

## Course 27411 Exercises 4/3 2013

### PLSR Exercise 0: (“Basic practice”)

Look at the “PLS quick start” tutorial (McDonalds meals data).

#### A way to get clear on “Raw” and “Weighted” regression coefficients:

1. Run MLR on these data – note the four beta-coefficients
2. Run PCR or PLS on these data WITHOUT standardisation (do NOT define any X- or Y-weights. Look at the regression coefficients plots – BOTH “Raw” and “Weighted” – using all 4 components.
3. Run PCR or PLS on these data WITH X-standardisation (but NO Y-weights). Look at the regression coefficients plots – BOTH “Raw” and “Weighted” – using all 4 components.
4. Run PCR or PLS on these data WITH X-standardisation (X-weights) AND Y-standardisation (Y-weights). Look at the regression coefficients plots – BOTH “Raw” and “Weighted” – using all 4 components. (The Y-weights are actually not necessary as there is only a single Y here)

For the comparisons in 3) and 4) also find the standard deviations for all the variables.

### PLSR Exercise 1(IMPORTANT: to be presented by Team 4 Monday 11/3)

Use the Pectin data to be downloaded from file sharing in CN. Setup and validate a PLS-model following the steps in Esbensen page 171 (and the Unscrambler tutorial). Compare with PCR! (Cf. Esbensen page 150-152) Remember to check for outliers. Are any spectral ranges more important than others to predict DE? How precise can DE be predicted by the models?

### PLSR Exercise 2 (OPTIONAL technical exercise)

To be found as PLSexercise2.pdf on the website.