (Caffrey et al. 2001; Lyons, Reinhard, and Planavsky 2014). Varying degrees of O3 allow for redox reactions, forming as both a product and constituent of the natural environment (Chapleski et al. 2016; Xing et al. 2016; Zoran et al. 2014).

Anthropogenic sources have deeply affected these necessary cycles by shifting natural concentrations of O3 in unnatural manners (Chauhan, Gupta, and Liou 2023; Cheadle et al. 2017; Danyang Ma et al. 2023; Flynn et al. 2021). As climate change continues to abet abnormal temperatures and weather cycles, the development of high-resolution predictive models such as those shown by this thesis are even more necessary to combat the exponential rate of urbanization (Balk et al. 2018; EPA 2021; Iglesias et al. 2021). This thesis seeks to provide a novel methodology which better incorporates geospatial relationships into modern statistical methods via residual kriging to three of the most populous counties in Arizona. The Statistical Model and Residual Krige (SMaRK) methodology is overlayed with statistical representations of census data in Maricopa, Pima, and Pinal Counties to show that leveraging the advantages of both techniques can better depict complex systems like O3. Similar methods have already shown great promise in modeling PM2.5, NOx, and similar air pollutants as complex as O3 (Y. Liu et al. 2018).

I.1. Machine Learning/Artificial Intelligence Predictions Require Proper Incorporation of Geospatial Data

Policies set by world governments can help reduce overall surface ozone pollution, but this is only as effective as the models used in gauging vulnerable areas. Current numerical modeling approaches, such as WRF-Chem, GEOS-Chem, and GODfit-Algorithms (Flandorfer 2019; Lerot et al. 2010; C. Lin et al. 2016; Yu et al. 2018), are computationally expensive, restricting the output of surface O3 maps to coarse spatial resolutions that are not suitable for public health studies. Health experts build their own datasets, resulting in highly accurate, but non-rasterized depictions of surface O3. Most ozone representations of the surface take numerous days to produce their final products (Kwok et al. 2015; C. Lin et al. 2016; Travis and Jacob 2019; Wu et al. 2021) and modelling efforts based on remote sensing measurements still have trouble capturing the complexity of surface ozone in urban settings without further improvements made by the researcher (Balamurugan, Balamurugan, and Chen 2022; Wang et al. 2023). When predictions from modelled O3 reactions are compared against surface observations from monitors, they tend to have difficulty simulating O3 concentrations at high-temporal resolutions. This suggests that the underlying geospatial patterns used during observation may not fully characterize regions accurately and/or that the resolution of the models is not adequate to simulate the photo-chemical environment of these finer observations. There is a compelling need in recent literature to improve high resolution surface O3 concentrations by incorporating simple spatial patterns into complex models.

Machine learning methods like Random forests can account for complex relationships between ozone and other covariates but tend to ignore spatial correlations of remote sensing (Niu et al. 2022; Telesca et al., n.d.; Wright and Ziegler 2017). With large data, linear and weighted regression tends to be exponentially faster, at the cost of egregious error (Feng et al. 2016; Huang et al. 2017; Watson et al. 2019). Combining an advanced model with its corresponding geospatial residuals helps account for the spatial correlation between modeled values while simultaneously accounting for complex relationships. Regression kriging is a commonly used kriging method based on multiple linear regressions and variograms (Yakowitz and Szidarovszky 1985; Q. Meng, Liu, and Borders 2013; Kleijnen 2017). In application to surface O3 values, this helps in incorporating co-funding covariates from a non-geospatial perspective. Five ensemble learning models were compared: Adaptive boosting, Stochastic Gradient Boosting, Extreme Gradient Boosting, Random Forest bagging, and a 2D recursive convolutional neural network (RCNN). These were created over a study area containing Arizona’s most populous counties of Maricopa, Pinal, and Pima from 1980-2023. Each model was created using a hyper-parameter tuner available through sci-kit learn in python (Raschka and Mirjalili 2019).

I.2. Why Surface Ozone? – Relations to Urban Air Quality

O3 has been detected in Earth’s stratosphere, troposphere, and more recently, on its surface (Claeyman et al. 2011; Davies and Schuepbach 1994; He and Carmichael 1999; M. Lin et al. 2012; Richter 2009; Xing et al. 2016). In 1955, the United States of North America (USNA) issued the Air Quality Control Act which dedicated the nation’s vast resources to additional monitoring, addressing air pollution concerns post-scientific revolution enticed by the Space Race of 1950. The acting President of the United States (POTUS) at the time; Richard Nixon, aided in the establishment of an Environmental Protection Agency (EPA) and National Oceanic and Atmospheric Administration (NOAA) to combat this newfound enemy with extreme prejudice (Nixon 1970). In doing so, new environmental movements have emerged due to unprecedented economic growth at the time; regulation policies which initially slowed some sectors, later exhibited long-term beneficial human and economic trends, as was theorized in the early 90s by Dr. Micheal E. Porter (Ambec and Barla 2002). Geographic Informational Science (GIS) has been dedicated to the proper implementation of these goals set forth in the early 1970s. With it came a new way to write Earth’s history via digital transformation of newfound resources; relating to trends near and far to answer difficult questions associated with life. From micro- to macro-scales, a geographer specializes in observations and predictions from planetary to microbial systems, inadvertently weaving complex knowledge of space and time beyond the scope it represents (Goodchild 1992).

Many communities at risk of high surface ozone concentrations are further threatened by urban heat island effects, vehicle emissions and industrial processes attributing to a variety of pollutants due to the mechanism which drives O3. It’s a precursor to many things due to its highly degenerative state (Afonso and Pires 2017; Bojkov and Fioletov 1995; Harithasree et al. 2024; J. Li et al. 2014). After zooming-in, ground-level O3 has been found to have a lasting impact on human health via reductions in life expectancy, abrupt changes to normalized Earthly air chemistries, and related oxo-based cycles for its development (Barzeghar et al. 2020; Ding, He, and Liu 2021; C. Lin et al. 2016; Manisalidis et al. 2020; Schlink et al. 2006; WHO 2013; Zhang, Wei, and Fang 2019). Surface O3 exposure has been found to contribute to several adverse respiratory symptoms, childhood cancers, adverse birth outcomes, overall mortality, and neurological disorders (Ni et al. 2024; Ghozikali et al. 2015; Tang et al. 2024; Turner et al. 2016). In addition, atmospheric studies have found the most significant constituents of ground-level O3 reactions to be nitrogen-oxides (NOx) and volatile organic compounds (VoCs) (Brown-Steiner and Hess 2011; Cheng et al. 2018; Girach et al. 2012).

When these are combined with large amounts of UV radiation, O3 begins to form and can have numerous effects on organic and in-organic material. Surface ozone has been found to be one of the leading pollutants on the Global Burden of Disease (GBD) (Anenberg et al. 2018; Brauer et al. 2024; Sun et al. 2024), harboring stealthy consequences that can only be seen with appropriate consideration of both formation and exposure to fully understand its impacts. Varying concentrations of O3 have been found to have numerous beneficial and adverse effects on various systems in a myriad of ways due to interactions with surrounding ecosystems (US EPA 2015b). This thesis applies the three laws of Geography to create a high-resolution representation of surface O3 at tiled resolutions ranging from 300m down to 25m. While the starting area is a small section of three counties within the United States, the framework applied here can be utilized for representations of O3 across the world as the incorporation of GIS and improvement of computational systems continue to progress in this era of Big Data (Cao 2022; Tamiminia et al. 2020; Bughin 2016; Curry 2016; Xu et al. 2023).

I.3. A Tale of Two Layers

Two layers in Earth’s atmosphere are known to house this reaction. It is generally beneficial to the environment and can act as a catalyst for certain biological and chemical systems whose main constituent is oxygen. Therefore, the patterns observed by researchers of specifically surface O3 (i.e 2m above the ground), have been difficult to follow. Generally, O3 is highly reactive and decomposes quickly, therefore increasing the probability for a reactive oxygen species (ROS) to “unnaturally” exist in any environment/system which it’s found to be a part of. Highly concentrated O3 areas near Earth’s surface typically affect populations outside highly industrialized zones with high vegetation, as the byproduct of plants is mainly CO2. Studies interested in surface ozone exposure within one’s activity space have noted severe differences in health outcomes among varying populations. To better understand the harmful cycles of surface O3, the beneficial aspects of O3 are worth mentioning in detail.

In the Stratosphere, O3 protects the surface of Earth by absorbing UV rays. Due to the chemical composition of this layer, stratospheric O3 naturally follows seasonal cycles, as these correlate to the distance from the sun and positioning of Earth’s tilt in its rotational pattern. However, due to rising temperatures, this beneficial, and natural cycle is threatened, potentially mixing with surface air quality and chemistries. As the Ozone Layer doesn’t absorb all UV radiation, what’s left over reflects off the surface of the Earth. Remote sensing is a field dedicated to measuring these reflections, correcting for the numerous atmospheric and geographic distortions provided by optical, electrical, and human error.

Ground-level ozone combined with other reactive gases will tend to correlate to the quality of air encompassing human communities (Bojkov and Fioletov 1995; Díaz et al. 2018; Gaudel et al. 2018; Schultz et al. 2017). As this dual formation involves titrations with varying chemicals, complex, non-linear associations begin closer to the source of common pollutants; later being reincorporated into the environment at some distance away. This makes it difficult for these O3 reactions to be identifiable and effectively modelled for decision making and regulatory entities. (Abdullah et al. 2019; Balamurugan, Balamurugan, and Chen 2022; Gaudel et al. 2018; Huang et al. 2017; Yamashita et al. 2010). In addition, concentrations of stratospheric ozone in the future will depend on the decrease of O3-depleting substances (ODS)s found near the surface due to reducing the frequency and hence; likelihood of these interactions (Huang et al. 2017; Manisalidis et al. 2020; Zhao et al. 2021).

I.4 Surface O3 Exposure and Transport

While most hazardous pollutants are emitted directly, complex pollutants such as surface O3 form as byproduct, later becoming a constituent for other chemicals. O3 is known as a secondary pollutant (J.-T. Lin et al. 2012; Watson et al. 2019; Venkanna et al. 2015) wherein it can act as an ingredient and result of chemical processes. The slightest change in wind speeds, environmental conditions (coastal to arid), and ecological elements (available greenspace vs. concrete) can influence O3 formation and degradation (Badia et al. 2023; K. Meng et al. 2022; Xing et al. 2016). The data provided by these, and numerous other works gives insights into historical transport of O3 due to urban, suburban, and rural development which were incorporated during development. Studies which gathered similar data products have found several links between urbanization and populations which are exposed to unhealthy levels of air pollution; typically well above those of current standards set by the Environmental Protection Agency and World Health Organization (EPA 2021; Kumar et al. 2015; X. Liu et al. 2022; WHO 2013) set at 70 ppb (EPA 2013). The EPA establishes an AQI for communicating daily air quality in which other major air pollutants are also regulated under the Clean Air Act. Ozone has direct interactions with all pollutants labeled hazardous by these agencies due to its molecular instability.

The trajectory of these emissions has a direct impact on policy decisions affecting numerous socio-economic statuses (SES) due to inherent constituents. Sand, smoke, volcanic plumes, dust, other gaseous components like clouds can affect the overarching operations of O3 cycles and complexity as seen in many studies (Harithasree et al. 2024; Venkanna et al. 2015; Tong et al. 2017). The precursors for its existence are risks to human health, as indicated by informed policies limiting exposures to other pollutants (e.g. Particulate matter (PM), Carbon monoxide (CO), Nitrogen dioxide (NO2), and more) per the CDC, EPA, and WHO (CDC 2024; US EPA 2015a; WHO 2013). Policies which limit the general reduction of emissions; like carbon dioxide (CO2), formaldehyde (HCHO or CH2O), methane (CH4) and nitrous oxides (NOx), tend to reduce surface O3 reactions as well, decreasing the probability for a reaction to occur in populated areas.

Current representations and remote sensing methods used for surface ozone can be too coarse for urban analysis, and might not highlight key details known to interact with urbanization and natural disasters in communities at finer spatial scales (Nawaz 2023; Zhang, Wei, and Fang 2019; Abdullah et al. 2019). These instruments often rely on novel approaches to aerosol forecasting and implement a slew of corrective algorithms for proper representation of meteorological variables. A Statistical Model and Residual Kriging methodology is proposed to refine S5P’s tropospheric O3 representation into a surface O3 estimates with a spatial resolution of 250m, a resolution suited for urban analysis (Wang et al. 2023)

I.5. Structure of Thesis

This thesis seeks to compare the performance of common machine learning (ML) and artificial intelligence (AI) methods with the enhancements made by the Residual Kriging method on forecasted O3 values for further development into a python-based air pollution modelling library. Beginning with a substantial literature review on the formation of O3, it’s found that almost every aspect of it can impact local ecologies, health, and people. These are heavily discussed to provide a high-quality basis for feature creation and model tuning based on scientific evidence. Some drivers included in the initial dataset were not utilized in the final model, albeit all data initially gathered was due to the synthesis of literature. A section dedicated to data sources and materials delves into further reasoning for the features best suited for ML/AI ensembles and integration with the RK method.

After understanding the fundamental drivers, constituents, and numerical model tuning methods, a geospatial regression krige is applied to the resulting uncertainty left by the estimated trend. The full combination of these techniques creates daily high spatial resolution rasters for the urban cities of Phoenix and Tucson in Arizona. These cities are encompassed in two counties, with a third sitting in between them. An extremely brief demographic analysis depicting income, total population, and occupied households is conducted via census data provided by the U.S. Census Bureau followed by an assessment of possible health outcomes due to excessive exposure to surface O3 above concentrations of 70 ppb.

The main portion of the thesis is concluded with a detailed description of future directions, model improvements, and further reasonings for why high-spatial resolution surface O3 models are needed, especially within the contiguous United States. A small portion on the use of Geographical laws and theory in historical scientific literature is presented as the final notes to this thesis to depict a proposed economic solution garnered from the betterment of air pollution modelling. Methodology used in this thesis can be best described as a common case-study using the Scientific Method, Geo-spatial statistical analysis, and application of the three main laws of geography to modern ML/AI modelling methodologies.

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