Environmental Computations Course Project

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Introduction

The study "Assessment of per- and polyfluoroalkyl substances (PFAS) in the Indian River Lagoon and Atlantic coast of Brevard County, FL, reveals distinct spatial clusters" by Emily K. Griffin, et al. details results of water samples tested for Per- and polyfluoroalkyl substances (PFAS), a class of human developed chemicals that have been linked to negative health implications to humans and wild animals. The results of Griffin's study includes the highest PFAS levels found at sample locations, cluster analysis for sample locations, and the potential impacts of PFAS on public and environmental health. Results also concluded that there were "site and region differences" between PFAS concentrations in 2019 and 2021. Based on these results, this project aims to test the hypothesis of whether PFAS compounds across different testing sites exhibit different temporal patterns.

Literature Review

According to the article "Occurrence, fate, sources and toxicity of PFAS: What we know so far in Florida and major gaps" written by Danni Cui et al., PFAS are characterized by their strong fluorine and carbon bonds making them highly durable in many chemical and thermal environments. Therefore, they are widely used substances, found in items like water repellent sprays, adhesives, and paints. Their durability is problematic because of links found between PFAS and negative effects like decreased immune systems, cancer, liver damage, and infertility (Cui, et al.; 2020; Abunada, et al.; 2020). In addition, according to a study in 2020 by Ziyad Abunada, et al., PFAS are being found in sediments, water bodies, organisms, and air. Water is one of the main pathways leading to PFAS contact with humans, making elevated levels in water bodies an area of concern. Possible sources for PFAS from human activity in Florida specifically are landfill leachate, substandard removal of PFAS in wastewater treatment, and military fire training facilities (Cui, et al.; 2020). Increasing activity of these sources may lead to differences in concentration levels in water bodies each year. Research and publications on PFAS and its effects have been steadily increasing from 2007 to 2020, something that could potentially impact the levels of PFAS concentration in water (Abunada, et al.; 2020). A study in Sweden by Stockholm University found a decreasing average sum concentration of PFAS through the years of 1996-2017 most likely because of increased mitigation efforts (Miaz, et al., 2020).

Data Description

Abunada et al. tested fifty seven sample sites in December 2019 over various locations along the Indian River Lagoon and Atlantic coast in Brevard County, FL. Sites were then resampled in February 2021, where resampling was still possible. A 250 mL bottle was used to take a surface water sample at each location and then stored at -20 degrees celsius in order to stop degradation of any chemicals in the samples. The data for this project detailed table S3 of the study which highlighted PFAS concentrations in 11 of the sites sampled in both 2019 and 2021. Data specifics include that sample sites were divided into 11 columns and different PFAS types were divided into rows. Each PFAS type had a row for 2019 data and a row for 2021 data. Summations of concentrations by sample site and by type of PFAS can be found in the last row or column in the table. This project will focus on the summations of each type of PFAS by year and sample site in the last column of the table in order to find patterns and correlations between type of PFAS, yearly trends, and location sites.

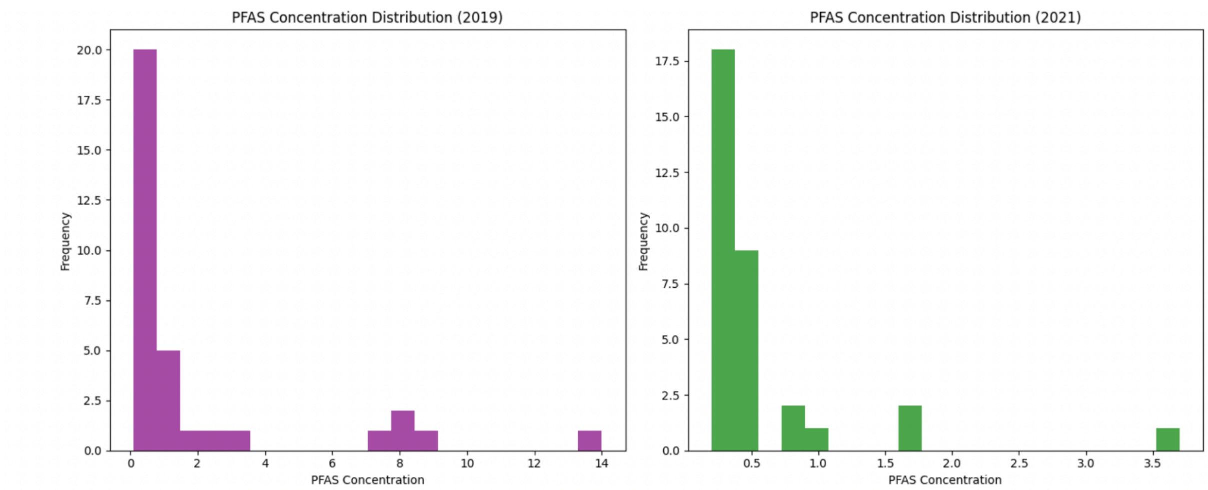
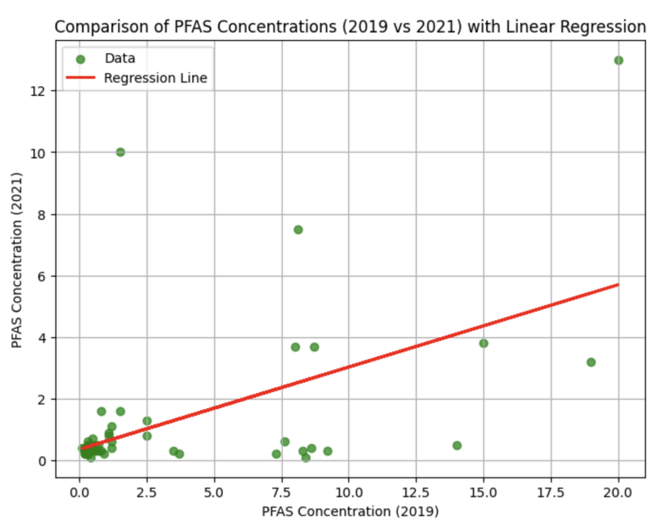


Figure 1: Histograms demonstrating PFAS concentration and frequency at testing sites in 2019 and 2021 sampling groups.

Results A

In both histograms, concentration values are skewed to the right indicating that most PFAS concentrations at test sites were low or close to zero. Both years had a couple outliers with higher concentrations, suggesting that some sites had higher PFAS levels. Higher frequencies and more variability of PFAS concentrations were found in 2019 with 9 different PFAS concentrations while in 2021 there were only 6 different concentrations. The 2021 histogram shows smaller spikes in the data and smaller intermediate values which means PFAS levels in 2021 appear lower and more uniform than in 2019. Therefore, the general trend of the data indicates that PFAS concentrations have dropped from 2019 to 2021. As demonstrated by the scatter plot and linear regression in Figure 2, there is a positive linear relationship between PFAS concentrations measured in 2019 and 2021. This suggests that sites with higher concentrations in 2019 tended to have higher concentrations in 2021 as well. The regression has a moderate level of strength because points on the scatter plot do not perfectly line up with the regression line. The Pearson and Spearman coefficients show weak negative correlations between PFAS and year, strengthening the idea that PFAS concentrations slightly decreased over time.



Pearson Correlation between Year and PFAS Site Concentrations: -0.2872090089599895

Spearman Correlation between Year and PFAS Site Concentrations: -0.15639706640801798

Figure 2: Scatter plot with regression line and Pearson and Spearman correlation coefficients for relationship between year and PFAS site concentrations

Results B

Principal Component Analysis (PCA) is a technique used to identify patterns of variability within a set of data to find general trends. The PC1 is the axis of greatest variance in the data. The PC2 shows additional patterns in PFAS distribution across sites or years that are independent of the main pattern captured by PC1. For this analysis, the data was color-coded by year (2019 and 2021) to explore whether PFAS concentrations exhibit distinct trends over time. The year variable was picked for color coding because it is most in line with my hypothesis of whether different PFAS compounds exhibit different temporal patterns. The PCA plot shows that the first two principal components explain a significant portion of the variance, with noticeable clustering of data points by year. This suggests that there are differences in PFAS concentrations between 2019 and 2021. One or two outliers from the cluster (especially in the positive PC1 direction) might indicate unusually high or unique PFAS concentration patterns at certain test sites. Temporal grouping of year indicates some shifts in PFAS profiles over time.

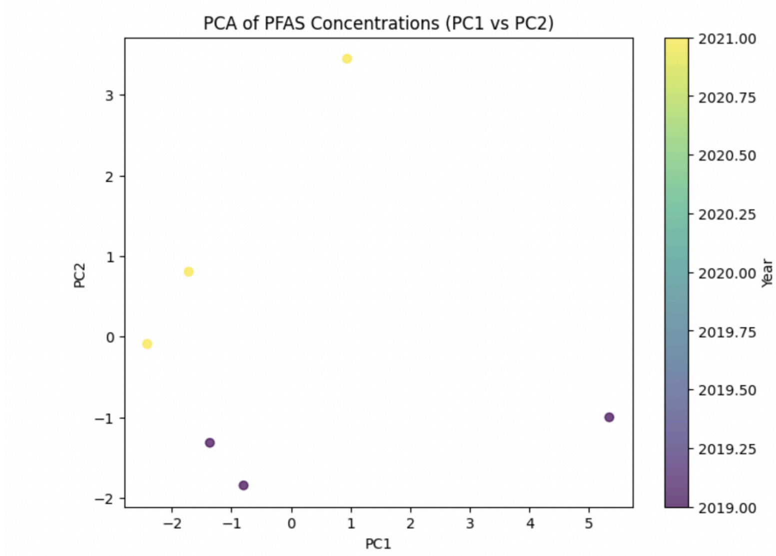


Figure 3: PCA plot demonstrating PFAS concentrations across sites and years.

Conclusion

In conclusion, there are apparent differences in PFAS concentrations across the sites between 2019 and 2021. Figure 1 showing histograms of PFAS concentration per year was evidence of lower PFAS concentrations occurring in 2021. This idea was further supported by the PCA analysis and plot which showed clustering patterns that indicated a reduction in total PFAS concentrations over time. The PCA further showed that the 2021 data had lower variation and magnitude compared to 2019 data. The Pearson coefficient of -0.287 suggests a weak inverse correlation because it is negative and below one. This coefficient signals from 2019 to 2021, the PFAS concentrations decreased slightly. However, the fact that this correlation is not strong indicates that other factors might also influence PFAS concentrations. The Spearman coefficient of -0.156, is also negative and low, implying that the decrease in PFAS levels is inconsistent across the sites. The scatter plot and linear regression line in Figure 2 demonstrated that site concentrations stayed similar from 2019 to 2021. Based on these results, my hypothesis that PFAS concentrations experience temporal patterns is moderately supported. Support was weaker because of low correlation coefficients, low amounts of data points in the PCA plot, and a large number of points off of the regression line in Figure 2. On a broader scale, the results suggest that temporal and spatial patterns in PFAS contamination may be influenced by environmental or anthropogenic factors.

Limitations and Future Work

The study is limited by its small sample size, with only two years and 11 test sites, restricting the ability to observe long-term trends. Expanding the dataset to include more years and sites could address this. In addition, many PFAS concentrations are reported as missing or "-" which could reduce the accuracy of PCA. In the future, sampling could be more comprehensive or methods could be changed to reduce the amount of missing values. Additionally, secondary variables like weather, remediation efforts, and human activities were not considered, potentially weakening conclusions. Including these factors in future analyses could enhance accuracy.

Bibliography

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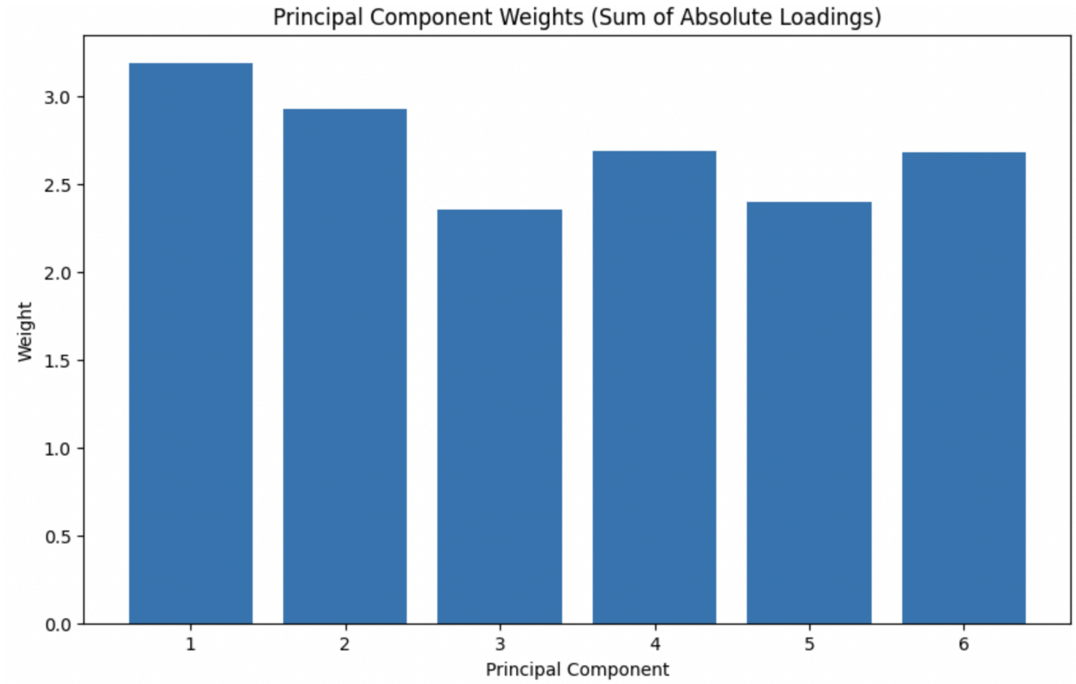
Supplementary Figures

Data Description For Each Site Tested

	Site 1	Site 2	Site 3	Site 4	Site 5	Site 6	Site 7
mean	1.812500	0.381818	11.790909	0.384615	6.658333	1.268750	1.664286
median	0.400000	0.400000	5.150000	0.300000	7.050000	0.350000	0.600000
std	3.724988	0.183402	24.400525	0.273393	5.969773	2.422868	2.332251

	Site 8	Site 9	Site 10	Site 11
mean	0.692857	0.571429	0.483333	0.876923
median	0.350000	0.350000	0.300000	0.500000
std	0.637862	0.541264	0.361395	0.925701

Supplementary Figure 1: Mean, median, and standard deviation for each testing site.



Supplementary Figure 2: Principal Component weight bar chart.