Rapid COVID-19 Diagnosis using Raman Spectroscopy and Machine Learning

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Raman and ML
Data Wrangling
Exploratory Data Analysis
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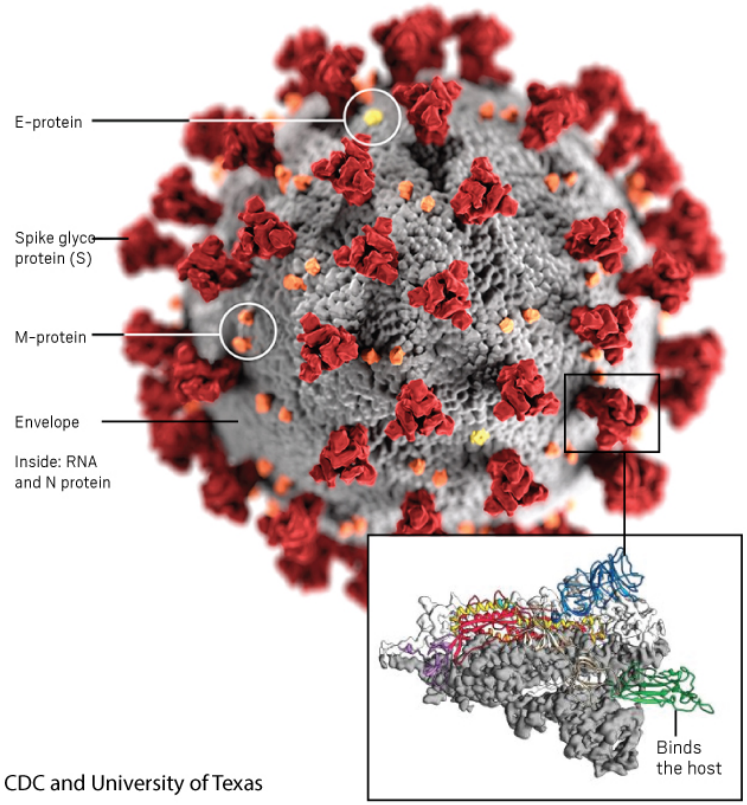

Author: Isaac Ghebregziabher

Capstone Project One

July 4, 2021

Springboard

World under COVID-19 pandemic crisis

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- > 171 million active cases
- 3.5+ million deaths
- Fast and reliable diagnostic is needed

RT-PCR – Current COVID-19 detection method is time consuming and expensive

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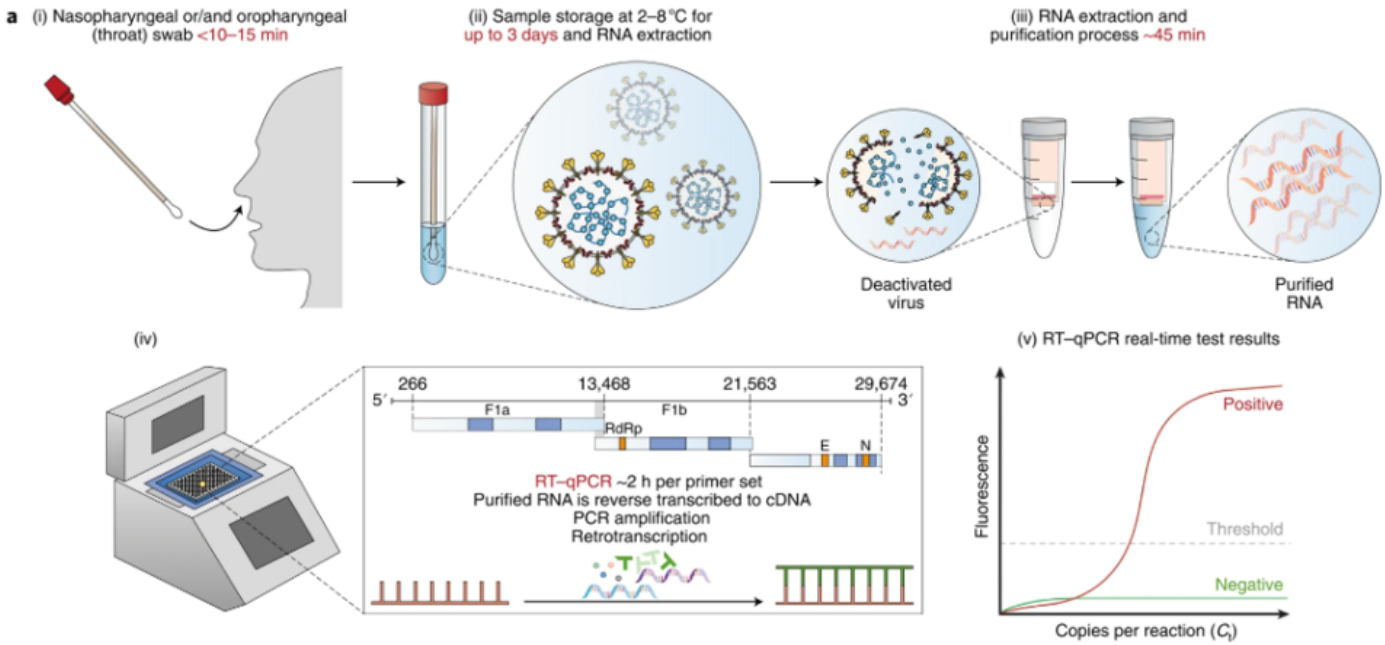
- 3 days for sample preparation and RNA extraction
- Expensive PCR



Springboard

Principle of Raman effect

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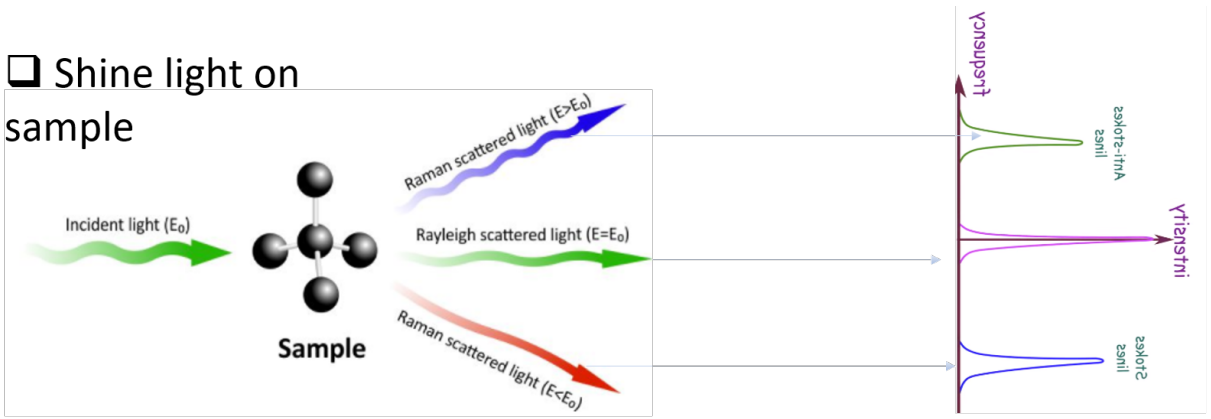
- Most light scatters unaffected (Rayleigh scattering)
- A few percent gets Raman scattered
- Raman Scattered light is signature of molecular composition

❑ Shine light on sample



❑ Most of the light is unaffected
❑ Small percentage of light undergoes frequency shift

Rapid detection of Covid-19 using Raman spectroscopy and Machine Learning

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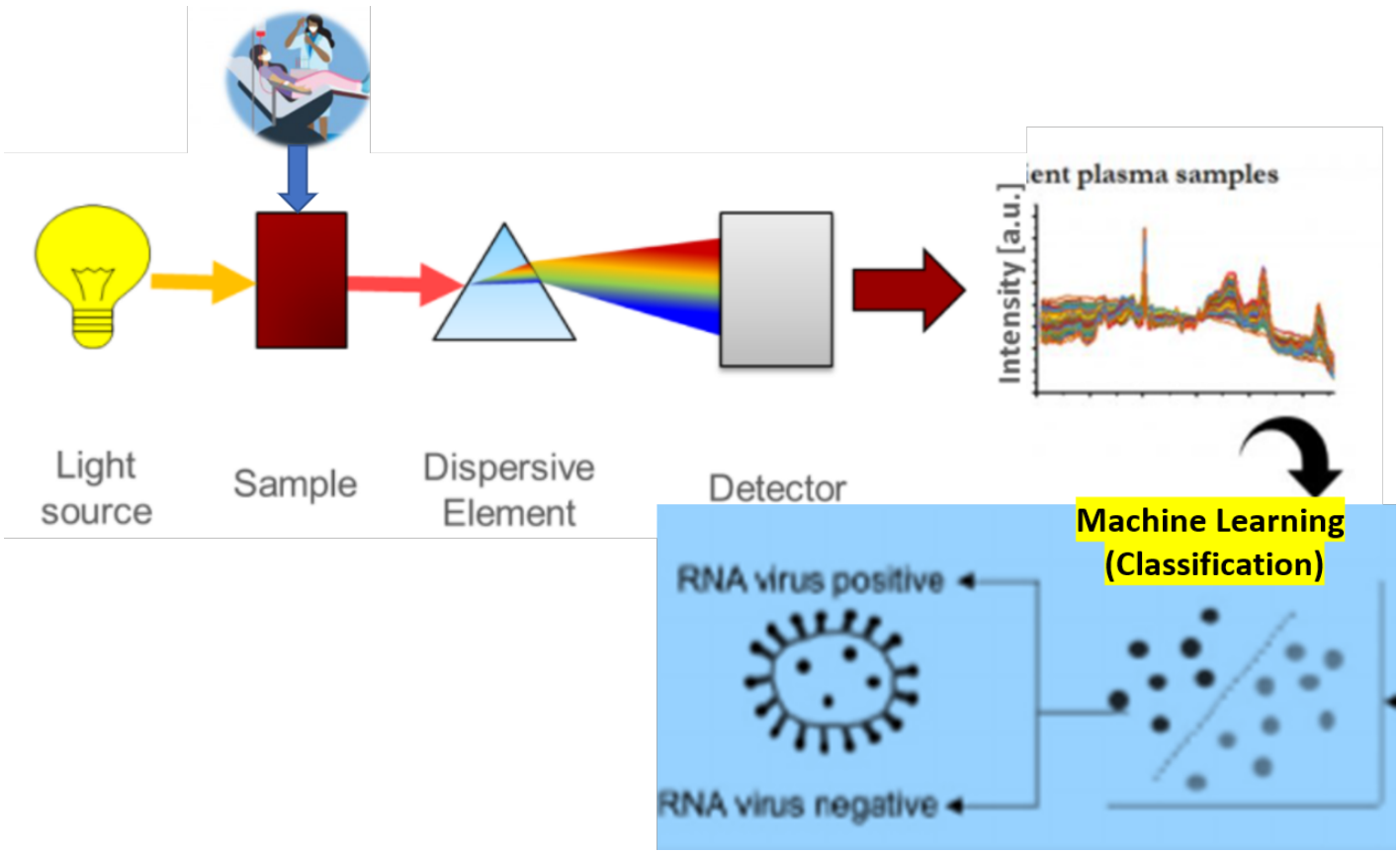

Springboard

Overview of Dataset obtained from Kaggle

- 309 rows X 901 columns
- Each column → Raman Wavenumber
- Rows → Intensity for wavenumbers
- Each row corresponds to one observation
- Last column '***diagnostic***' is target variable

Feature names = Wavenumbers in units of cm-1

	400	402	405	407	410	412	415	417	420	422	...	diagnostic
0	0.0	-0.015237	-0.030607	-0.038309	-0.039078	-0.035809	-0.031176	-0.030395	-0.033311	-0.031603	...	Healthy
1	0.0	-0.012098	-0.028164	-0.035189	-0.036138	-0.031050	-0.026015	-0.027539	-0.028084	-0.027075	...	Healthy
2	0.0	-0.013000	-0.029058	-0.035021	-0.034994	-0.033025	-0.028413	-0.028470	-0.029737	-0.029198	...	Healthy
3	0.0	-0.015728	-0.034346	-0.045140	-0.047671	-0.044334	-0.040807	-0.040474	-0.041417	-0.040699	...	Healthy
4	0.0	-0.020355	-0.045839	-0.060556	-0.065805	-0.064988	-0.062097	-0.061955	-0.064759	-0.066886	...	Healthy

Raman scattered intensities for each Wavenumber

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Raman detector might have dead pixels corresponding to all zero value intensities

- No missing values in dataset
- 9 features wave-numbers with 0 intensity value
- Drop null features (treated as missing)

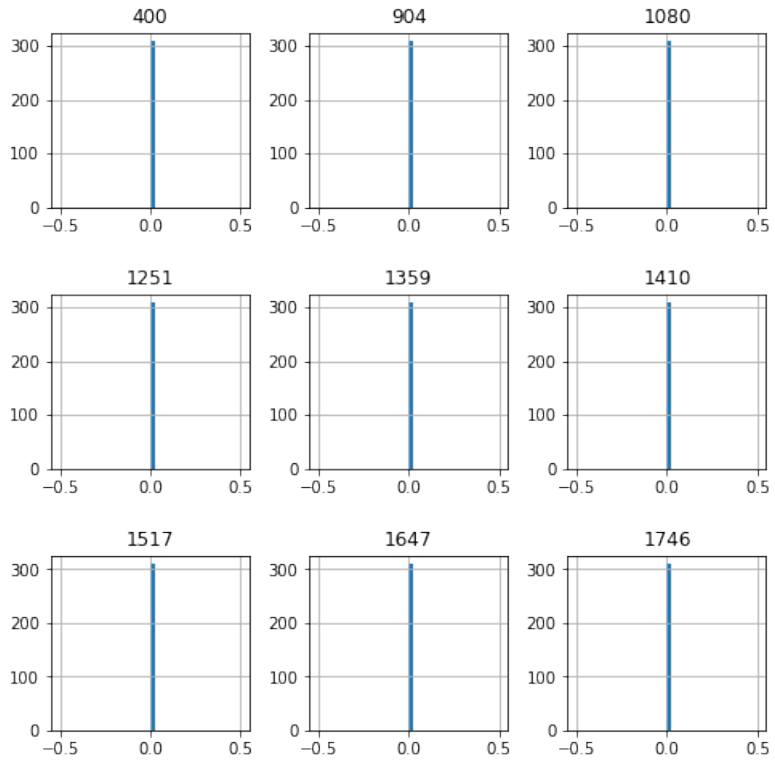

Figure: Single valued features (dropped).

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Dataset is balanced

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- No class imbalance issues
- Dataset is balanced with ≈ 50:50 class ratio.

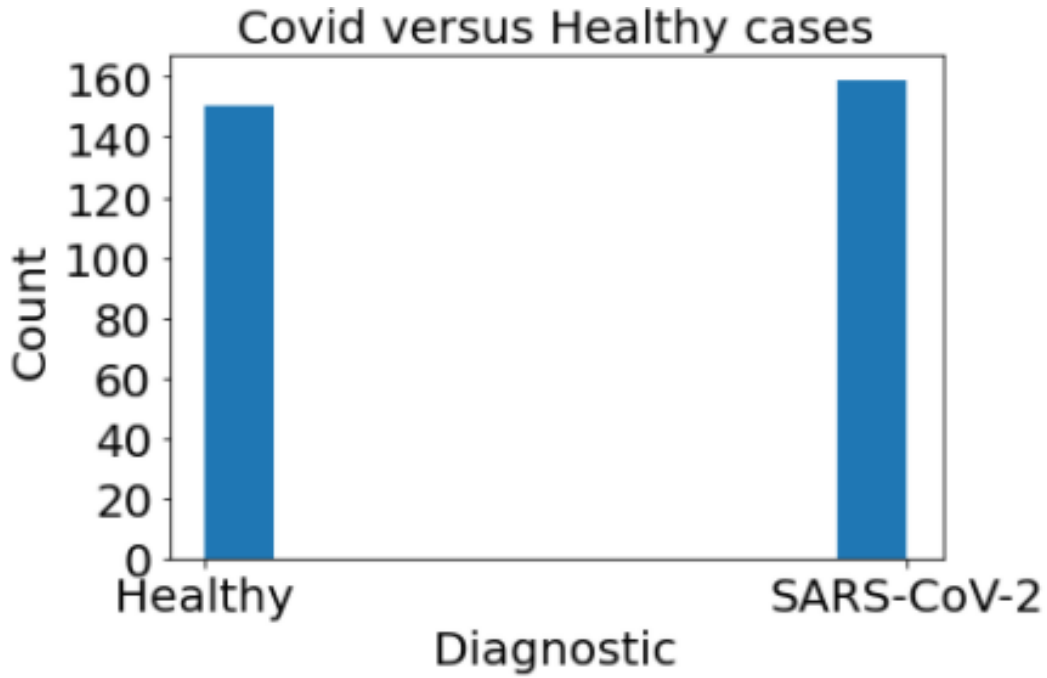
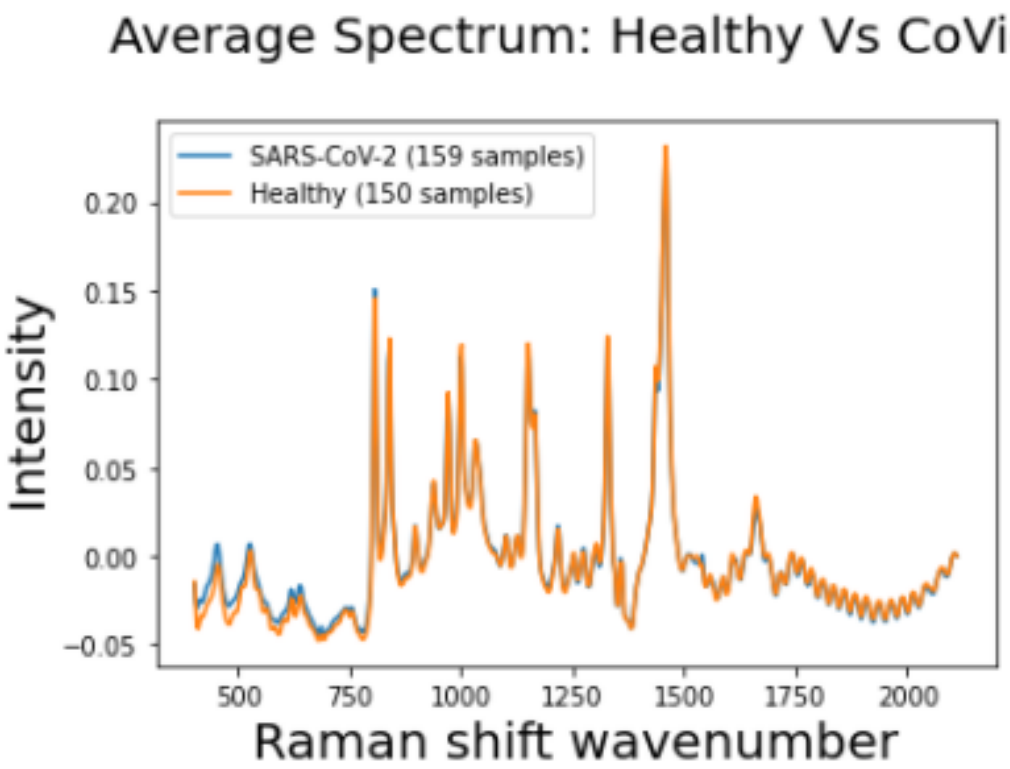


Figure: ≈ 50 : 50 COVID to Healthy class ratio.

Visually indiscernible Raman spectrum

- Visually difficult to easily identify COVID from Healthy.
- Machine Learning model is needed for fast and reliable COVID diagnosis.



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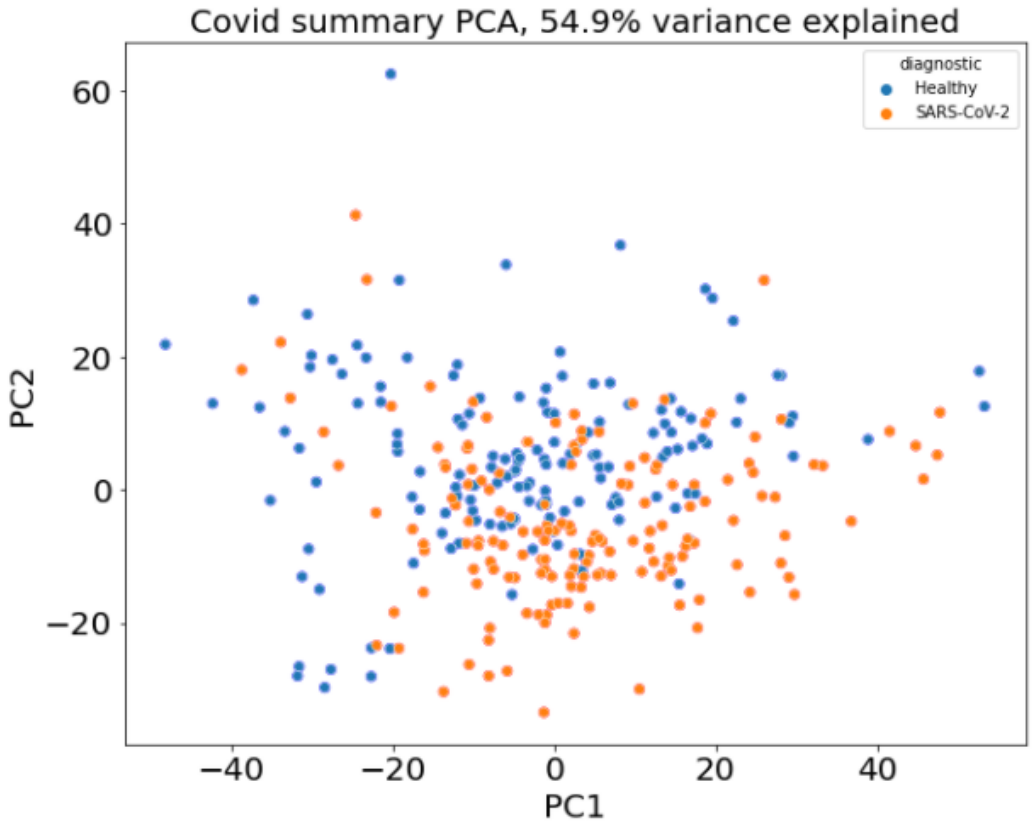
High dimensional data visualization - PCA

- Over 50 percent variance explained with two principal components.
- No visual class separation



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Principal component analysis – feature reduction

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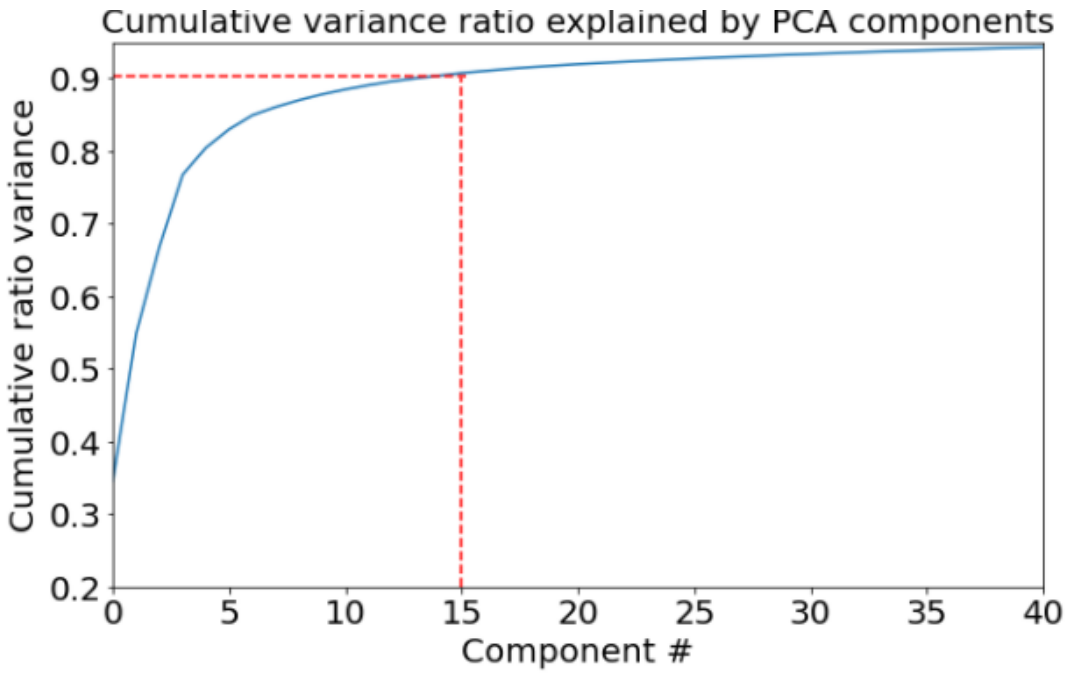
- Over 90% data variance explained with 15 components.
- Feature reduction to 15 from 900!



Modeling: Supervised Machine Learning

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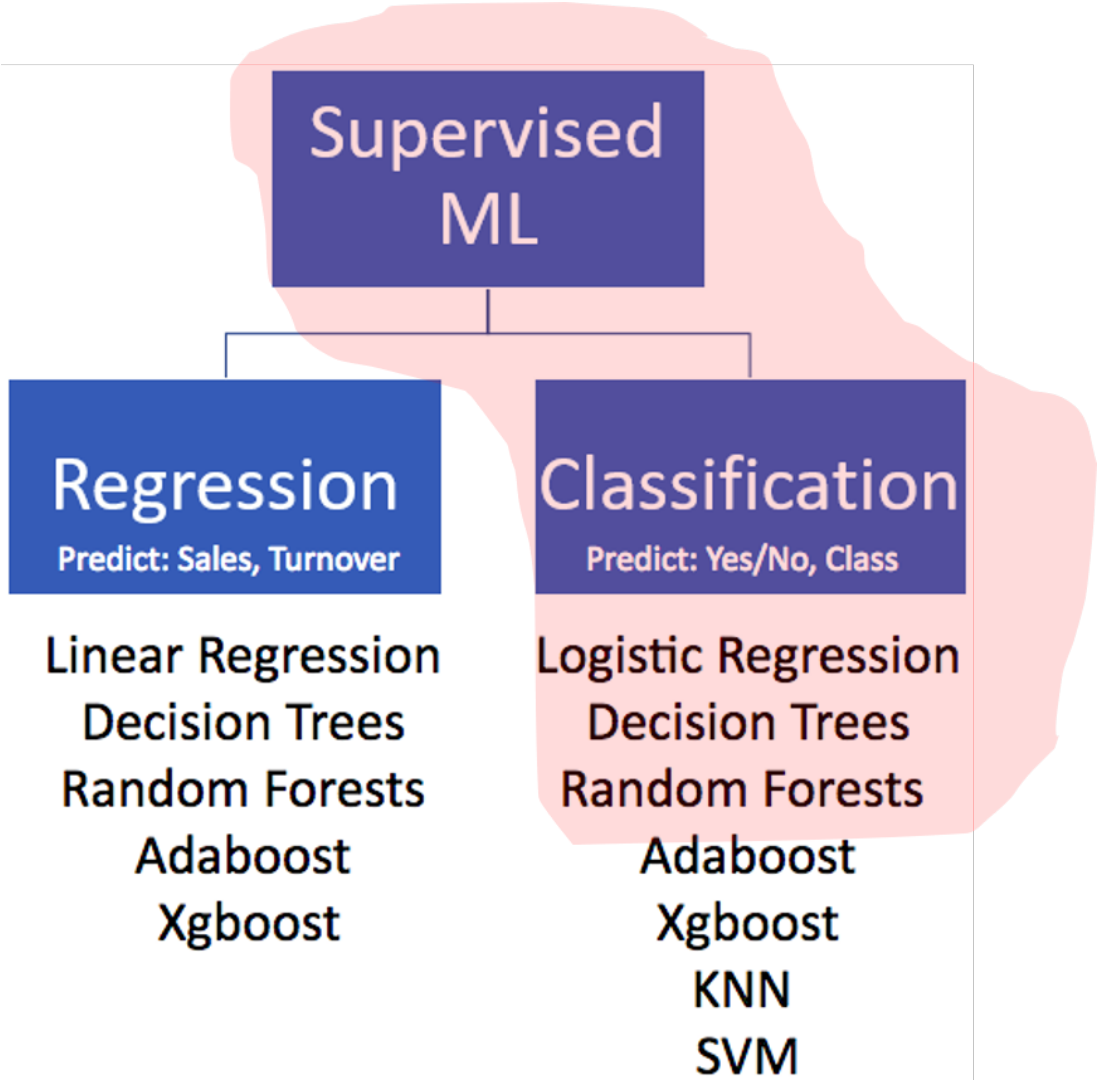
Three models considered:



Classification Report Training dataset: Logistic Regression

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```
Misclassified samples: 6
Logistic regression: PCA 15 components
 Classification report for train-dataset:
              precision    recall  f1-score   support

     Healthy       0.98      0.96      0.97       112
   SARS-CoV-2      0.97      0.98      0.97       119

    accuracy                           0.97       231
   macro avg       0.97      0.97      0.97       231
weighted avg       0.97      0.97      0.97       231
```

97 percent accuracy!

Need to be tested with the test split.

Classification Report Training split: Decision Tree

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```
Misclassified samples: 0
Decision tree: PCA 15 components
 Classification report for train-dataset:
              precision    recall  f1-score   support

     Healthy       1.00      1.00      1.00       110
   SARS-CoV-2      1.00      1.00      1.00       121

    accuracy                           1.00       231
   macro avg       1.00      1.00      1.00       231
weighted avg       1.00      1.00      1.00       231
```

100 percent accuracy! Model might be over-fitting.

Need to be tested with the test split.

Classification Report Training split: Random Forest

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```
Misclassified samples: 0
Random Forest: PCA 15 components
 Classification report for train-dataset:
              precision    recall  f1-score   support

     Healthy       1.00      1.00      1.00       110
   SARS-CoV-2      1.00      1.00      1.00       121

    accuracy                           1.00       231
   macro avg       1.00      1.00      1.00       231
weighted avg       1.00      1.00      1.00       231
```

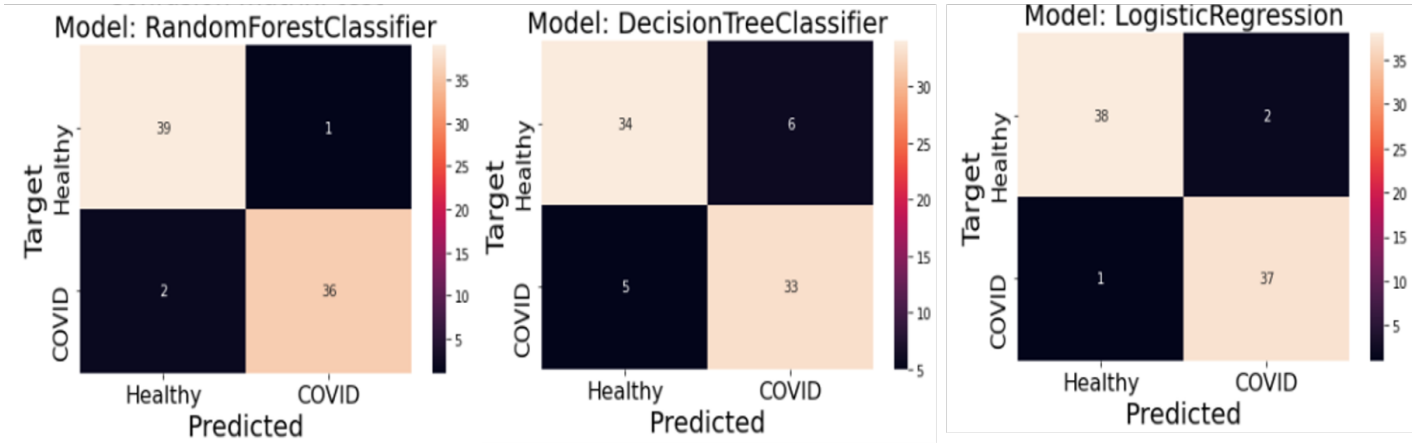
100 percent accuracy! Model might be over-fitting.

Need to be tested with the test split.

Models Testing With Test Split

- All models performed well
- RF and Logistic regression have highest accuracy

Confusion matrix: Test dataset



Accuracy = 96%

Accuracy = 86%

Accuracy = 96%

With PCA physical meaning of features is lost.

Need to model using all features without PCA to gain physical insight on features.

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Random forest classifier is the best performing model

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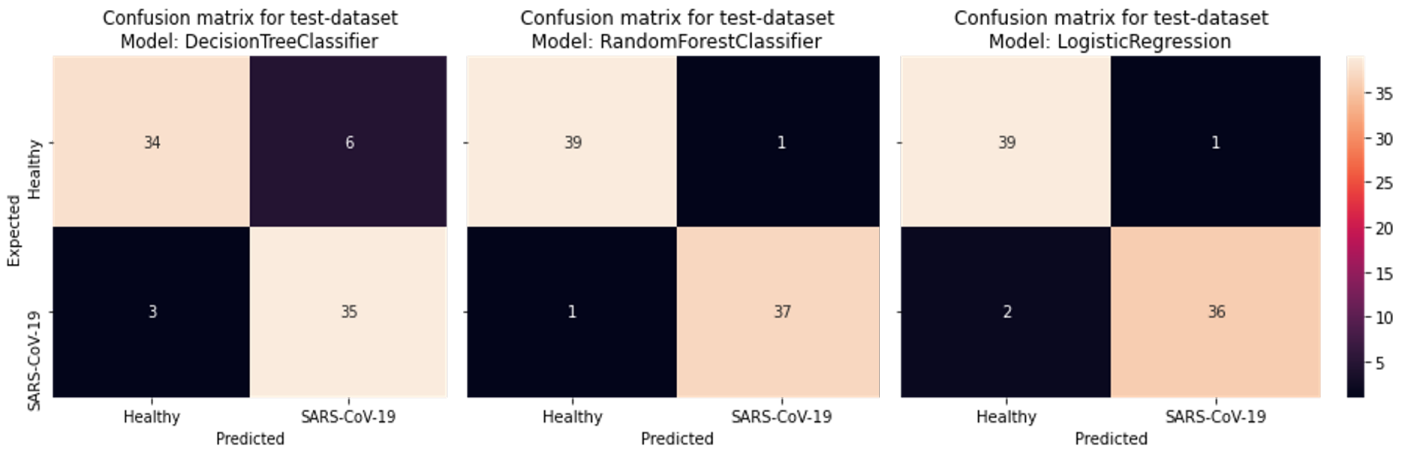
Though all models persisted with good accuracy:

- Random fores performs the best
- 97% classification accuracy
- Random forest chosen for deployment



Accuracy = 0.88 Accuracy = 0.97 Accuracy = 0.96

Important features with high predictive power

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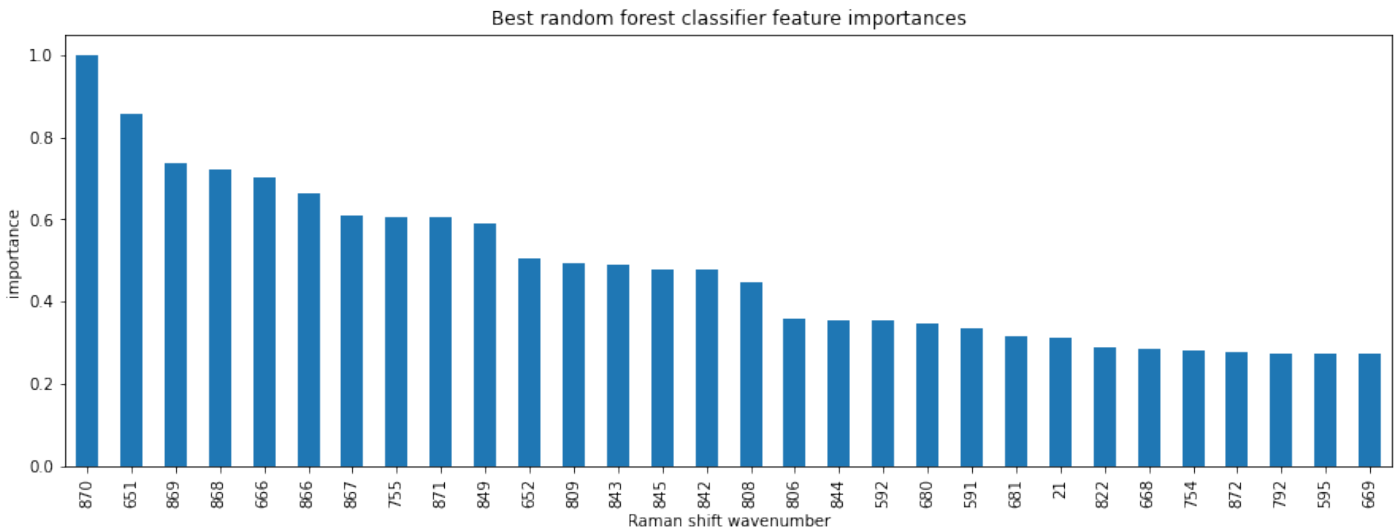
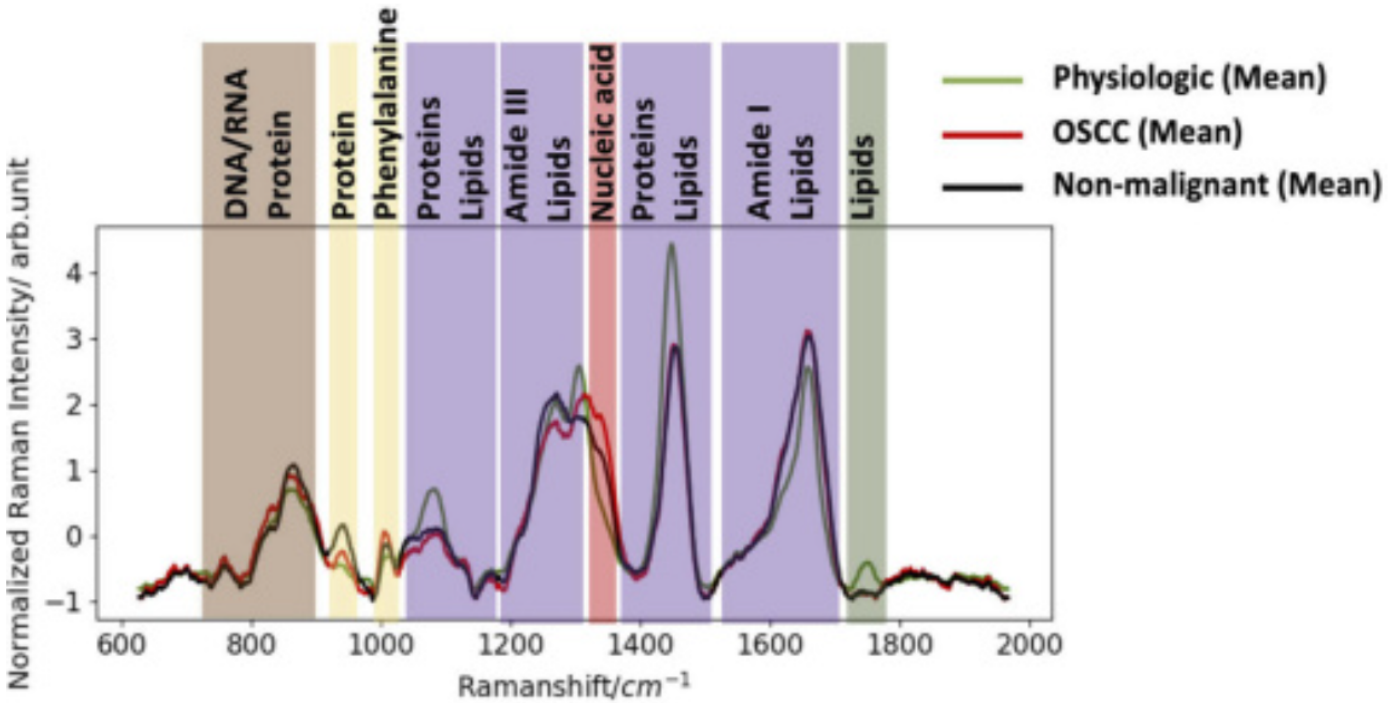
15 features out of 901 are the most important.

- Wavenumber in range [650, 870] has high predictive power
- feature 870 has the highest predictive power



Important features Raman band corresponds to RNA/DNA band

- Virus is an RNA/DNA protein
- Band $[700, 900]$ is prominent for RNA/DNA
- Band corresponds to predicted important features



Do we need more data to enhance model performance?

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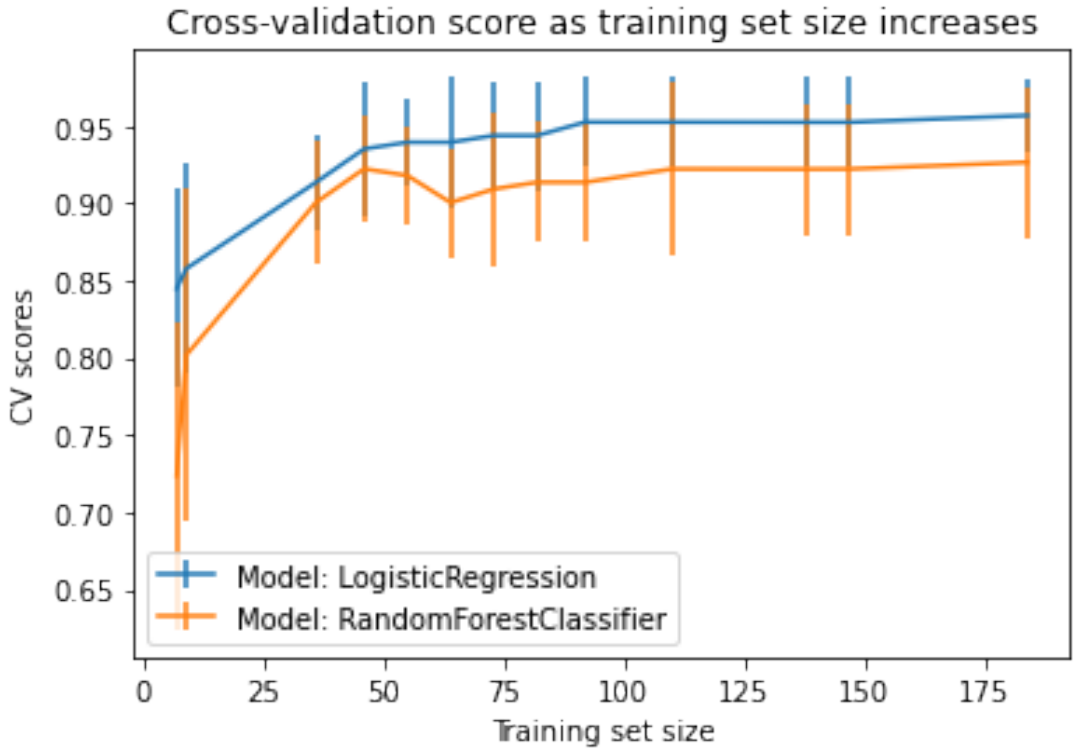
Model accuracy saturates well before the end of available data.



No need for more data.

Summary and Future Work

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- We developed supervised machine learning models COVID detection using Raman spectroscopy data.
- Logistic regression, decision tree, and random forest supervised machine learning algorithms were considered.
- We find COVID detection using Random forest results in highest detection accuracy of 97 percent.
- Future works needs to be done with covid suspect and covid survived data for more comprehensive and reliable conclusion.

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for time generous and insightful discussions