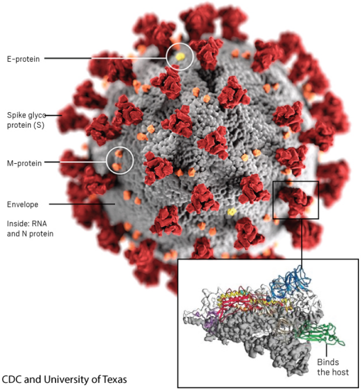
Rapid COVID-19 Diagnosis using Raman Spectroscopy and Machine Learning



CDC and University of Texas

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Capstone Project One

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Springboard

Side Deck - Capsone 1

Introduction

Current diagnostic method

Raman spectroscopy

Raman and ML

Data Wrangling

Exploratory Data Analysis

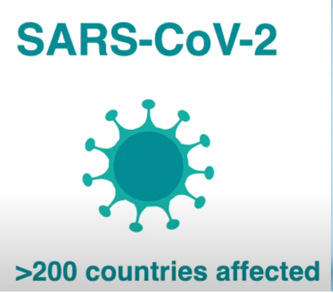
Modeling

Summary

Acknowledgement

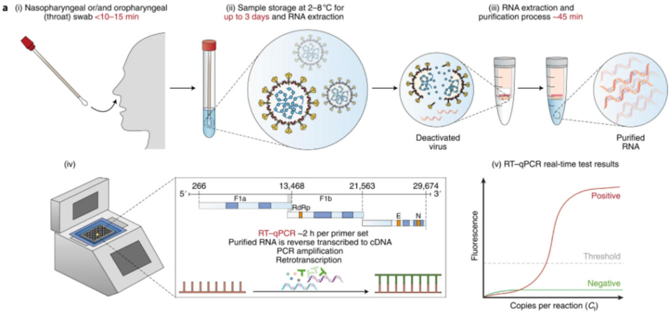
World under COVID-19 pandemic crisis

- > 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

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



a
(i) Nasopharyngeal or/and oropharyngeal (throat) swab <10–15 min
(ii) Sample storage at 2–8 °C for up to 3 days and RNA extraction
(iii) RNA extraction and purification process ~45 min
Deactivated virus
Purified RNA
(iv)
266
13,468
21,563
29,674
5′
3′
F1a
F1b
RdRp
E
N
RT–qPCR ~2 h per primer set
Purified RNA is reverse transcribed to cDNA
PCR amplification
Retrotranscription
(v) RT–qPCR real-time test results
Fluorescence
Positive
Threshold
Negative
Copies per reaction (C_t)

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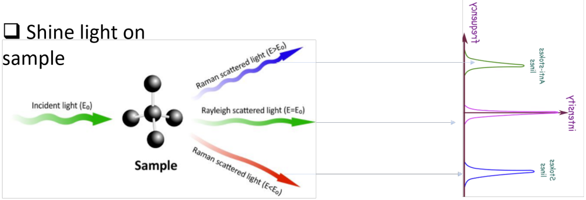
Principle of Raman effect

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

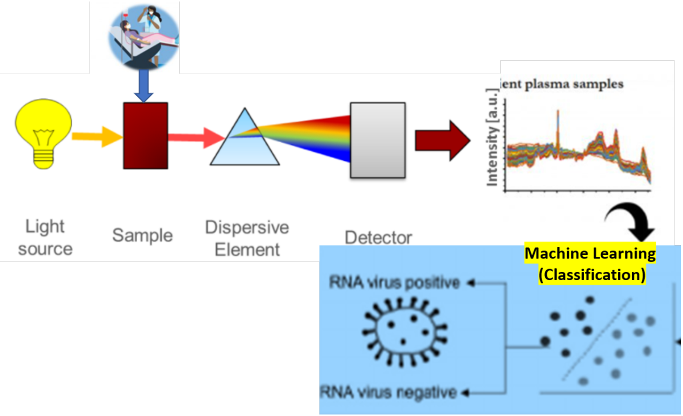
❑ Shine light on sample


Incident light (E_0)
Sample
Raman scattered light ($E>E_0$)
Rayleigh scattered light ($E=E_0$)
Raman scattered light ($E<E_0$)
frequency
intensity
Anti-stokes lines
Stokes lines

❑ 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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Drop features with all values equal to 0

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

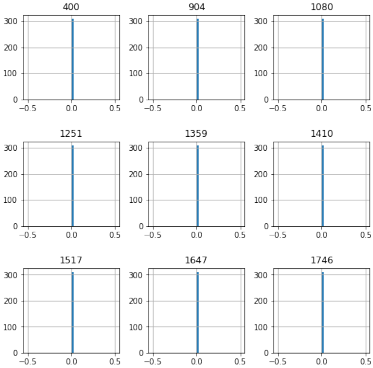


Figure: Single valued features (dropped).

Remaining features have normal distribution

- No concern on feature distributions.
- Most close to normal.
- little skew on several features.

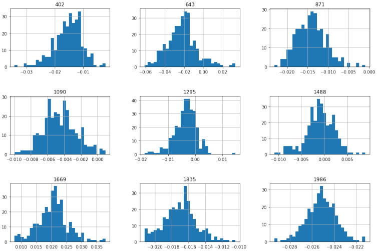


Figure: Close to normal feature distributions.

Dataset is balanced

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

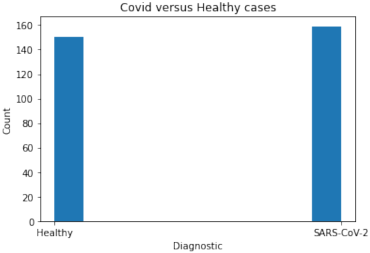
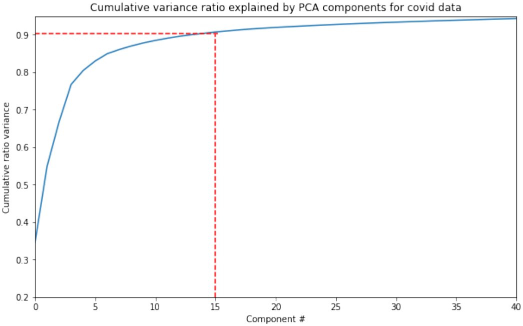


Figure: ≈ 50 : 50 COVID to Healthy class ratio.

Principal component analysis – feature reduction

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

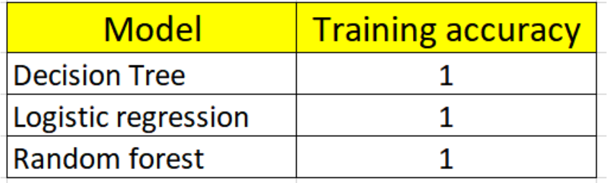


Springboard

Model training and accuracy

Three models considered:

- Decision tree
- Logistic regression
- Random forest



Model	Training accuracy
Decision Tree	1
Logistic regression	1
Random forest	1

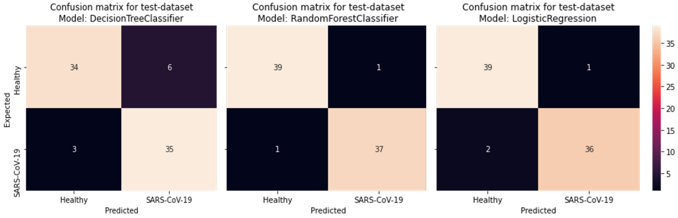
All models seem to over-fit.

Need to be tested with the test split.

Random forest classifier is the best performing model

Though all models persisted with good accuracy:

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



Accuracy = 0.88

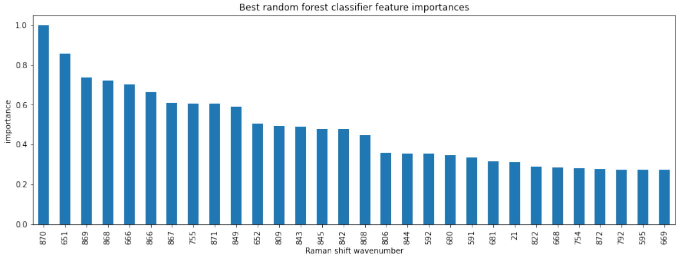
Accuracy = 0.97

Accuracy = 0.96

Important features with high predictive power

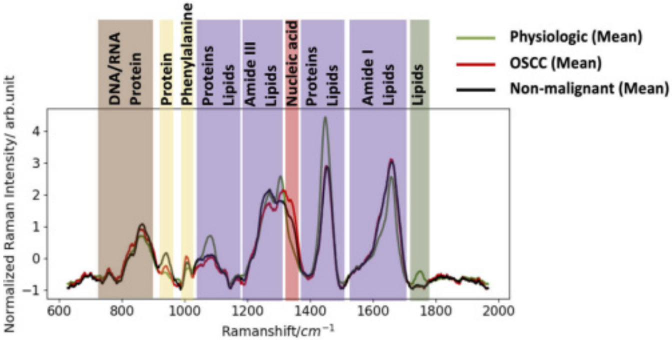
15 features out of 901 are the most important.

- 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



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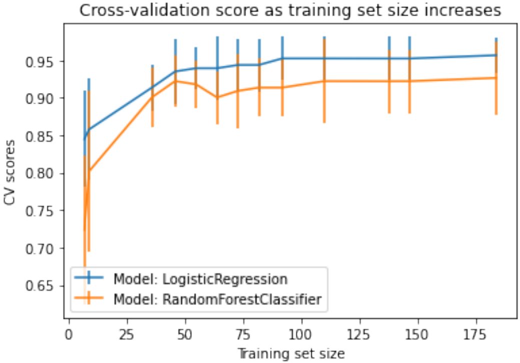
Do we need more data to enhance model performance?

Model accuracy saturates well before the end of available data.



No need for more data.

Summary

- We obtained Raman spectroscopy for COVID detection experimental dataset from Kaggle.
- To get insight We applied data cleansing, wrangling, and exploring techniques.
- We compared and contrasted the performance of Logistic regression, decision tree, and random forest classification models
- We find Random forest to be the best with diagnostic accuracy of 97%

Acknowledgement

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for time generous and insightful discussions