# My amazing title

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# Abstract

The abstract should be a short summary of your thesis work. A paragraph is usually sufficient here.

# Acknowledgments

Use this space to thank those who have helped you in the thesis process (professors, staff, friends, family, etc.). If you had special funding to conduct your thesis work, that should be acknowledged here as well.

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# Chapter 1 Introduction

## 1.1 Background

Coal is one of the most dangerous combustible fuels which is being burned in all across the world as one of the largest methods of obtaining energy. Yet, although it is a fossil fuel which is naturally abundant and easy to utilize, it is comprised of a long list of dangerous chemicals including – but not limited to: arsenic, radium, boron, and a large list of other chemicals which prove to be dangerous to humans and animals alike. (Kelderman et al., 2019)

Power plants produce electricity by burning this coal, and as a result of how prevalent it is within the US - over 100 million tons of coal ash are produced every year. This side-product as a result of the coal combustion is often disposed by directly being dumped into landfills and waste ponds. (Kelderman et al., 2019)

Only recently have these complaints and lawsuits regarding the disposing practices made by non-profit environmental organizations been heard. Due to the onslaught of pressure put on the Environmental Protection Agency – the Coal Ash Rule was bor in 2015. (Kelderman et al., 2019)

This rule has forced over 265 coal power plants – about 3/4 of all coal power plants in the US - to make data regarding chemical concentrations publicly available to the general population. (Kelderman et al., 2019)

In their analysis using this data, the Environmental Integrity Project – a non-profit

organization dedicated to issues involving environmental justice have concluded that essentially all groundwater under coal plants are contaminated. (Kelderman et al., 2019)

However, is this really the case? There are many naturally occurring chemicals existing in groundwater as as such, perhaps their claims are overstated.

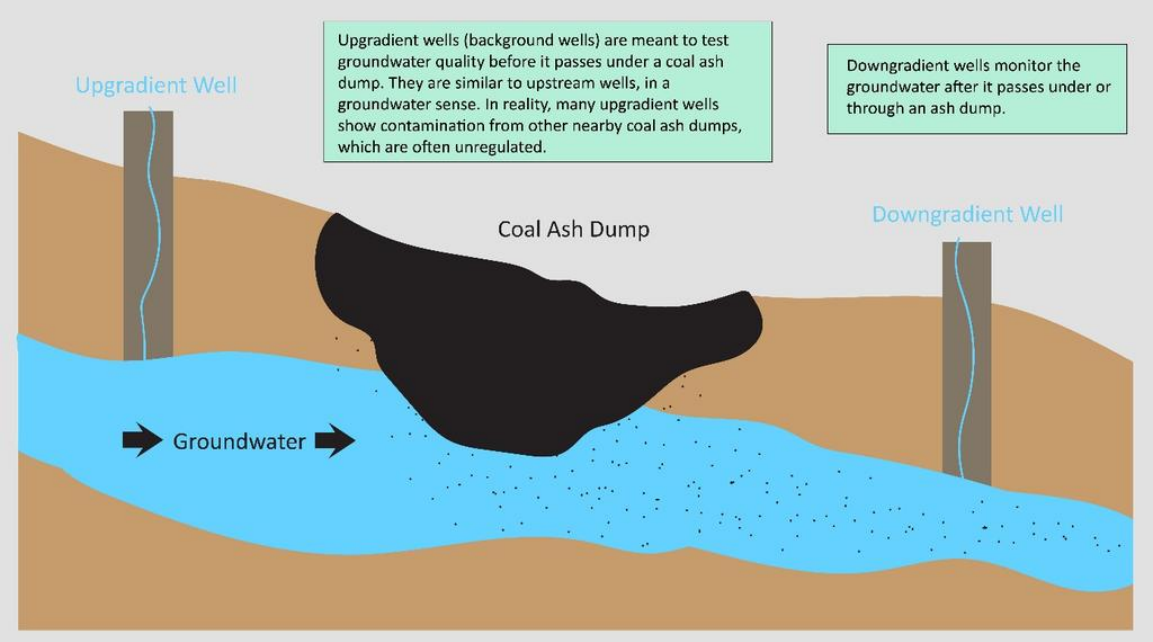


Figure 1.1: Difference Between Upgradient and Downgradient Wells

Typically in a coal ash plant, there exists two types of wells: upgradient wells and downgradient wells. These wells are essential to measure the amount of contamination being caused by coal ash. Upgradient wells, also known as background wells, measures the concentrations of chemicals in groundwater before it passes through an coal ash dump. Conversely, downgradient wells measure the concentrations of chemicals in groundwater after it passes through a coal ash dump.

- "80% of the US population is served by 14% of the utilities," so if something were to get into the water distribution system, it can easily spread amongst the

US population which is why contamination in water services is so important. (Byer & Carlson, 2019)

With this information, typically – one estimates the amount of chemical contamination caused by a coal as dump by subtracting the upgradient concentration from the downgradient concentration of a chemical (downgradient concentration - upgradient concentration).

However, due to the lack of proper reporting guidelines prior to the enactment of the Coal Ash Rule, we believe that there may be retired or even unregulated upgradient wells which can cause the concentrations of chemicals being recorded from these upgradient wells to be inaccurate or even completely wrong.

Our end goal remains the same as the EIP: to identify contaminated groundwater in coal plants – but to attempt to find a way to effectively correct the improper/inaccurate values resulting from LOD errors and other factors which the EIP may not have considered.

The limit of detection problem stems from the measuring devices' inability to obtain chemical concentrations smaller than a certain threshold amount, thus affecting the measurements recorded.

Our plan is to utilize bootstrapping and imputation techniques to correct for these measurements by accounting for the innate contamination which may be caused by factors such as retired and unregulated wells that were mentioned before.

## 1.2 Data

### 1.2.1 Coal Ash Rule

A large coal ash spill at the Tennessee Valley Authority (TVA) which occured on December 22, 2008 in Kingston, TN – prompted the Environmental Protection Agency

(EPA) to propose a set of standardized regulations and procedures to address the concerns regarding coal ash plants nationwide in the US. (Environmental Protection Agency, 2020)

This was known as the Coal Ash Rule, passed on December 19, 2014. (Environmental Protection Agency, 2020)

Changes were made to the Coal Ash Rule over the years in the form of 'amendments,' one of which made required facility information and data to be made publicaly available to the public (April 15, 2015 rule change) (Environmental Protection Agency, 2020)

### 1.2.2 Source of Data

The data used in the study are from the results published in "Annual Groundwater Monitoring and Corrective Action Reports" which were made available to the public in March 2018 as a result of the Coal Ash Rule. (Environmental Integrity Project, 2020)

These reports are in PDF format and are thousands of pages long, which makes it difficult for individuals to look through the data in a meaningful way. (Environmental Integrity Project, 2020)

The EIP obtained the data from an online, publicly available database containing groundwater monitoring results from the first "Annual Groundwater Monitoring and Corrective Action Reports" in 2018 which was collected from coal plants and coal ash dumps under the Coal Ash Rule (Environmental Integrity Project, 2020)

They wrangled the data into a more accessible machine-readable format which contains information from over 443 annual groundwater monitoring reports posted by 265 coal ash plants, which is downloadable from the EIP's website. (Environmental Integrity Project, 2020)

### 1.2.3 Variables

The dataset contains information regarding chemical concentrations at coal plants. A coal plant consists of multiple disposal areas for the coal ash that it produces. At each disposal area, there are specific locations that groundwater is being measured, known as wells which represent an observation in the dataset. There are two types of wells – upgradient and downgradient wells. The variables consist of information regarding the specific chemical concentrations of each well. From the 19 different contaminants (antimony, arsenic, boron, etc.) a major problem is that some wells only have measurements for certain chemicals and don't have them for others.

### 1.2.4 Plan of Action

Within the report, the EIP mentions certain restrictions within the data that have caused their data to potentially be inaccurate (specifically, with limit of detection problems, and a large amount of missing chemical data). The limit of detection problem comes when measuring devices used to measure chemical concentrations are unable to detect below a certain threshold, causing large numbers of observations to have duplicate, wrong values – which can cause for misguided analysis.The other issue is less guided/formed, but for brevity, we think that a lot of the issues in the data comes from the potential possibility of contamination during data collection from investigators from non coal-ash sources. This may include things like: retired/unregulated wells which are old and have chemicals leaking into the groundwater, mismanagement in measuring, etc.My project hopes to work with methods on handling this missing data – alongside investing potential uses of bootstrapping and other resampling methods (potentially?) in order to try to come up with a more statistically accurate and sound result by looking to assuage the problems that the EIP faced in their analysis. Specifically, to

find a way to split up the data into ”uncontaminated” and ”contaminated” wells in order to find the natural distribution of chemicals in each – and doing to so in the face of data corrupted by LOD problems and inaccuracies. I'm hoping to apply and compare different ways of altering the data to account for these myriad of issues in order to look for more salient findings that the EIP might have missed or if not, to see if improvements can be made regarding the way that contaminated coal ash wells are being identified.

# Chapter 2 Methodology

## 2.1 Overview

- What is the of detection (LOD)? LOD is often thought of as being closely related to analytical chemistry, but it actually lies close to the realm of statistics as well. By definition, a limit of detection is the lowest value reported which is different than the blank (generally zero) with some confidence level.

- What is the problem with LOD? As a concept closely related to missing data, LOD values are often can lead to bad practices (in terms of statistical analysis) leading to analysis and/or conclusions which are heavily flawed if not accounted for and dealt with.

- [FIND SOURCE TALKING ABOUT LEFT CENSORED VS RIGHT CENSORED DATA]

- Some individuals have argued for simply just throwing away/discarding values that are below of the LOD, which is of course the easiest way to deal with them – but that gets rid of tons of useful information (Berthouex, 2020) and honestly, is not good statistical practice.

- These LOD entries still contain information that a lot of people don't realize – specifically information that the values is between 0 and the LOD, which is

actually very useful information. (Chen et al., 2011)

- On the same vein, reporting limits can often be used be misleading as non-statisticians (practices in environmental law) may often interpret ND (non-detect) as nullity, when in fact it only means that the measurement falls below a certain limit (Elias & Goodman, 1999)

- Statisticians over past century have come up with methods to deal with this issue (some good... and some... kind of absolutely terrible). There are many different ways that researchers are dealing with detection limits, which are ubiquitous in the scientific realm. Some of the most common methods involve substitution, nonparametric, and maximum likelihood methods. (Lafleur et al., 2011)

- Of course, these methods aren't the only way to deal with it, but it is what we have come up with for now. Detection limits are constantly changing as time passes and because of that – techniques and ways to combat it will gradually evolve and change (for the better) to deal with it

- Detection limits are constantly changing: as technology improves, so too does our ability to accurately measure substances (Elias & Goodman, 1999)

## 2.2 Reporting

- The way that chemists/researchers indicate whether or not if a value is a LOD value or not varies across labs and as such isn't standardized... Some may use`ND`, `< value`, `0`, `some value between 0 and LOD`, etc. (Berthouex, 2020)

- The general form of the equation used to determine LOD is of the form:

$$LOD = k * s_{zero}$$

where “k is the constant for defining LOD” and $s_{zero}$ is the standard deviation of the zero/blank" (Akard, Tsurumi, Oestergaard, & Inoue, 2002)

- 2 or 3 SDs is often what is used, refer to picture (I think it’s neat) (Akard et al., 2002)

- [INCLUDE SOME MORE MATH ABOUT THIS WHEN WRITING THIS UP, refer to these papers]

## 2.3 Approaches

- Substitution is the worst way, nonparametric ways do better, maximum likelihood methods are the best (Lafleur et al., 2011)

### 2.3.1 Substitution Approach

- Substitution methods are biased but easy to implement which is why they are often used (common values: LOD/2, LOD/sqrt(2), LOD) but are discouraged b/c results in estimates of parameters being biased (Chen et al., 2011)

- In a study performed by [Glass] to investigate the effectivenss of LOD approaches, they used a variety of substitution methods. The first method they implemented was replacing all values with LOD/2, they claim these method was recommended for datasets where lots of data is below LOD or when data is highly skewed with a geometric sd of 3 or more. Some people also use LOD/sqrt(2) and which recommended to be used when few data us below LOD or when data is not

highly skewed. However, through their study, they found that there really isn't a difference between these two methods. (Glass & Gray, 2001)

### 2.3.2 Kaplan-Meier Estimate Approach (#Kaplan-Meier)

- Kaplan-Meier Estimation is a common technique used to deal with right-censored data, but can also be used for left-censored values as well – in the form of the Reverse Kaplan-Meier Estimation.

- Suggests using the reverse Kaplan-Meier (KM) estimator to estimate the distribution function and population percentiles for data where there is "left-censored data" (data point is below a certain value but known by how much) (Gillespie et al., 2010)

- After their study, they found that even though THEORETICALLY the reverse KM is for left-censored data (just like KM is for right-censored data), it is still limited in its usage since all it does it estimate a distribution function (it's really just an exploratory thing, they said) (Gillespie et al., 2010)

### 2.3.3 Distribution-Based Multiple Imputation Approach (#DBML)

- Study exploring different options to handle LOD laboratory data – specifically with regards to multiple imputation methods for left-censored data. They concluded that "the distribution-based MI method" worked well for bivariate data where the values were $<$ LOD. (Chen et al., 2011)

- They also ivnestigated distribution-based multiple imputation methods – they used MLEs to estimate distribution parameters based on all datas ($<$ LOD and those not). They repeatedly imput the values to create multiple complete sets of data, and then analyzed each one individually (Chen et al., 2011)

- Mathematically, they created a log-likelihood function with all the data, then derived MLEs of each parameters on multiple bootstrapped datasets. Each bootstrap data gives different estimates for the mean, sd, etc. (refer to article for math) (Chen et al., 2011)

### 2.3.4 Write about other approaches here

- Another method is "Cohen's Method" where one extrapolates the left hand side of distribution based on the distribution of the uncensored data and then calculate the MLE estimate of the arithmetic mean – found to be unreliable with data with outliers, this method can ONLY be used with data where there is a single LOD. From their study they found that this method gave high, unlikely results of the mean (Glass & Gray, 2001)

- Imputing from a uniform is useful when you don't know the distribution of the data (Canales, 2018)

### 2.3.5 Comparison between different methods

- Compared 5 methods: found that in terms of performance: imputation method using MLE to estimate distribution parameters and then imputing censored data points with values from this distribution below the LOD > imputation from a uniform distribution > other 3 methods (substitution, log-normal MLE to estimate mean and SD, and kaplan-meier estimate) (Canales, 2018)

- KM method is better than MLE for data where there are TONS of missing data or if data is highly skewed (distribution not assumed in KM method) (Canales, 2018)

- Uses RMSE (root mean squared error) to see how close the estimated values

are to the true values (lower RMSE means closer estimation to known values) (Canales, 2018)

### 2.3.6 Packages

- Probably will not be included, just here for my own reference!
- "MLE and KM methods were implemented using the NADA package (https://cran.r-project.org/web/packages/NADA/NADA.pdf) in R (`cenmle` and `cenfit` functions) where data is labeled as censored or uncensored, for censored values, LOD is used as a placeholder, since these methods aren't imputation methods – these censored values weren't replaced. Instead, summary statistics were generated with the entire data set (including the censored data)" (Canales, 2018)
- "The imputations methods used mostly followed the general ideas: we have to assume the entire data set follows a particular distribution. Then we use this distribution to impute in values for the censored data. The MLE imputation method uses MLE methods to estimate the parameters of a distribution to fit the dataset, then values lower than the LOD are imputed FROM this dataset for all censored values (they used the function `fitdistcens` from the R package `fitdistRplus`). The second uniform imputation method assumes a uniform distribution with minimum 0, maximum LOD – for all values less than the LOD, then the left-censored values are replaced with a number randomly selected from this uniform distribution." (Canales, 2018)

# Corrections

A list of corrections after submission to department.

Corrections may be made to the body of the thesis, but every such correction will be acknowledged in a list under the heading "Corrections," along with the statement "When originally submitted, this honors thesis contained some errors which have been corrected in the current version. Here is a list of the errors that were corrected." This list will be given on a sheet or sheets to be appended to the thesis. Corrections to spelling, grammar, or typography may be acknowledged by a general statement such as "30 spellings were corrected in various places in the thesis, and the notation for definite integral was changed in approximately 10 places." However, any correction that affects the meaning of a sentence or paragraph should be described in careful detail. The files samplethesis.tex and samplethesis.pdf show what the "Corrections" section should look like. Questions about what should appear in the "Corrections" should be directed to the Chair.

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