**Intro to gas analysis and chemometrics**

**Experimental setup**

Describe system a.d.h.v. figure

Use Adonis’ paper, Zhe’s thesis, questionspaper

**Data calibration**

Wavenumber calibration – (compare with Adonis’) sound system calibration

H2O & CO2 calibration

**Concentration and compound determination**

Acetone and other molecules determination

Finding p-values + Explanation of p-values

Determine compounds with high intensity in regions of low p value

Determine compounds without need for p-values (and explain pros/cons)

Remove CO2 in order to better estimate underlying ethyl-alcohol (check Adonis’ Analytical Chemistry paper for theory/understanding)

**Clustering and classification**

Got 80% accuracy on sorting healthy vs. asthmatic using SVM

**Discussion**

Cause of noise (in rawest signal): Thermal fluctuations expand laser box(, causing different wavelengths to be stable and emitted, seen in the signal as intensity fluctuations? [source: Adonis]). Piëzo hysteresis causes wavenumber (horizontal) shift and stretch. Mode-hopping is caused by piëzo + grating allowing short periods were multiple wavelengths are supported [source: Adonis]. Mode-hopping is also caused by random gas fluctuations?

In order to achieve higher accuracy with the QCL setup the intensity fluctuations should be minimized. The main cause X could be replaced by …. The wavenumber shifting and stretching caused by the hysteresis of the piëzo can be fixed using a similar method as for the wavenumber calibration.

Optional/what else was done during this project

Get NEC as in Florian’s paper

CO2H2O concentration determination

Acetone concentration determination (Done by Adonis, not me)

Learned R: reading and editing of Erasmus people their exhaled.r script

Learned Python: used for machine learning data ordering and CO2 removal script