



APPLICATION OF ARTIFICIAL INTELLIGENCE IN CHEMICAL SCIENCES

BTP-1

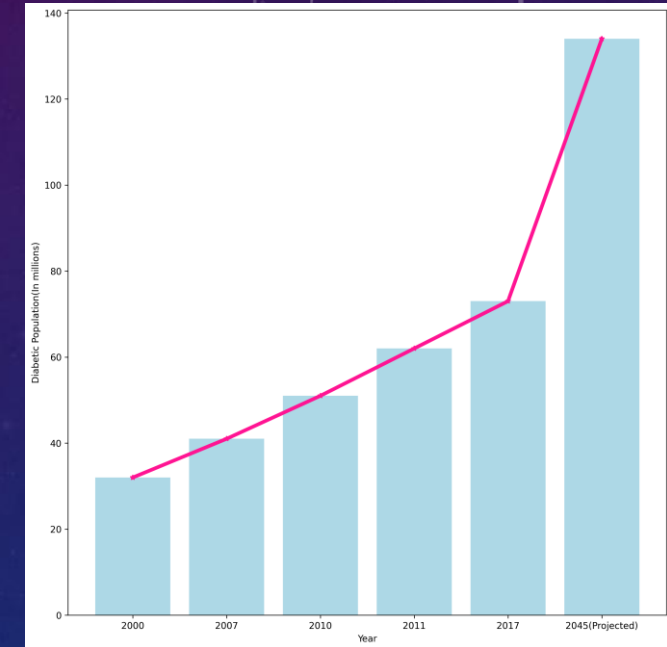
VEER GAJARLAWAR | 21CY10013

GUIDE: PROF. MAHESH MOHAN MR

INTRODUCTION AND MOTIVATION

DIABETES: A GROWING EPIDEMIC IN THE MODERN WORLD

- Diabetes is a major public health problem that is approaching epidemic proportions globally. About 18 million people die every year from cardiovascular disease, for which diabetes and hypertension are major predisposing factors. India ranks second after China in the global diabetes `epidemic with 77 million people with diabetes.
- This emphasizes the need for a non-invasive technique to improve diabetes detection and monitoring. FTIR spectroscopy in combination with AI can be potential solution.



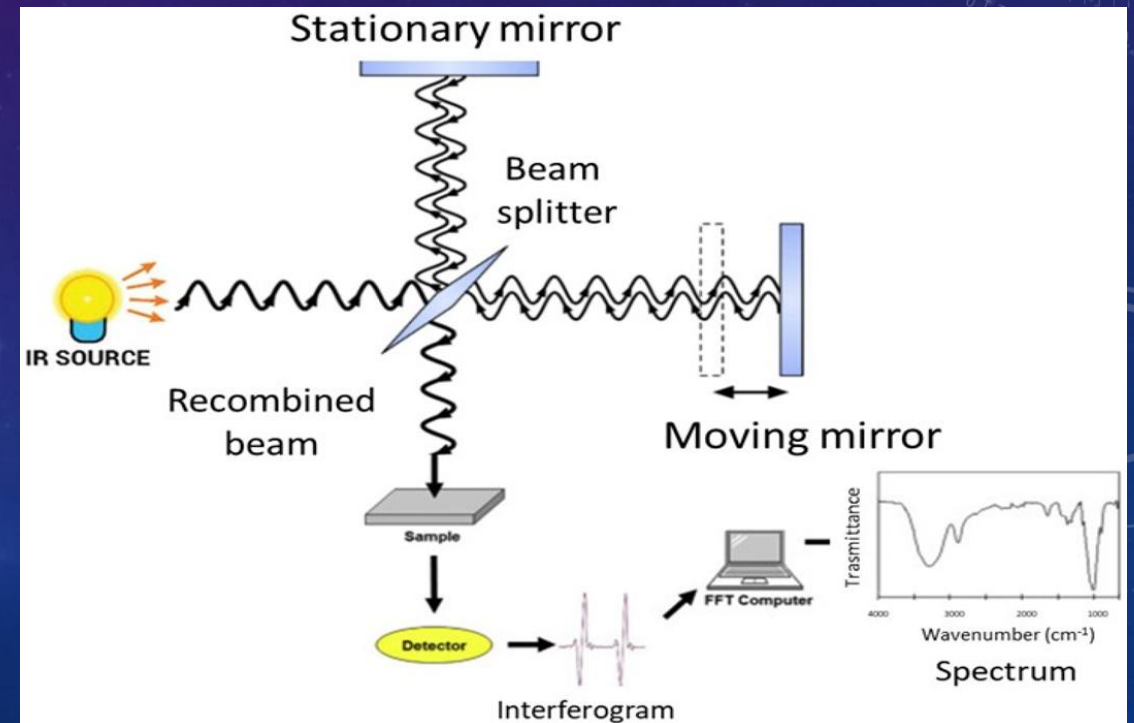
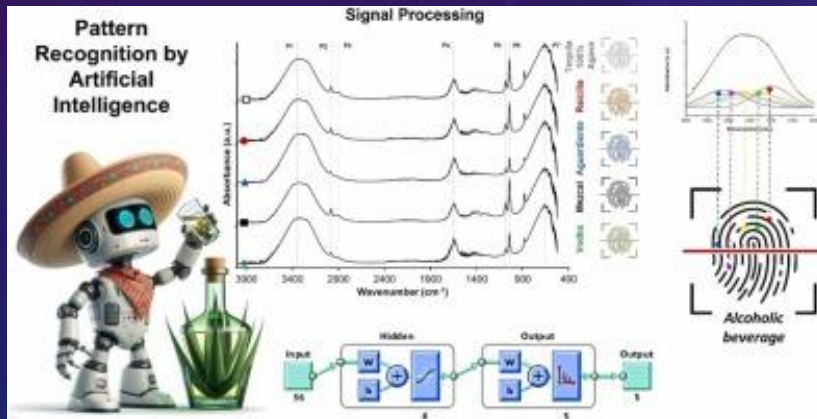
NEED FOR A NON-INVASIVE APPROACH

- Unlike traditional analytical techniques, use of FTIR spectroscopy is a non-invasive and cost effective approach.
- The consumables required for FTIR spectroscopy are minimal, as it primarily relies on the instrument's ability to analyze samples directly or with simple substrates, reducing ongoing costs.
- It provides a rapid analysis as it provides the results in minutes.
- TIR instruments are generally durable and require less frequent maintenance.



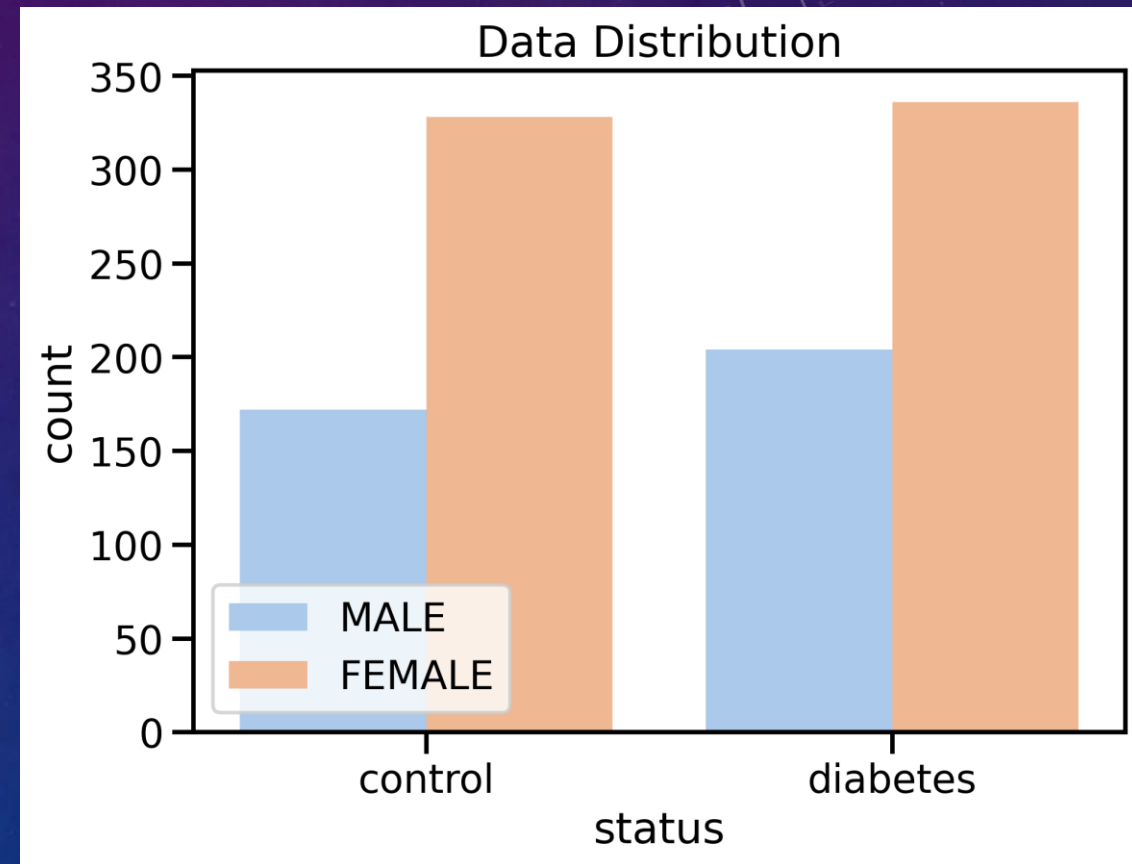
APPLICATION OF AI IN FTIR SPECTROSCOPY

- When integrated with AI, FTIR spectroscopy has applications in a variety of domains, including medical diagnostics for disease detection, material categorization, etc.
- Some of the applications we explored were pollen grain classification, estimation of age of herbarium samples and disease detection.

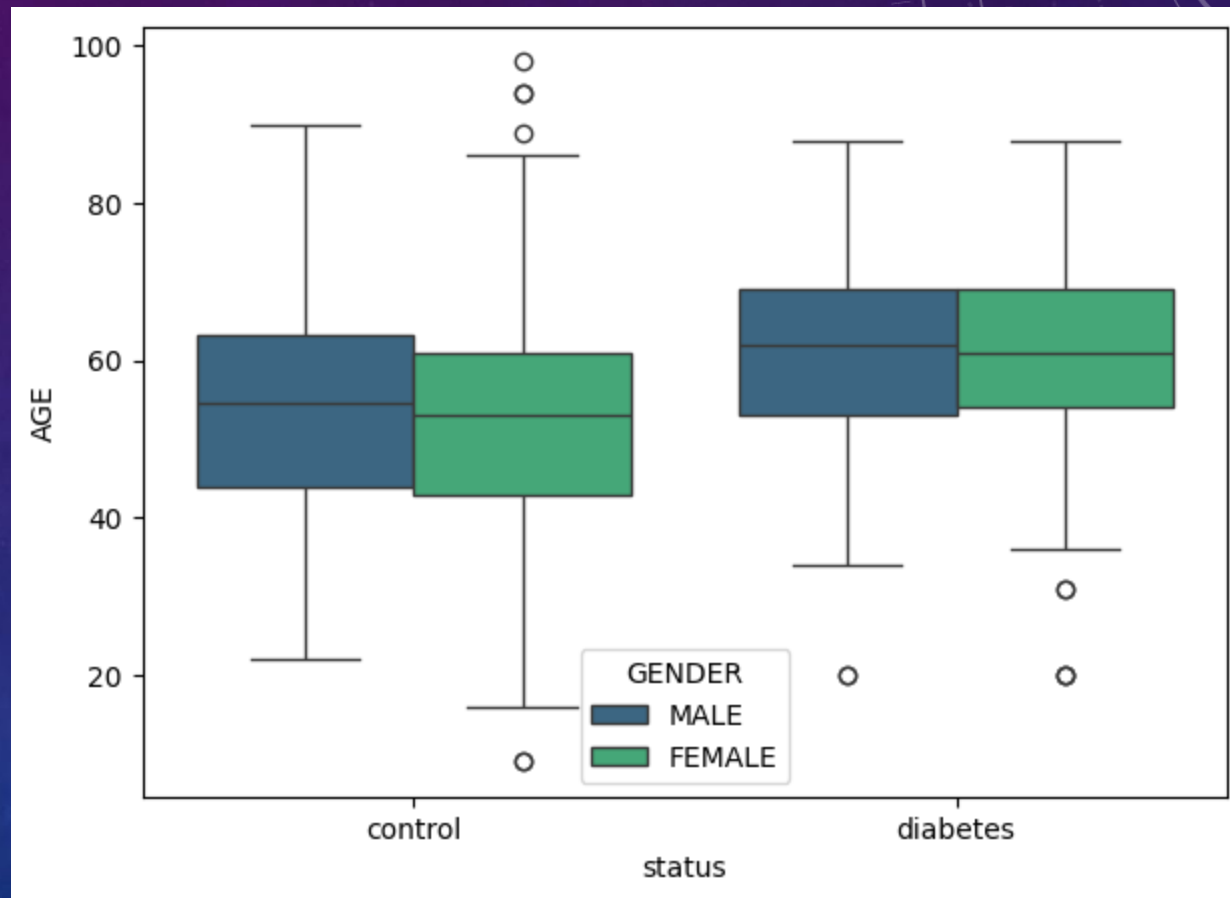
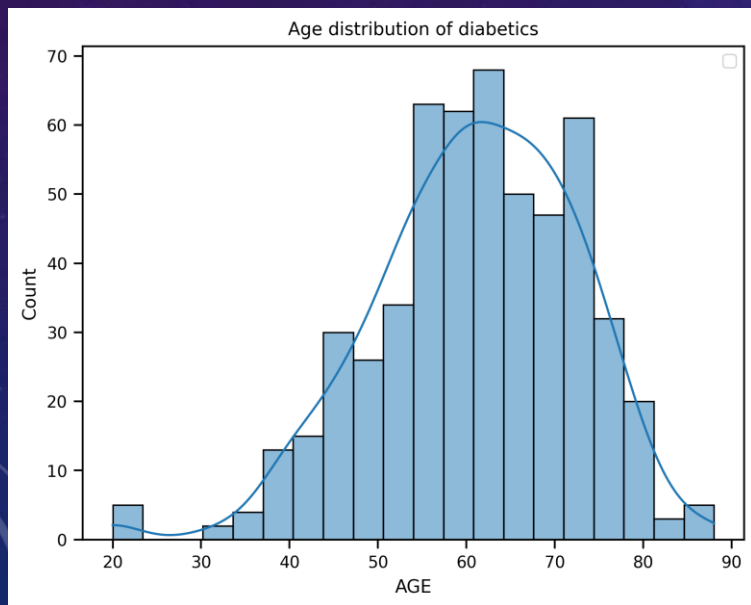
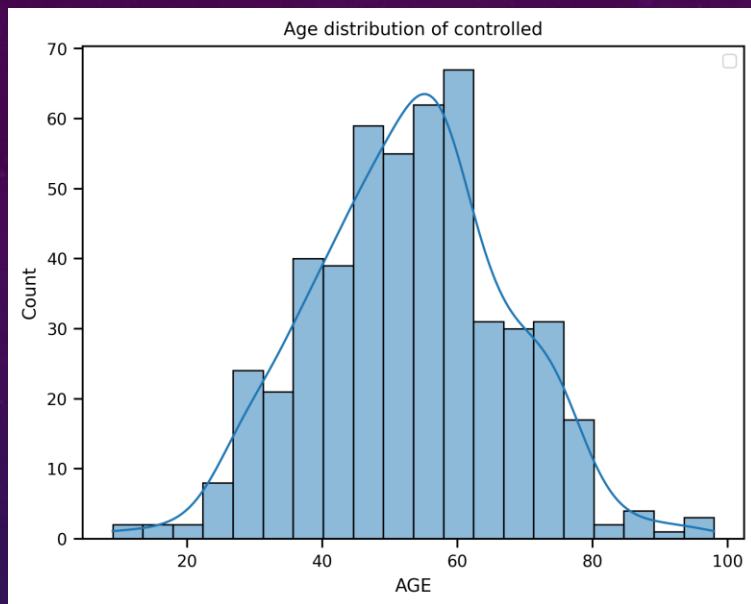


DATASET CONSIDERED FOR DIABETES DETECTION

- **DATASET:**
- Total number of male diabetes spectra: 204.
- Total number of female diabetes spectra: 336.
- Total number of male control spectra: 172.
- Total number of female control spectra: 328.
- Total number of features (Wavenumbers): 3737.

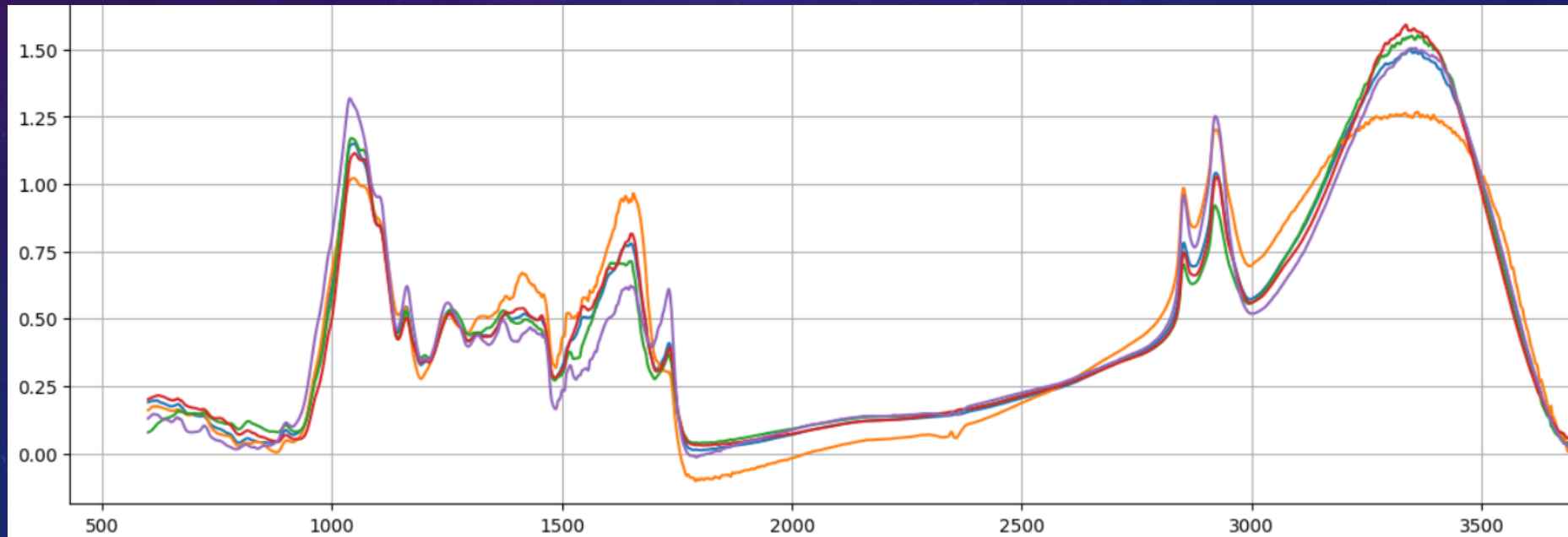


DISTRIBUTION WITHIN THE DATASET



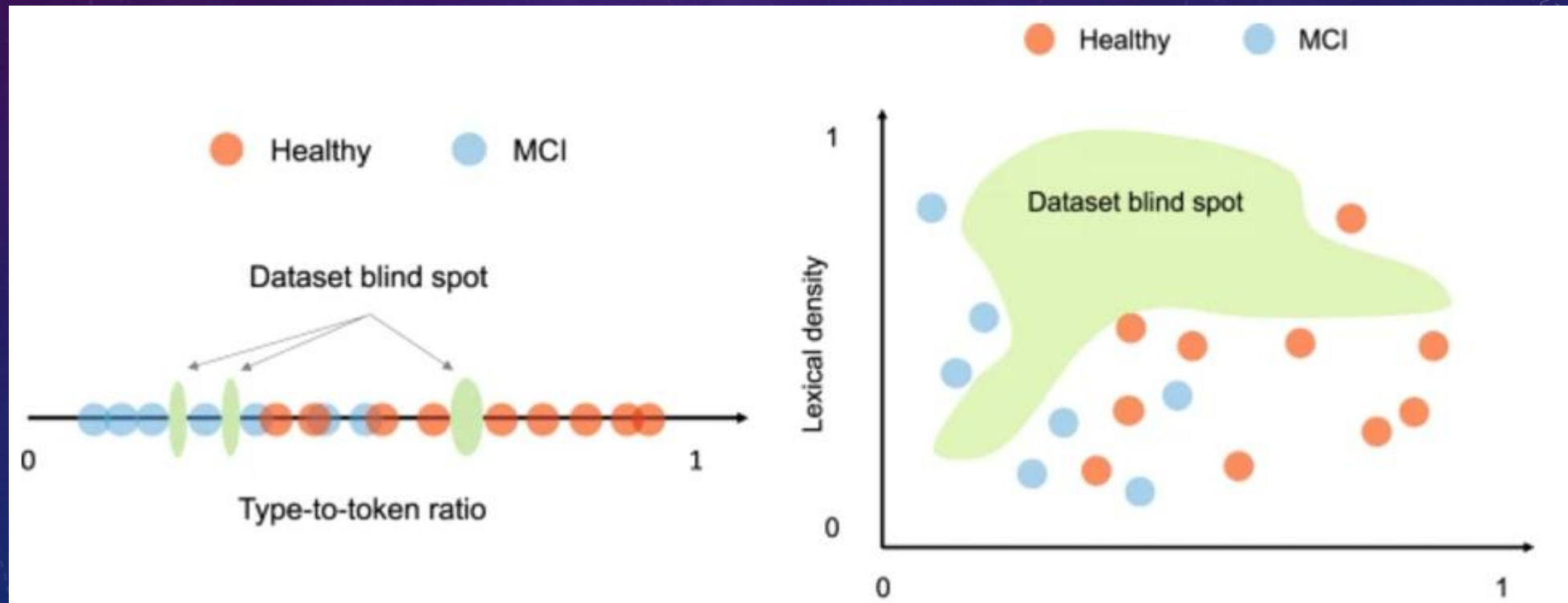
MAJOR CHALLENGES WITH FTIR SPECTROSCOPY DATA

- Interpreting complex patterns in FTIR spectral data involves understanding how the spectral features relate to the underlying chemical or biological processes.
- Each peak or feature in an FTIR spectrum corresponds to a specific bond or group of atoms vibrating in a unique way. However, in real-world samples, especially biological ones like saliva or blood, multiple compounds are present.
- This sometimes makes spectral data unreliable for analysis.
- Machine learning can help us work with such data.



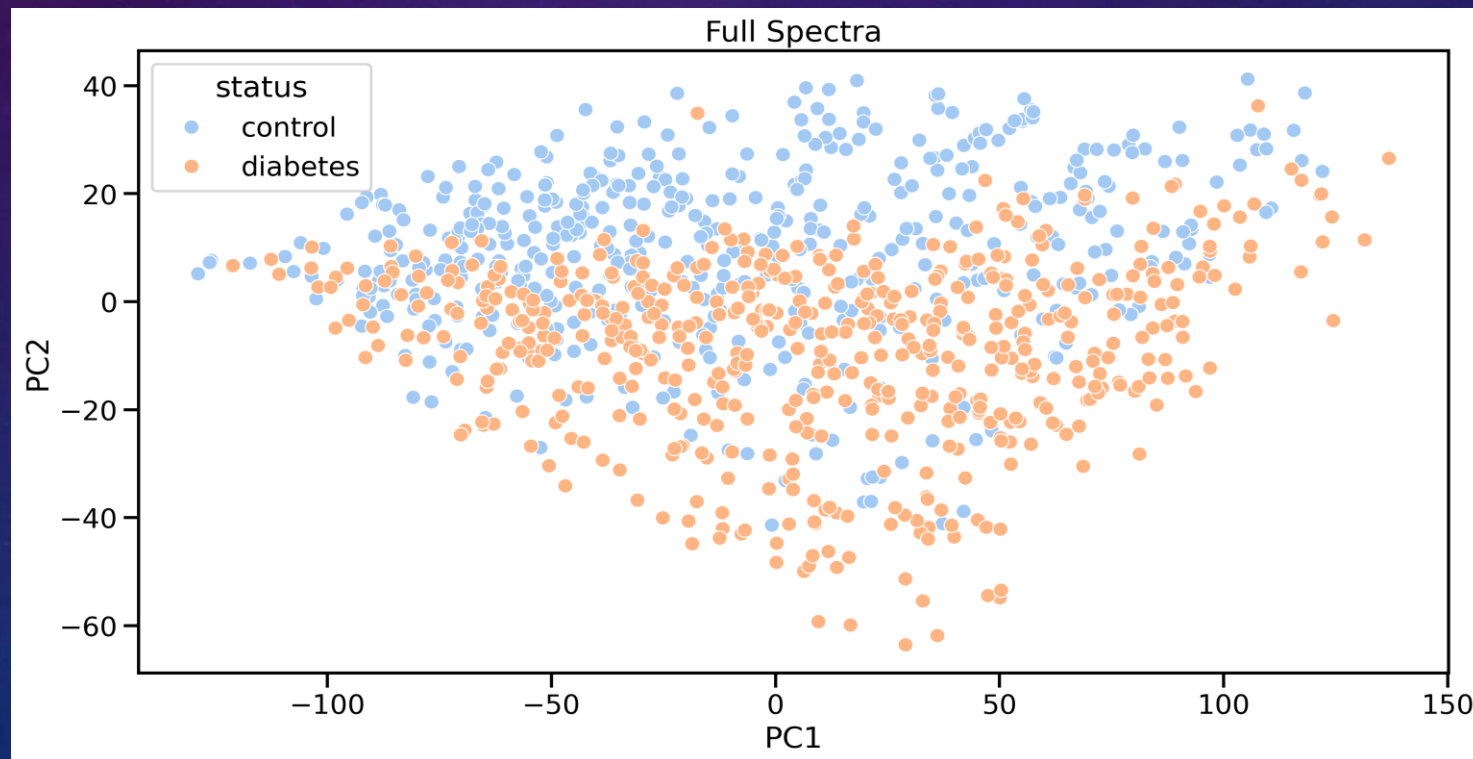
MAJOR CHALLENGES WITH FTIR SPECTROSCOPY DATA

- A major challenge is the high-dimensional nature of the spectral data obtained. FTIR spectroscopy generates data that represent absorbance at hundreds or even thousands of wavenumbers, resulting in a vast number of features or variables for analysis.
- This phenomenon is referred to as the *curse of dimensionality*.



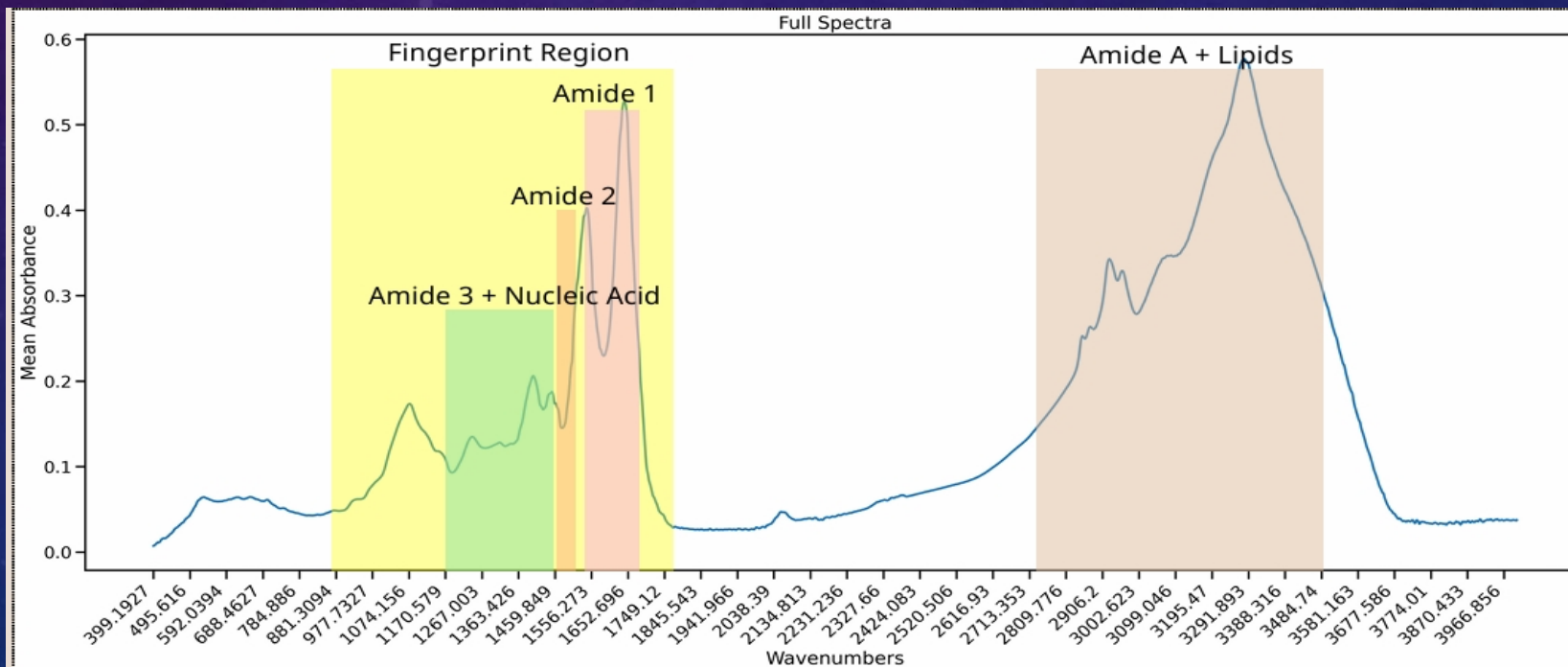
EXISTING SOLUTION

- To effectively tackle the issue of high dimensional FTIR spectral data, we can use dimensionality reduction techniques that are critical for simplifying the data while retaining as much of the underlying structure and information as possible.
- Principal Component Analysis (PCA) is a widely used dimensionality reduction technique in data science and machine learning. However, it may not always prove to be helpful.

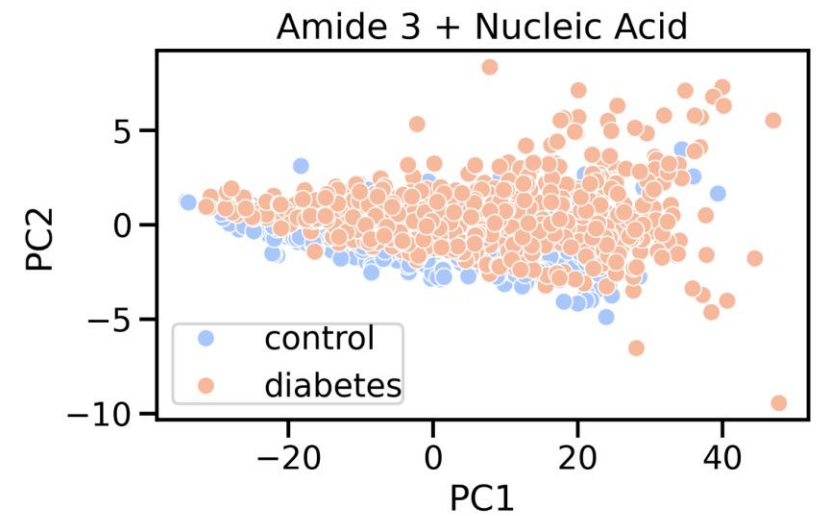
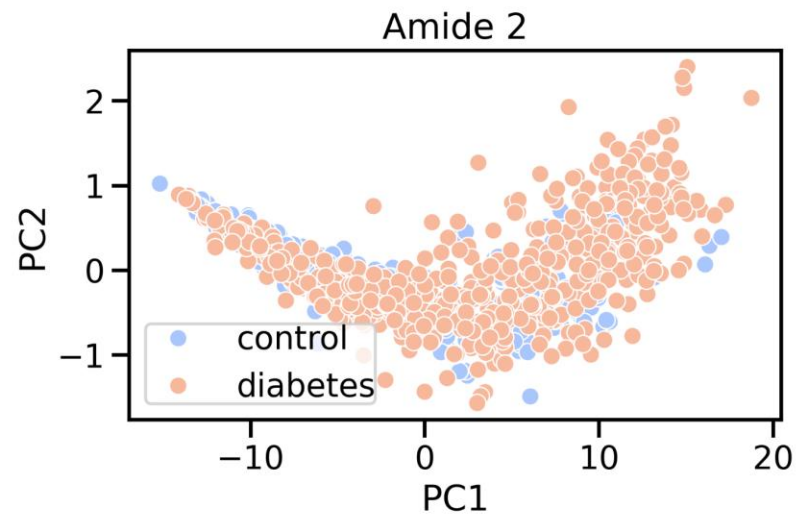
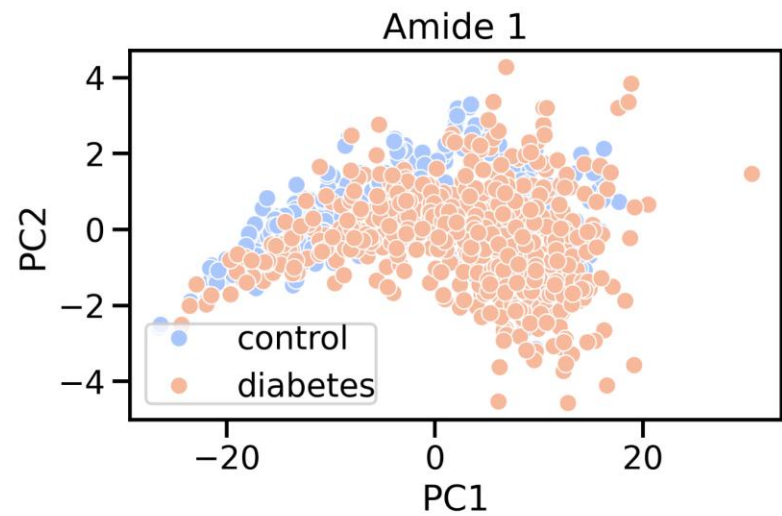
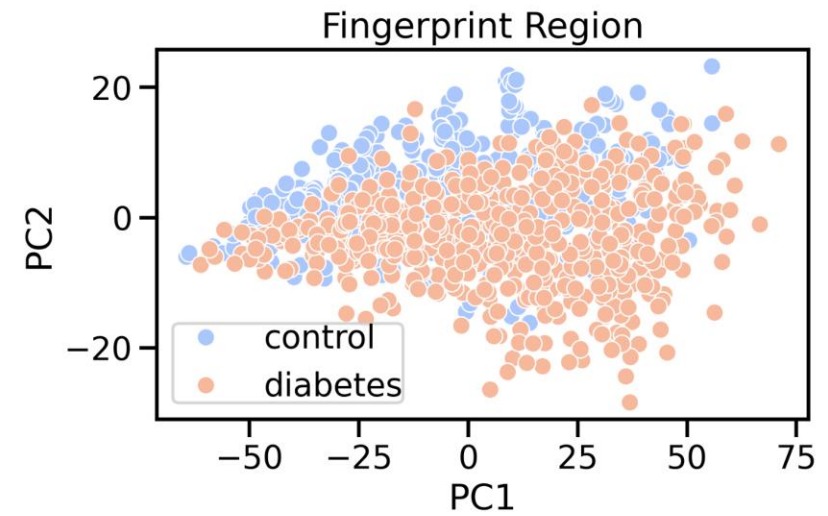
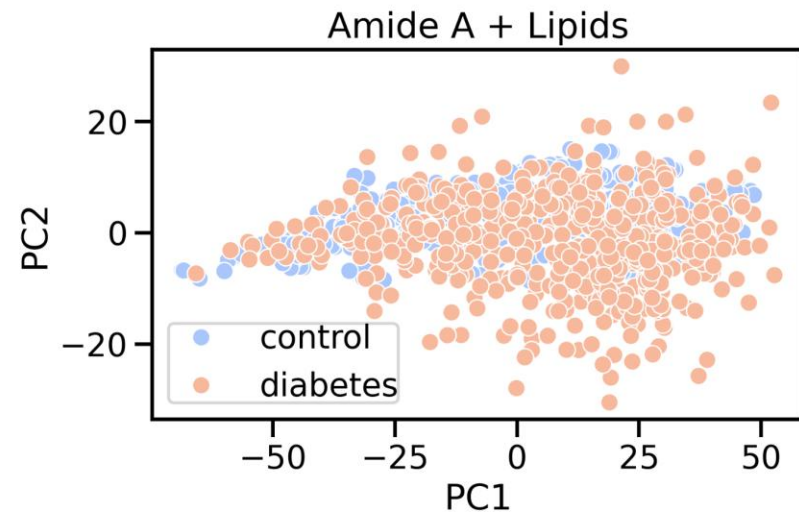
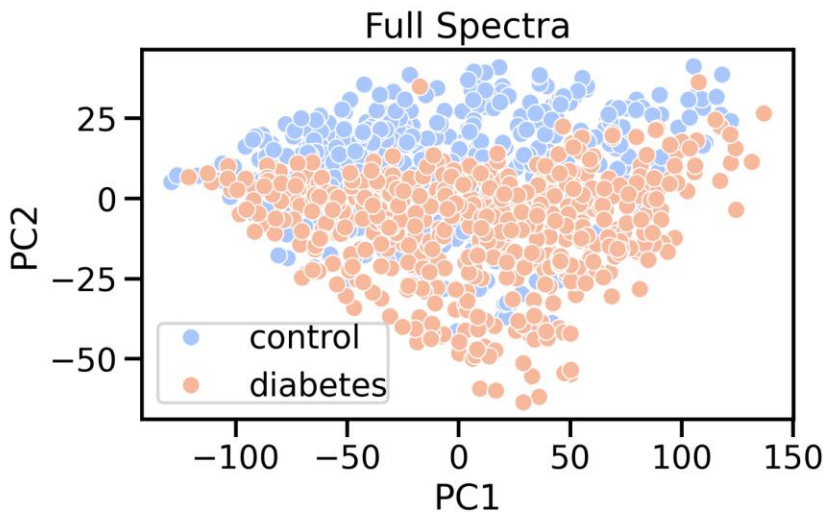


METHODOLOGY: DIVIDE AND CONQUER APPROACH USING AI

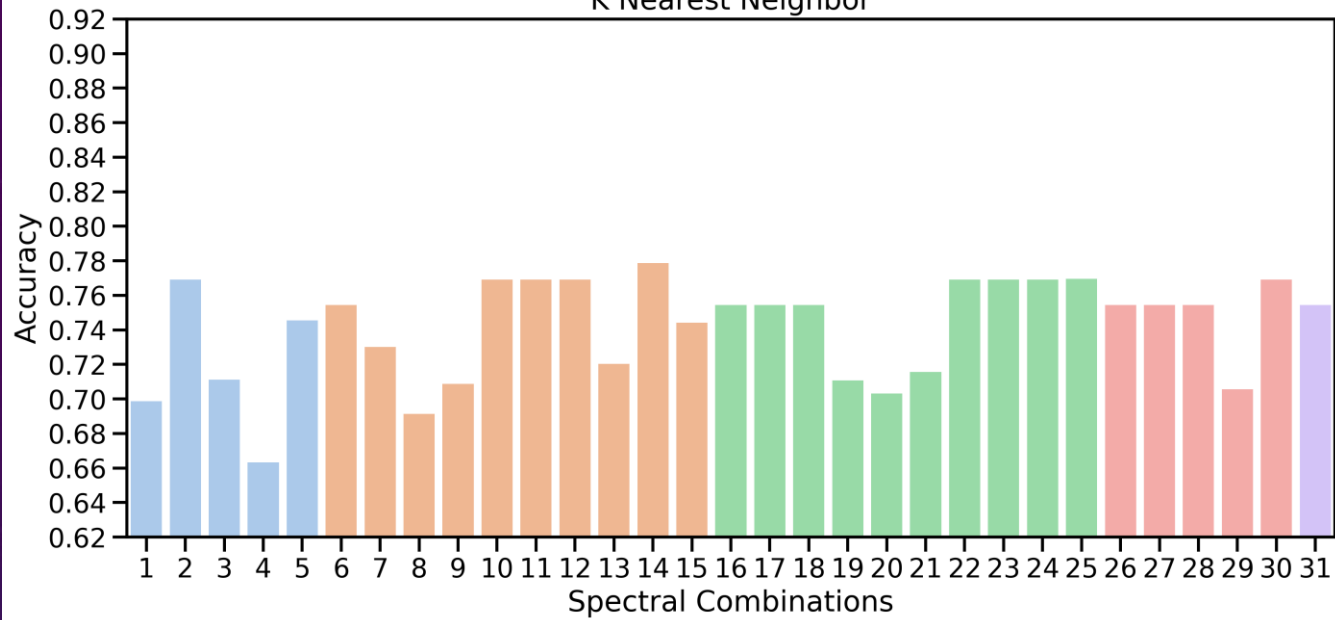
- we analyzed various different regions like Amide A + Lipids region (2800 cm^{-1} - 3500 cm^{-1}), Amide 1 region (1600 cm^{-1} - 1700 cm^{-1}), Amide 2 region (1500 cm^{-1} - 1560 cm^{-1}), Amide 3 + Nucleic Acid region (1200 cm^{-1} - 1500 cm^{-1}) and fingerprint region (900 cm^{-1} - 1800 cm^{-1}).
- Performing PCA in these different regions independently, did not prove to be of much help as data points from both categories showed great amount of overlap.
- The machine learning algorithms used for the analysis were Support Vector Machines (SVM) and K Nearest Neighbour (KNN) coupled with Leave One Out Cross Validation on all possible combinations of regions.



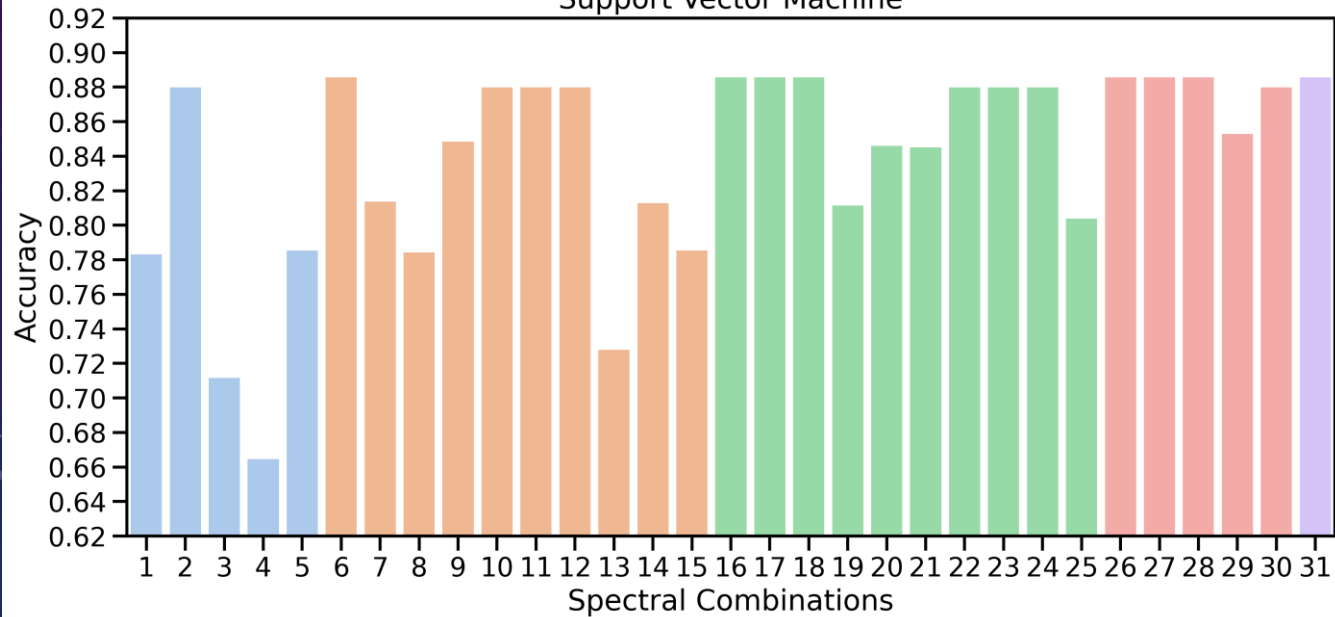
PCA ON DIFFERENT REGIONS



K Nearest Neighbor



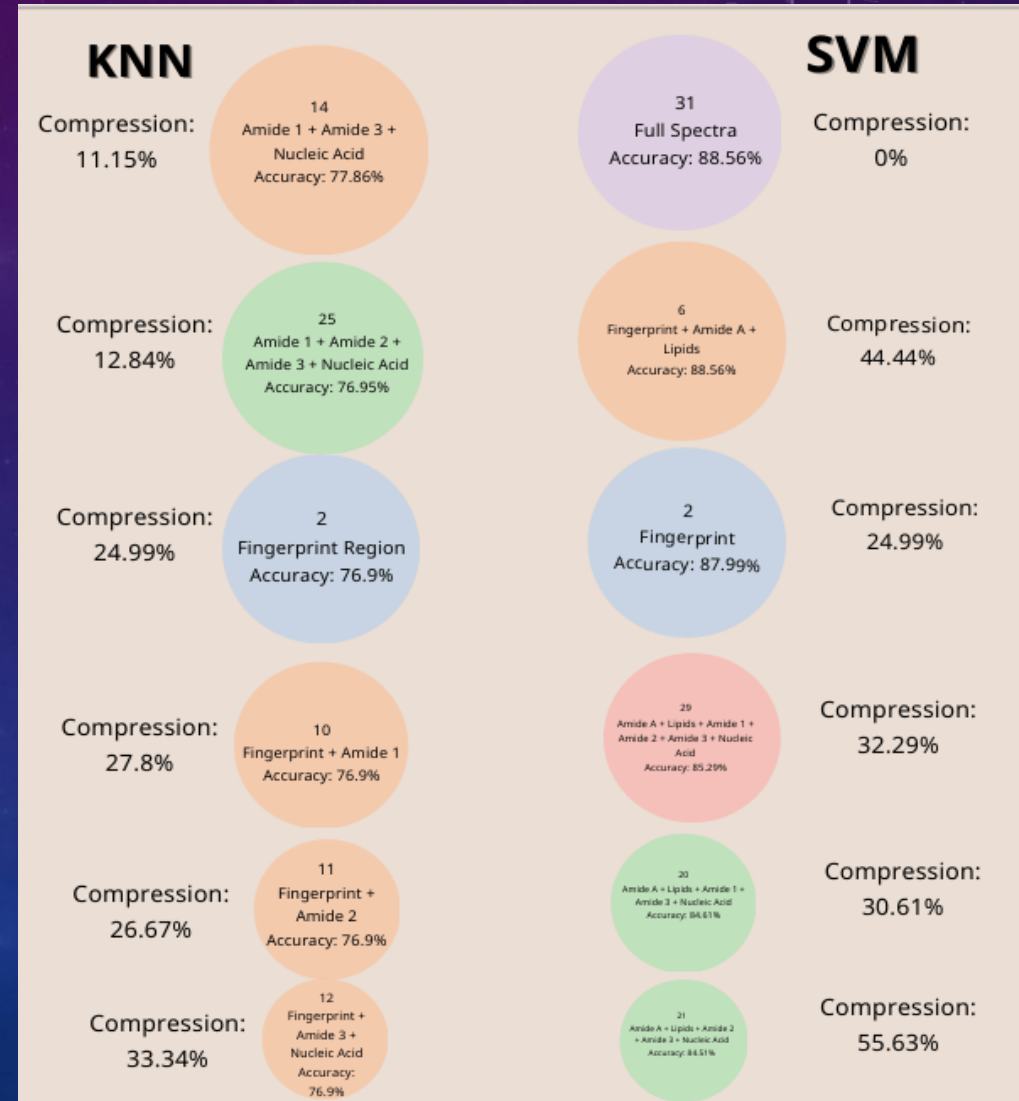
Support Vector Machine



- 1 Amide A + Lipids
- 2 Fingerprint region
- 3 Amide 1
- 4 Amide 2
- 5 Amide 3 + Nucleic Acid
- 6 Amide A + Lipids + Fingerprint region
- 7 Amide A + Lipids + Amide 1
- 8 Amide A + Lipids + Amide 2
- 9 Amide A + Lipids + Amide 3 + Nucleic Acid
- 10 Fingerprint region + Amide 1
- 11 Fingerprint region + Amide 2
- 12 Fingerprint region + Amide 3 + Nucleic Acid
- 13 Amide 1 + Amide 2
- 14 Amide 1 + Amide 3 + Nucleic Acid
- 15 Amide 2 + Amide 3 + Nucleic Acid
- 16 Amide A + Lipids + Fingerprint region + Amide 1
- 17 Amide A + Lipids + Fingerprint region + Amide 2
- 18 Amide A + Lipids + Fingerprint region + Amide 3 + Nucleic Acid
- 19 Amide A + Lipids + Amide 1 + Amide 2
- 20 Amide A + Lipids + Amide 1 + Amide 3 + Nucleic Acid
- 21 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid
- 22 Fingerprint region + Amide 1 + Amide 2
- 23 Fingerprint region + Amide 1 + Amide 3 + Nucleic Acid
- 24 Fingerprint region + Amide 2 + Amide 3 + Nucleic Acid
- 25 Amide 1 + Amide 2 + Amide 3 + Nucleic Acid
- 26 Amide A + Lipids + Fingerprint region + Amide 1 + Amide 2
- 27 Amide A + Lipids + Fingerprint region + Amide 1 + Amide 3 + Nucleic Acid
- 28 Amide A + Lipids + Fingerprint region + Amide 2 + Amide 3 + Nucleic Acid
- 29 Amide A + Lipids + Amide 1 + Amide 2 + Amide 3 + Nucleic Acid
- 30 Fingerprint region + Amide 1 + Amide 2 + Amide 3 + Nucleic Acid
- 31 Amide A + Lipids + Fingerprint region + Amide 1 + Amide 2 + Amide 3 + Nucleic Acid

RESULTS AND FINDINGS

- Based on the analysis of various combinations, SVM emerged as the better performing algorithm with the top accuracy of 88.56%, obtained using the combination of Fingerprint + Amide A + Lipids region. This result is comparable to the one achieved by considering the entire spectra while also achieving a compression of 44% in feature extraction.



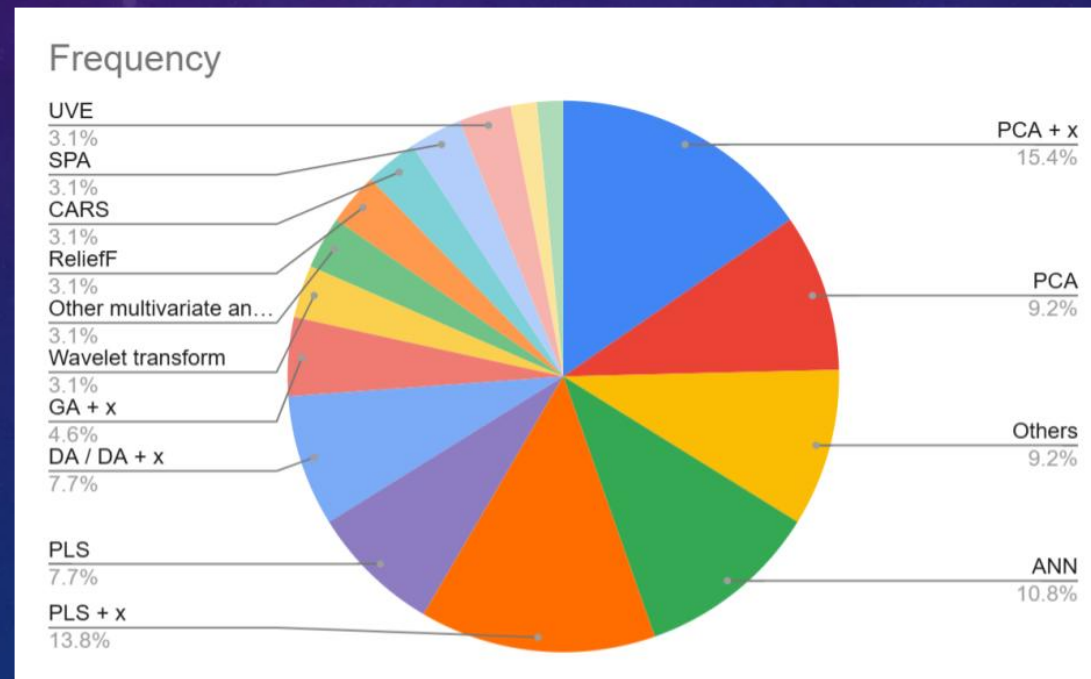
VIEW THE CODE

You can view the code used for all the analysis and predictions by scanning this barcode.



FUTURE WORKS

- As discussed early on, feature extraction is one of the key applications of AI in FTIR spectroscopy. However, the exact technique algorithm to be used is highly case sensitive and depends on factors like kind of spectral data in question and approach of the author.
- *A generalized feature extraction technique* would allow researchers to automate feature selection and dimensionality reduction without manual intervention, enabling more efficient and unbiased analysis.





ACCOMPLISHMENTS

- Our abstract titled “AI Assisted Spectral Analysis for Diabetes Detection” was selected for poster presentation at the Symposium on Emerging Nanotechnologies for Sensors-Organization and Recognition Systems 2024 (SENSORS 2024)

AI Assisted Spectral Analysis for Diabetes Prediction

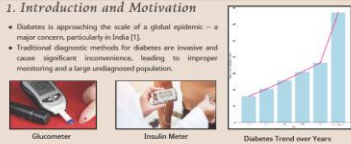
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1. Introduction and Motivation

- Diabetes is approaching the scale of a global epidemic – a major concern, particularly in India [1].
- Traditional diagnostic methods for diabetes are invasive and cause significant inconvenience, leading to irregular monitoring and a large undiagnosed population.
- Thus, there exists an urgent need for non-invasive methods to improve diabetes detection and monitoring.
- Fourier transform infrared (FTIR) spectroscopy, combined with Machine Learning (ML), offers a non-invasive approach for analyzing saliva, providing a potential breakthrough for diabetes diagnosis [2].

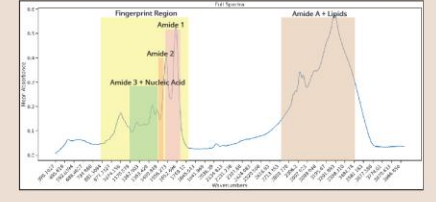


2. Challenges

- A major challenge is the high dimensional data obtained by FTIR which contains absorbance at hundred or even thousands of wavenumbers.
- High dimensional data points necessitate large datasets to train an AI model (due to increase in blind spot).

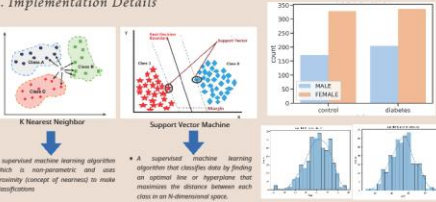
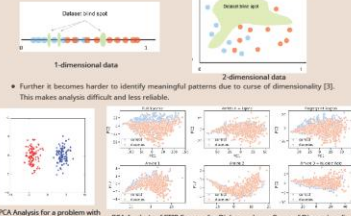


3. Methodology: Divide and Conquer Approach using AI




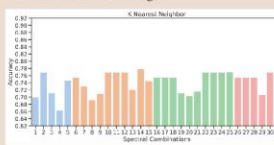
- To find the most relevant wavenumber region for diabetes diagnosis using the FTIR spectra of human saliva, we analyzed various different regions like Amide A + Lipids region (2800-3500), Amide 1 region (1600-1700), Amide 2 region (1500-1560), Amide 3 + Nucleic Acid region (1200-1500) and Fingerprint region (500-1800).
- We used dimensionality reduction technique of Principal Component Analysis (PCA) to explain the variance in these regions, but it didn't prove to be very helpful.
- We used ML algorithms like Support Vector Machine (SVM) and K-Nearest Neighbor (KNN) on all the possible combinations of the above-mentioned regions in order to find the region most applicable for the purpose of diagnosis.
- In order to determine the biomarkers, we used the decision tree algorithm which helped us to find the wavenumber that provided with the best prediction results.

4. Implementation Details



- A supervised machine learning algorithm which is non-parametric and uses proximity (similarity) of instances to make classifications.
- A supervised machine learning algorithm that classifies data by finding an optimal line or hyperplane that maximizes the distance between each class in a high-dimensional space.

5. Results and Findings



Model	Region	Compression	Accuracy
KNN	1 Amide A + Lipids	14	11.53%
	2 Fingerprint region	31	17.86%
	3 Amide 2	21	12.84%
SVM	1 Amide A + Lipids + Fingerprint region	4	44.44%
	2 Amide A + Lipids + Amide 2	3	24.99%
	3 Amide A + Lipids + Amide 3 + Nucleic Acid	2	24.99%
	4 Amide A + Lipids + Amide 1	10	27.8%
	5 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid	11	26.67%
	6 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid + Amide 1	10	27.8%
	7 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid + Amide 1 + Amide 2	11	26.67%
	8 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid + Amide 1 + Amide 2 + Amide 3	11	26.67%
	9 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid + Amide 1 + Amide 2 + Amide 3 + Amide 1	11	26.67%
	10 Amide A + Lipids + Amide 2 + Amide 3 + Nucleic Acid + Amide 1 + Amide 2 + Amide 3 + Amide 1 + Amide 2	11	26.67%


6. Conclusion

- AI-assisted analysis of FTIR spectra of human saliva samples is performed to differentiate healthy and diabetic people.
- We show that the combination of Fingerprint region (~1500) and Amide A + Lipid Region (2800-3500) with SVM are optimal for diabetes diagnosis.
- This leads to a 44.4% dimensionality reduction, while delivering the same performance as that of full FTIR spectrum.
- FTIR analysis of saliva samples can be developed as low cost and noninvasive alternative method for diabetes monitoring.

7. References

1. Tabák S. A. Is Diabetes Becoming the Biggest Epidemic of the Twenty First Century? *International Journal of Health Sciences*. 2007; 1(2): V-VIII.
2. Sanchez-Brito, M., Luna-Roson, F. J., Mendoza-Gonzalez, R., Vazquez-Zapien, G. J., Martinez-Ramos, J. C., Mata-Miranda, M. M. Type 2 Diabetes Diagnosis Assisted by Machine Learning Techniques through the Analysis of FTIR Spectra of Saliva. *Biomedical Signal Processing and Control* 2021, 69, 102855.
3. Altman, N., Krzywicki, M. The Curse of Dimensionality. *Nature Methods* 2018, 15 (6), 399-400.

Code Available



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1. Tabish S. A. Is Diabetes Becoming the Biggest Epidemic of the Twenty-first Century? *International Journal of Health Science*, 2007, 1(2), V–VIII.
2. Sanchez-Brito, M.; Luna-Rosas, F. J.; Mendoza-Gonzalez, R.; Vazquez-Zapien, G. J.; Martinez-Romo, J. C.; Mata-Miranda, M. M. Type 2 Diabetes Diagnosis Assisted by Machine Learning Techniques through the Analysis of FTIR Spectra of Saliva. *Biomedical Signal Processing and Control* 2021, 69, 102855.
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4. Baum, Zachary J., Yu, Xiang, Ayala, Philippe Y., Zhao, Yanan, Watkins, Steven P., Zhou, Qiongqiong. (2021). Artificial Intelligence in Chemistry: Current Trends and Future Directions. *Journal of Chemical Information and Modelling*. Received: June 1, 2021; Published: July 15, 2021.