

Exploratory data analysis – Tablets data

Goal: Can you predict the assay value (the active ingredients) in a pharmaceutical tablet?

Filename: tablets.lxf / tablets4matlab.mat

Number of measurements: 195 (calibration) and 460 (test set)

Xcal (195 x 650): NIR spectra of the milled barley samples.

Xval (460 x 650): NIR spectra of the milled barley samples (test set samples).

Ycal (195 x 1): Assay value; the active ingredients in a pharmaceutical tablet.

Description:

This data consists of a series of NIR diffuse transmission spectra of intact tablets, collected using a Multitab spectrometer (Foss NIRSystems, Silver Spring MD). Each spectrum covers the spectral range 600 – 1898 nm, in 2 nm increments. Each tablet has an assay value for its active ingredient, which is in the range of 152 to 239 mg, with a nominal value of 200 mg and estimated precision of +/- 1.3 mg.

The objective of this analysis is to develop and test an NIR method for determining the assay value of these tablets