**CIND 820: Big Data Analytics Project**

*Literature Review, Data Description, and Approach*

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Containing nearly 20% of the earth’s fresh surface water, the Great Lakes are a global treasure. The coastlines of the great lakes and St. Lawrence River stretch from beyond Thunder Bay in the west to Atlantic Ocean in the east. These waters underpin Ontario’s high quality of life.

The Government of Ontario has been taking action to protect, conserve and restore the Great Lakes with partners, individuals, and communities to support the vision of healthy Great Lakes for a stronger Ontario – Great Lakes that continue to be drinkable, swimmable, and fishable.

In 1972 the United States and Canada signed the Great Lakes Water Quality Agreement (GLWQA) to protect and restore the waters of the Great Lakes Basin Ecosystem. Since the original version, the agreement has been revised several times and was renegotiated from 2010 to 2012. Its strengths include a structure and process that place focus on strategies for restoring and protecting the ecosystem rather than prioritizing national agendas (Alliance for the Great Lakes, 2007).

Today more than 35 million people live in the Great Lakes basin in Canada and the United States. The Great Lakes are important sources of drinking water, irrigation, transportation, and recreation opportunities such as fishing, hunting, boating, and wildlife watching. The Great Lakes are a critical component of the regional economy on both sides of the border.

Despite their great size, the Great Lakes are actually very vulnerable to [pollution](https://www.nwf.org/en/Educational-Resources/Wildlife-Guide/Threats-to-Wildlife/Pollution). The amount of water entering and leaving the lakes each year is less than one percent of the total in the lakes. Persistent chemicals that enter the lakes can remain for many years, with many building up in the food web. The source of toxic pollutants includes decades of industrial waste, raw sewage overflows, runoff from cities, and mining operations. Excess nutrients that throw the ecosystem out of balance enter the lakes from agricultural runoff and untreated sewage.

Given the spatial and temporal changes in water chemistry, regular monitoring programmes are needed to reliably estimate water quality. This leads large and complex data matrices composed of a large number of physical and chemical parameters, which are often difficult to interpret, making it challenging to draw meaningful conclusions.

Robust scientific inference is crucial to ensure evidence-based decision making. Accordingly, the selection of appropriate statistical tools and experimental designs is integral to achieve accuracy from data analytical processes. Environmental monitoring of water quality has become increasingly common and widespread as a result of technological advances, leading to an abundance of datasets. After conducting a scoping review of the water quality literature, it was found that correlation and linear regression are by far the most used statistical tools. However, the accuracy of inferences drawn from ordinary least squares (OLS) techniques depends on a set of assumptions, most prominently: (a) independence among observations, (b) normally distributed errors, (c) equal variances of errors, and (d) balanced designs. Environmental data, however, are often faced with temporal and spatial dependencies, and unbalanced designs, thus making OLS techniques not suitable to provide valid statistical inferences. Generalized least squares (GLS), linear mixed-effect models (LMMs), and generalized linear mixed-effect models (GLMMs), as well as Bayesian data analyses, have been developed to better tackle these problems. Recent progress in the development of statistical software has made these approaches more accessible and user-friendly.

An understanding of how to select the most appropriate statistical methods is critical if practitioners are to make informed decisions. When inappropriate or suboptimal methods are applied to even the most robust datasets, consequences may include drawing false conclusions, including missing environmentally critical changes.

Primary studies that focused on investigation of water quality or monitoring of water quality in ecosystems were identified by conducting a search using a pre-established list of statistical techniques and keywords. Eighteen statistical methods were identified as a basis for initial identification of studies including: Analysis of Variance (ANOVA), Bayesian Analysis, Cluster Analysis, Control Charts, Correlation, Correspondence Analysis, Factor Analysis, Kruskal–Wallis, Machine Learning, Mann-Kendall, Mann–Whitney, Generalized Linear Mixed-Effect Models (GLMMs), Linear Mixed-Effect Models (LMMs), Principal Component Analysis (PCA), Non-metric Multidimensional Scaling (NMDS), Regression, Simulation and Forecasting, and t-test.

The four most used statistical approaches included various simulation and forecasting methods (N=5,374, 34.4%), correlation (N=3,701, 23.7%), linear regression (N=1,727, 11.1%), and PCA (N=1,258, 8.1%)

This section will provide exploratory analysis of the All Ontario Great Lakes dataset. All statistical analyses were conducted by using R software. Please use the following link to access a repository of the codes used to create this work: <https://github.com/SvShaki/the-All-Ontario-Great-Lakes> The data is obtained from Ontario Data Catalogue published by the Government of Ontario on November 30, 2020. URL: <https://files.ontario.ca/moe_mapping/downloads/2Water/GLIP/All_Lakes_GLIP.csv>

As previously mentioned, the dataset includes information on sampling locations, water chemistry and chlorophyll collected at 18 locations in the Great Lakes-St. Lawrence River and 4 locations in Lake Simcoe. Data range: January 1, 1976 – December 31, 2019. Last updated: November 30, 2020.

In total the dataset contains 425011 rows and 14 attributes. The attributes, their data type and description can be found in the table below:

|  |  |  |
| --- | --- | --- |
| Attribute | Data Type | Description |
| LAKE | Character | the name of the lake where the measurement or observation was taken |
| FACILITY\_NAME | Character | the name of the facility responsible for collecting the data |
| STATION | Integer | represents a station identifier where the measurement was taken |
| DATE\_YYYYMMDD | Character | the date of the measurement in the format YYYYMMDD (Year, Month, Day) |
| YEAR | Integer | represents the year portion of the date when the measurement was taken |
| MONTH | Integer | represents the month portion of the date when the measurement was taken |
| WEEK | Integer | represents the week number corresponding to the date when the measurement was taken |
| ANALYTIC\_METHOD | Character | represents the method used for the analysis or measurement |
| TEST\_CODE | Character | represents a code associated with the specific test conducted |
| PARAMETER | Character | represents the parameter being measured or observed |
| VALUE | Numeric | represents the numeric value of the parameter measured or observed |
| UNIT | Character | represents the unit of measurement for the parameter |
| VALUE\_QUALIFIER | Character | represents a qualifier associated with the value measured |
| VALQUAL\_DESCRIPTION | Character | represents the description or explanation of the value qualifier |

The dataset initially contained 153 missing values. To ensure the integrity and accuracy of the analysis presented in this research, these missing values were addressed by removing them from the dataset prior to analysis.

The distribution of a numeric variable "VALUE" was checked by plotting a histogram of the dataset. The conclusion we have made that the distribution appears to be skewed to the right, indicating a longer right tail and a concentration of values towards the lower end. This suggests that a significant portion of observations has lower values, while a smaller proportion exhibits higher values.

Another statistical test for normality was applied - the Kolmogorov-Smirnov test. Based on the output provided, the KS test yielded a test statistic (D) of 0.4012 and an extremely small p-value (p < 2.2e-16). This indicates strong evidence against the null hypothesis that the data follows a normal distribution. Therefore, based on the KS test results, we can conclude that the variable "VALUE" in the Lakes dataset significantly deviates from a normal distribution. This implies that the assumption of normality may not be appropriate for analyses or modeling techniques that rely on this assumption. It suggests the need for alternative approaches or techniques that do not assume normality. Additionally, the warning message "ties should not be present for the Kolmogorov-Smirnov test" suggests that there might be tied values (i.e., identical values) in the dataset, which can affect the accuracy of the KS test results. It's important to address this issue if tied values are present in the dataset.

We have standardized the numeric columns using z-score standardization. Given that the data do not follow a normal distribution, standardization may be a more appropriate choice than normalization. Standardization (Z-score normalization) does not assume a specific distribution for the data and can handle non-normally distributed data effectively. It centers the data around its mean and scales it by its standard deviation, which can still be useful for algorithms and analyses that assume normally distributed data or work better with standardized features.

Normalization (Min-Max scaling), on the other hand, might not be as effective with non-normally distributed data, especially if the distribution is skewed or has outliers. Normalization could potentially amplify the effects of outliers and distort the relationships between the variables.

Therefore, based on the results of the Kolmogorov-Smirnov test indicating non-normality, standardization would likely be the better choice for preparing the data for analysis.

At the column level, some basic analysis is also offered at this point. The descriptive statistics of each column are provided.

Exploratory data analysis revealed significant insights into the "Lakes" dataset, including the distribution of sampling locations across lakes, associations between lake names and water parameters, and trends in sampling locations over time. Visualizations such as bar charts, pie charts, box plots, contingency tables, heatmaps, and time series plots were employed to elucidate patterns and trends within the dataset.

Analytical approach was begun by conducting the Decision Trees algorithm to assess the differences in researching pollution levels, ecosystem health, and human impacts among Lake Ontario, Lake Erie, Lake Huron, and Lake Superior. The confusion matrix and statistics obtained from the model reveal significant differences in researching between the Lakes. The overall accuracy of the model is 43.45%, which suggests that the model performs slightly better than random guessing. However, the Kappa value (0.0798) indicates poor agreement beyond chance. Sensitivity (True Positive Rate): Lake Ontario has the highest sensitivity (98.53%), indicating that the model can effectively identify instances of pollution, ecosystem health issues, or human impacts in Lake Ontario. Lake Erie, Lake Huron, and Lake Superior exhibit much lower sensitivity, suggesting that the model struggles to identify instances in these lakes. Specificity (True Negative Rate): Lake Superior has the highest specificity (99.996%), meaning the model can accurately identify instances where pollution, ecosystem health issues, or human impacts are not present in Lake Superior. Positive Predictive Value (PPV): Lake Superior has the highest PPV (99.5885%), indicating that when the model predict pollution, ecosystem health issues, or human impacts in Lake Superior, it is correct 99.5885% of the time. Lake Erie has the second highest PPV, indicating that when the model predicts pollution in Lake Erie, it is correct 69.887% of the time. Top of Form

Then, exploratory data analysis was implemented to understand the distribution of sampling locations across the lakes:

* Lake Erie 143,458 sampling locations
* Lake Huron: 68,025 sampling locations
* Lake Ontario: 167,809 sampling locations
* Lake Superior: 45,566 sampling locations

Lake Ontario and Lake Erie have the highest number of sampling locations, indicating a higher density of data collection and monitoring activities compared to the other lakes. Lake Huron and Lake Superior have the fewest sampling locations among the lakes, potentially indicating lower monitoring intensity or fewer sampling programs in this region. Using visualizations such as bar charts and pie charts, we examined the number of sampling locations associated with each lake, revealing insights into spatial patterns and disparities in sampling efforts.

Next, the association between lake names and specific water parameters was investigated. Through contingency table analysis and calculation of mean parameter values for each lake, we identified significant relationships and variations in water quality characteristics across lakes.

To assess the significance of differences in parameter concentrations among lakes and years, two-way ANOVA tests was performed. The analysis provided insights into variations in water quality dynamics over time and across different lake ecosystems. The analysis indicates that both the lake and year factors have a significant impact on parameter concentrations (p < 0.001 for both factors). Lake factor: The p-value associated with the lake factor is less than 0.001, indicating a highly significant difference in parameter concentrations among the lakes. Year factor: Similarly, the p-value associated with the year factor is less than 0.001, suggesting a highly significant difference in parameter concentrations across the years. Interaction effect: The interaction between lake and year is not explicitly reported in the summary, but it would be essential to check for interaction effects to see if the influence of one factor depends on the levels of the other factor.

The Chi-square test of independence was conducted to analyze the association between lake name and a specific water parameter. The calculated Chi-squared statistic is 543.17 with 48 degrees of freedom. The p-value associated with the test is less than 2.2e-16, indicating an extremely significant association between lake name and the specific water parameter under consideration.

The next step in our research was the finding how many facilities associated with each lake. The Lake Ontario has the highest number of sampling locations (7). The Lake Superior has the fewest sampling locations among the lakes analyzed (2).

The primary objective of answering the next question was to identify groups of sampling locations with similar water quality characteristics. This involves finding patterns or similarities among the sampled data points to aid in targeted interventions and management strategies for water quality improvement.

Clustering techniques, such as K-Means, are widely used in data analysis and machine learning for grouping similar data points together based on their attributes or features. In our case, we are interested in grouping sampling locations based on their water quality characteristics.

K-Means is a popular clustering algorithm due to its simplicity and efficiency. It partitions the data into K clusters by iteratively assigning each data point to the nearest cluster centroid and then recalculating the centroids based on the mean of the data points assigned to each cluster. K-Means is suitable for our research because it is capable of handling large datasets efficiently and provides relatively interpretable results.

By applying K-Means clustering to our dataset, we partition the sampling locations into K clusters based on their water quality characteristics. This process enables the classification of sampling locations into distinct groups with similar patterns of water quality attributes. Each cluster represents a group of sampling locations that share common characteristics in terms of water quality. By assigning cluster labels to the original dataset, we create a basis for classification, allowing us to identify and analyze groups of sampling locations with similar water quality profiles. Cluster 1: This cluster exhibits average values across most variables, with slight negative deviations in STATION and VALUE. Cluster 2:This cluster has notably high values for the variable VALUE, while other variables exhibit relatively low values. Cluster 3: This cluster shows negative deviations in MONTH and WEEK, while other variables are close to the mean. Cluster 1 is the largest group with 208,238 observations. Cluster 2 is the smallest group with 15,546 observations. Cluster 3 is the second largest group with 201,074 observations.

The visualization of clustering results using techniques like Principal Component Analysis (PCA) helps in understanding the structure of the data and the relationships between sampling locations. PCA reduces the dimensionality of the data while preserving its variance, making it suitable for visualizing high-dimensional datasets. By plotting the clusters obtained from K-Means clustering, we can visually inspect the grouping of sampling locations and observe any distinct patterns or trends present in the data.

By performing the Trend analysis using a Linear regression model to the time series data and analyzing the trend component, we have made the following conclusions:

* Intercept(2.347e+03): The intercept represents the estimated number of samplings locations at the beginning of the time series (YEAR = 0). In this model, it is estimated to be approximately 2347 sampling locations.
* Coefficient for YEAR (1.067e-02): The coefficient for the YEAR variable represents the estimated change in the number of sampling locations for each unit increase in the year. In this case, the coefficient is very small, indicating that there is a very slight increase in the number of sampling locations over the years.
* Significance levels: The p-value associated with the coefficient for the YEAR variable is 0.606, which is greater than the conventional significance level of 0.05. This indicates that the coefficient is not statistically significant, suggesting that there is no strong evidence to reject the null hypothesis that the coefficient is equal to zero.
* R-squared (0.001561): The R-squared value indicates the proportion of variance in the number of sampling locations that is explained by the linear regression model. In this case, the R-squared value is very low (0.001561), indicating that the linear regression model explains only a very small amount of the variance in the number of sampling locations.
* Residuals: The residuals represent the difference between the observed number of sampling locations and the number of sampling locations predicted by the linear regression model. The summary shows the minimum, 1st quartile, median, 3rd quartile, and maximum of these residuals.
* Overall, based on the results of the linear regression model, there doesn’t seem to be a significant trend in the number of sampling locations over time for each lake. The coefficient for the year variable is not statistically significant, and the R-squared value is very low, indicating that the linear model does not explain much of the variance in the data. Therefore, it seems that the number of sampling locations does not exhibit a clear linear trend over time.

Finally, for our time series analysis of the number of sampling locations over time for each lake, we have chosen to employ the AutoRegressive Integrated Moving Average(ARIMA) model. The ARIMA model is well-suited for capturing temporal dependencies and identifying underlying trends and patterns in time series data. To assess the performance of our ARIMA model, we have selected the following evaluation metrics:

* Mean Absolute Error (MAE): Represents the average magnitude of errors between the forecasted and actual values.
* Root Mean Squared Error (RMSE): Measures the square root of the average of squared differences between forecasted and actual values, penalizing larger errors more heavily.
* Mean Absolute Percentage Error (MAPE): Provides a percentage representation of the average forecast error compared to the actual values.

Based on our analysis, the ARIMA model yielded the following performance measures:

* ARIMA MAE: 136.3003
* ARIMA RMSE: 166.3437
* ARIMA MAPE: 12.86552%

These results indicate that, on average, our ARIMA model’s forecasts deviate by approximately 136.3003 units from the actual values. The RMSE of 166.3437 suggests that the model’s forecast exhibit larger discrepancies from the actual values, particularly for outliers or extreme values. The MAPE of 12.86552% represents the relative magnitude of forecast errors compared to the actual values.

In conclusion, our approach to analyzing the “Lakes” dataset involved a comprehensive exploration of water quality dynamics in lake ecosystems. Through a combination of machine-learning approaches, statistical tools and techniques, and visualization, we identified significant patterns, associations, and trends in water quality parameters across different lakes and sampling locations.

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