ANALYZING A LOW-COST, CUSTOM SPECTROMETER WITH MACHINE LEARNING METHODS TO PREDICT NITRATE CONCENTRATIONS IN HYDROPONIC NUTRIENT SOLUTIONS

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INTRODUCTION

- Hydroponics is a system that utilizes a nutrient solution medium to grow plants
- Managing the level of nutrients in a hydroponics system is essential to its success and ability to produce the plants desired
- Current methods to gather water quality data are tedious and expensive
- Monitoring environmental water quality is important for maintaining and managing water systems
- UV-VIS Spectroscopy measures light absorbed at various wavelengths[1] and is used to obtain water quality data
- Current UV-VIS methods are expensive

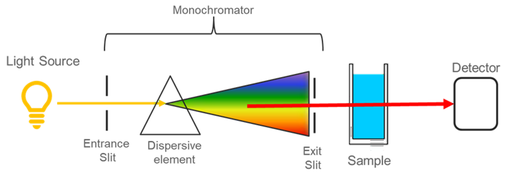

Figure 1: Diagram of UV-VIS Spectrometer[2]

OBJECTIVE

- Validate a low-cost, custom-built, open-source spectroscopy setup by comparing its ability to measure water quality data in hydroponic nutrient solutions with a state-of-the-art, off-the-shelf, standard laboratory spectrometer.

METHODS

- The GatorSpec, an open-source, custom-built, low-cost spectroscopy setup was created by J. Barrett Carter for an ongoing project to form the technological basis for deploying field-deployable water sensors
- Synthetic hydroponic nutrient solutions were created with 11 compounds dissolved in water

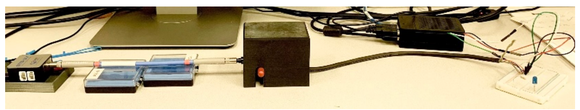

Figure 2: GatorSpec Spectroscopy Setup

Table 1: Compounds added to samples

Fe Chelate DTPA	**$Ca(NO_3)_2$**	**$CuSO_4$**	**$MgSO_4$**	**$MnSO_4$**	**KH_2PO_4**	**KNO_3**	**Na_2MoO_4**	**$Na_2[B_4O_5]\cdot 5H_2O$**	**$ZnSO_4$**	**HNO_3**

- Spectra was collected on the GatorSpec and Nanodrop to obtain absorbance values at wavelengths varying from 190nm-840nm for the raw and diluted samples with a 1:30 dilution
- Principal Component Analysis (PCA) is a statistical method used to reduce a dataset with many dimensions into a few principal components while preserving as much information as possible[5]
- PCA was performed on the absorbance data to compare the two machines

Figure 3: Nanodrop2000C[3]

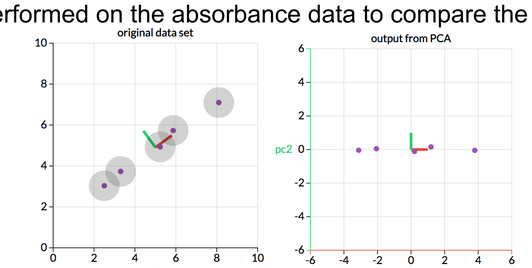

Figure 4: PC1 in Analysis represents most of the data variability[4]

RESULTS AND DISCUSSION

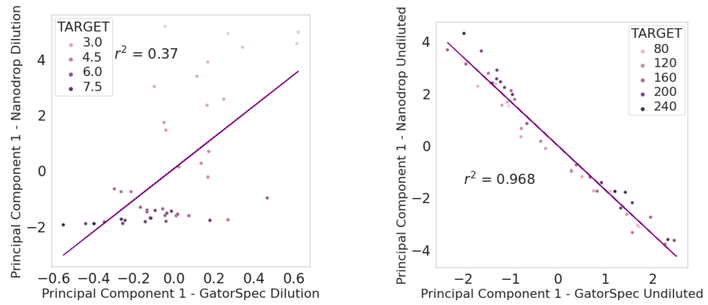

Figure 5: Principal Component 1 Comparison for Diluted Samples (left) and Undiluted Samples (right)

- Principal Components are the new set of variables that are linear combinations of initial variables[5]
  - Most of the information from the initial variables are compressed into the principal components[5]
- Explained variation is what percentage of the data is accounted for in the principal component[6]
- Correlation between PC1 for both instruments, indicating they behave similarly
- Nitrate concentration estimated better with diluted samples
- Same relationship between components that explain most of the variability in the data

Table 2: Explained Variation per Principal Component

Dataset	GatorSpec Diluted	GatorSpec Undiluted	Nanodrop Diluted	Nanodrop Undiluted
Principal Component 1	65.47%	97.37%	82.87%	81.45%
Principal Component 2	24.58%	1.11%	8.23%	6.790%

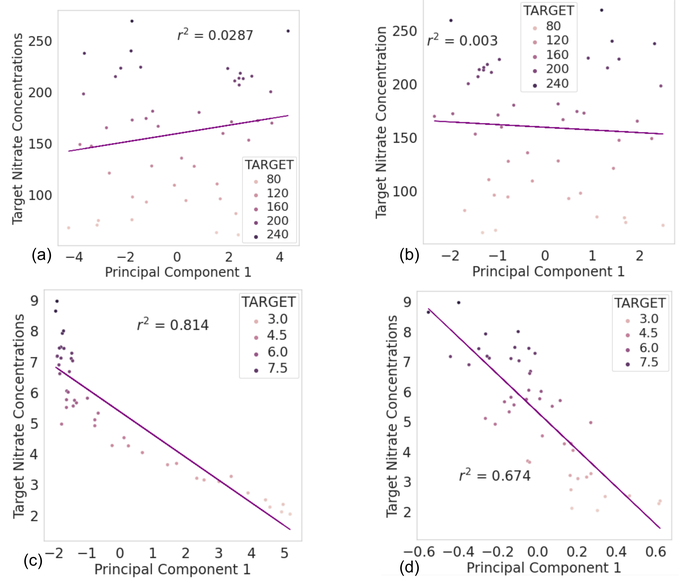

Figure 3: Principal Component 1 vs Principal Component 2 in (a) Nanodrop Undiluted Samples, (b) GatorSpec Undiluted Samples, (c) Nanodrop Diluted Samples, and (d) GatorSpec Diluted Samples

Table 3: Most Important Wavelengths

Sample Type	Principal Component	Wavelength
GatorSpec Diluted	PC1	229.4
	PC2	228.9
Nanodrop Diluted	PC1	219
	PC2	194
GatorSpec Undiluted	PC1	261.3
	PC2	242.6
Nanodrop Undiluted	PC1	244
	PC2	240

- In a PCA, features are variables that represent variance in the data[7]
- Table 2 shows the ”features” (wavelengths) that contribute the most to the variance of the absorbance data
- Wavelengths all close to known peak wavelengths nitrate is absorbed at
- Nitrate and absorbance are related
- PCA is an unsupervised analysis, meaning the dimensional reduction is only dependent on the features[2]

CONCLUSIONS

- Both spectroscopy setups behave similarly solely based on the absorbance values
- Some limitations of this study include:
  - Different cuvettes used with different methods of preparation for each instrument
  - Limited sample size (n = 46)
- Next steps:
  - Perform a Partial Least Squares Regression Analysis to perform dimensional reduction based on the target nitrogen concentrations
  - Estimate the concentration of nitrate in each sample using the absorbance data from each spectroscopy setup

REFERENCES

1. “UV-Vis Spectroscopy & Spectrophotometer FAQs.” *Chemical Analysis, Life Sciences, and Diagnostics | Aligent*
2. “UV-VIS Spectroscopy: Principle.” *UV-Vis Spectroscopy: Principle. | SMACgig WORLD*
3. “Thermo Scientific NanoDrop 2000/2000C Spectrophotometers - Spectroscopy, Spectrophotometry.” | *Fisher Scientific*
4. Powell, Victor, and Lewis Lehe. “Principal Component Analysis Explained Visually.” *Principal Component Analysis Explained Visually*
5. Jaadi, Zakaria. “A Step-by-Step Explanation of Principal Component Analysis (PCA).” *Built In*, 1 Apr. 2021
6. Lindgren, Isabella. “Dealing with Highly Dimensional Data Using Principal Component Analysis (PCA).” *Medium*, Towards Data Science, 28 Apr. 2020