Quantifying nitrogen oxides and ammonia via frequency modulation in gas sensors

Master Thesis - Mid term seminar

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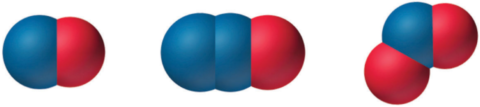
Outline

Problem in a nutshell

Motivation

NO_x[1]:



NO N_2O NO_2

- NOx are detrimental to the environment and humans.
- NOx are naturally ocurring in man-made processes. E.g. Combustion.
- Ammonia can "neutralize" NOx, producing water (H_2O) and nitrogen gas (N_2). Both harmless! - Selective catalytic reduction (SCR)
- But ammonia is also hazardous to the environment/humans.

[1] Image source: ENVIS Centre on Plants and Pollution

Problem in a nutshell

Motivation

- The dosing of ammonia in the catalyst is key:
  - Too much ammonia: NOx reduction will occur $\rightarrow$ Unnecessary ammonia emissions.
  - Too little ammonia: NOx reduction will occur partially/will not occur $\rightarrow$ NOx emissions.
- Gas sensors can be used to measure the concentrations of NOx to aid on ammonia dosing.
- However, the sensor also responds to ammonia.
- Operating the sensor in a cyclic operation (e.g. temperature) can enhance selectivity.
  - Different gasses react differently in different stages of the cycle.
- Temperature cycling.
- **Frequency cycling**.

Problem in a nutshell

Research questions

- Can frequency cycling be used to simultaneously quantify NOx and ammonia concentrations?
- Which method yield best prediction of gas concentrations?

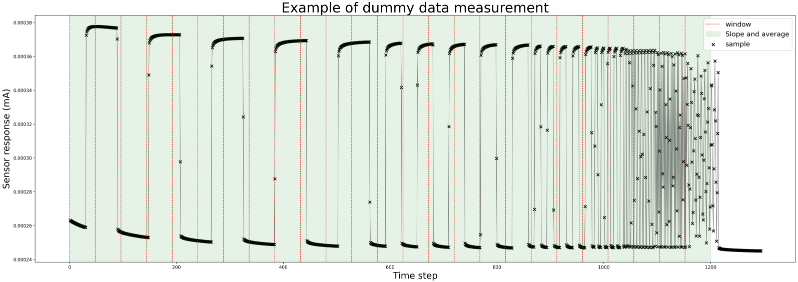
What has been done so far

- Writing
  - Introduction - Done.
  - Theory - Done.
  - Data - Partially done.
- Some preliminary implementation of the methods
  - Linear Regression
  - Principal Component Regression
  - Partial Least Squares Regression
  - Ridge Regression

Caveats

- Real data not yet available - lab problems
- Methods used on "dummy" data
- Dummy data has problems:
  - Small number of observations
  - Measurement of shape features
  - Naïve window of measurements
  - High frequencies problematic

(Dummy) data



Example of dummy data measurement
Sensor response (mA)
Time step
window
Slope and average
sample
0.00038
0.00036
0.00034
0.00032
0.00030
0.00028
0.00026
0.00024
0
200
400
600
800
1000
1200

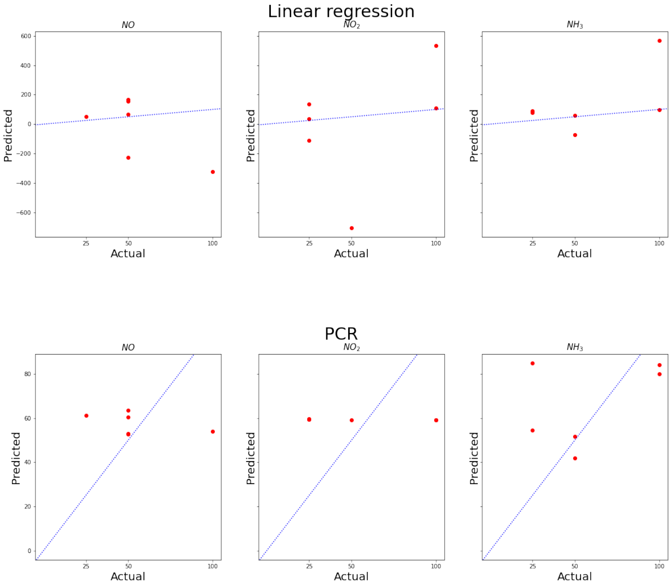
(Dummy) data

	NO2	NO	NH3	avg0	avg1	avg2	avg3	avg4	avg5	avg6	...	slope15	slope16	slope17	slope18	slope19	
0	50	100	25	-0.076323	0.915652	-0.970946	0.999202	-0.363800	-0.026400	0.603117	...	-11.274687	-10.370948	3.966974	-0.479340	-0.897105	-
1	100	25	100	-0.352834	0.854548	-0.934629	0.984386	-0.188594	0.027784	0.792582	...	-11.287665	-11.421536	1.860088	-2.393667	-3.398451	-
2	25	100	50	-0.141720	0.874015	-0.959047	0.999862	-0.352600	0.027594	0.561209	...	-4.754586	-11.580877	-3.583086	-3.218467	-1.802992	-
3	50	25	100	-0.249815	0.890990	-0.850049	1.123559	-0.242452	0.254415	0.645449	...	1.367344	-11.669267	-6.962770	2.391163	3.753269	
4	100	100	25	-0.188844	0.765447	-1.026246	0.960545	-0.511767	0.027451	0.372231	...	1.599057	-10.410155	-6.444129	3.060615	4.349158	

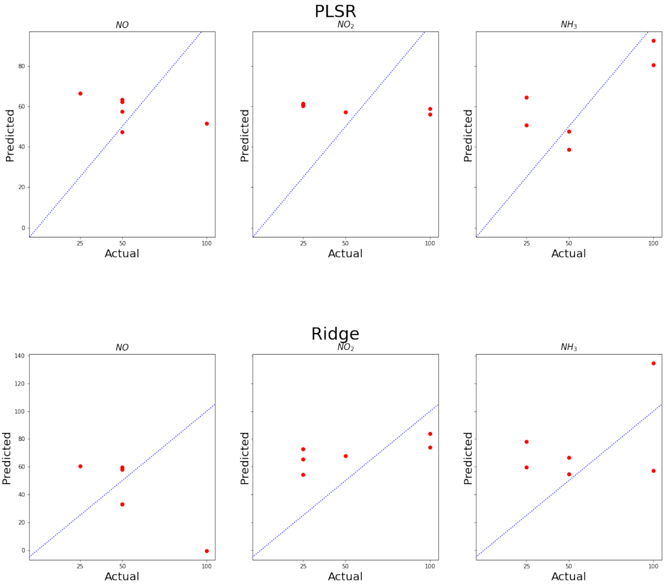
Methods

1. Linear Regression
2. Principal Component Regression
3. Partial Least Squares Regression
4. Ridge Regression
5. Some non-parametric regression - tbd

(Preliminary) Results



(Preliminary) Results



Real data will be much better!

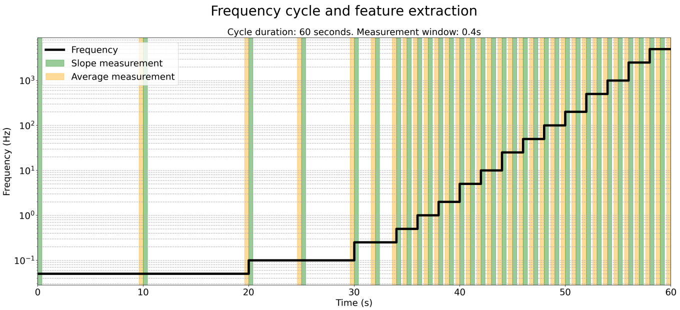
- More gas mixtures
- More frequencies
- More cycles
- Shape features directly measured

Real data will be much better!

Table: Data acquisition details

Parameter	Value
Factors (gases)	3
Levels (concentrations)	5
Frequencies	16
Features per frequency	4 (2 slopes and 2 averages)
Features per cycle	64
Number of cycles	5
Data points per mixture	320
Number of mixtures	125
Datapoints per experiment	40.000
Number of experiments	3
Total data points	120.000

Real data will be much better!



What is next

1. Apply methods to real data
2. Assess results
3. Define what is "good" in "good prediction levels"
4. Look into non-parametric alternatives
5. Keep writing!

Thank you!