Determining NDMA Formation during Disinfection using Treatment Parameters

Aleksandra Szczuka aszczuka@stanford.edu
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Motivation
In order to get rid of harmful viruses and bacteria, drinking water must be disinfected. However, when water is disinfected, harmful carcinogenic disinfection byproducts (such as Nitrosodimethylamine, NDMA) may form. Once formed, reducing NDMA concentrations is costly for drinking water utilities, and preventing NDMA formation is highly desirable. The goal of this project is to predict whether or not NDMA will be formed, reducing NDMA concentrations is costly for water treatment plants in the United States.

Data
The complete data set was obtained by merging datasets for water treatment utilities available through the EPA. In total, 10 data sets were compiled for 108,604 utilities located throughout the US. Features such as facility size, type of water disinfected, point of sampling, disinfectant used in the facility Features were chosen based on literature knowledge of what parameters may affect NDMA formation. Data was preprocessed for the ease of use in Matlab, for instance, categorical variables such as plant size were assigned numerical categorical values instead of the original categorical values.

Methodology

For the original data set, the highest AUC value for the test set occurred when decision trees were implemented. SVM (Linear and Gaussian kernel) performed the worst. When non-detect samples are randomly deleted, the AUC’s for the training data peak at a 2:1 Non-detect and Detect samples. SVM (Linear and Gaussian kernel) are most affected.

For Randomized Data augmentation, best results were achieved when data was averaged 10 times (2, 10, and 100 tested). However, the AUC’s were worse than classification with random deletion of non-detect samples. Therefore, only the classification algorithms were implemented on the test data. For the test set, the SVM (Gaussian kernel) predicted the most of the detect samples, however, it also showed a more false positives than other fitting methods. Decision Trees may be the more appropriate classification to use.

How Much will form?
In order to predict what the amount of NDMA formed in a treatment plant would be, two fitting methods were used: decision tree regression and a general linear model. The error associated with those fitting methods is shown below. Decision regression trees outperformed the general linear model, however, analytical method results usually have lower errors.

Future work
The results achieved in this project are a good starting point for future work. However, the data set that I was able to compile this quarter was very limited. Even though the EPA has been monitoring NDMA formation throughout the united states, they do not provide data for water quality parameters associated with the treatment plants, rather, they provide parameters such as disinfection technique used. While this is important information, it does not paint the full picture for NDMA formation. The main goal would now be to map the water quality parameters available online with the correct water treatment plants by either names used by the EPA or GPS coordinates. Further processing of obtained data to reduce skew would also be appropriate, using techniques such as stratified sampling. Cross validation would also likely improve the results.

References