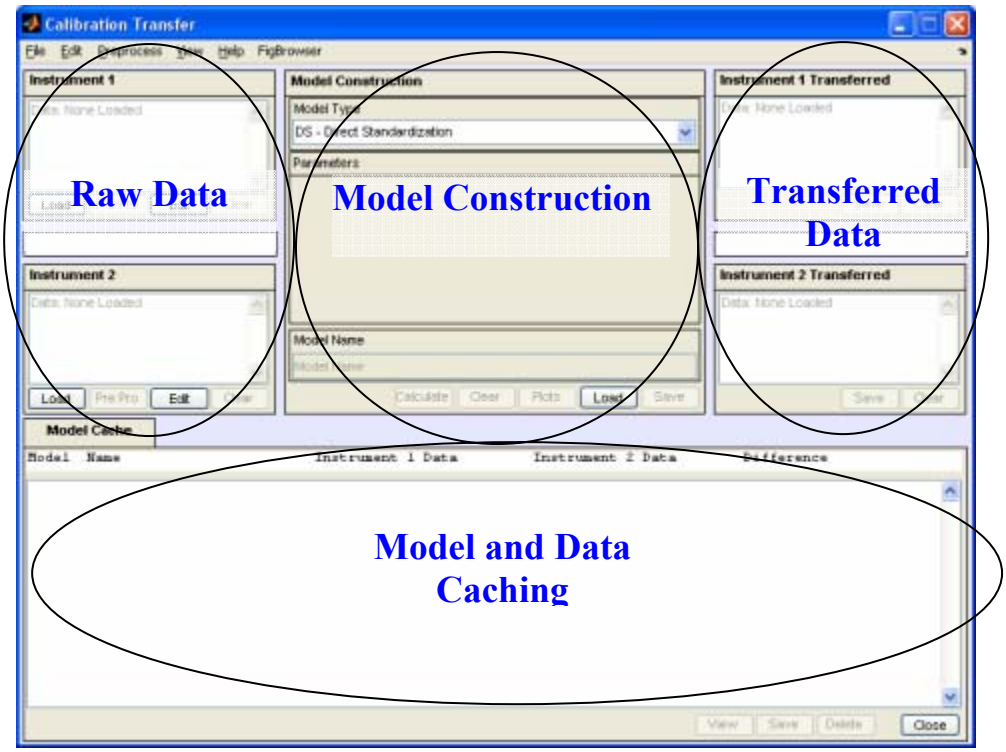
Getting Started with Calibration Transfer

About Calibration Transfer

Calibration transfer is useful when collecting data for similar samples on two or more different instruments (or on the same instrument at two or more different points in time). The goal is to create a model to compensate for differences in the instruments that can then be used to eliminate or reduce variation caused by the change in instrument. The following demonstration will show a simple example of creating a Piecewise Direct Standardization (PDS) model on some demonstration data included with PLS_Toolbox/Solo.

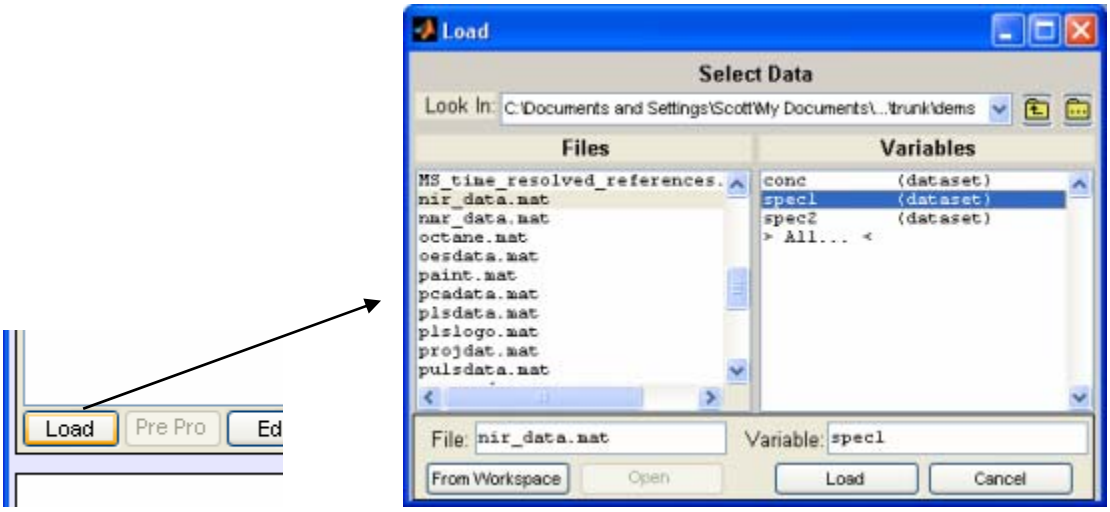
Working with the GUI

The easiest way to start the GUI is to click on its icon  in the **browse** interface. This will bring up the GUI:

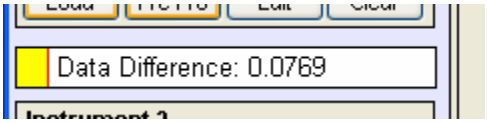


The general workflow in the GUI is from left to right. The first task when starting is to load raw data. This can be done with the **Load** button for Instrument 1 and 2. Go to the

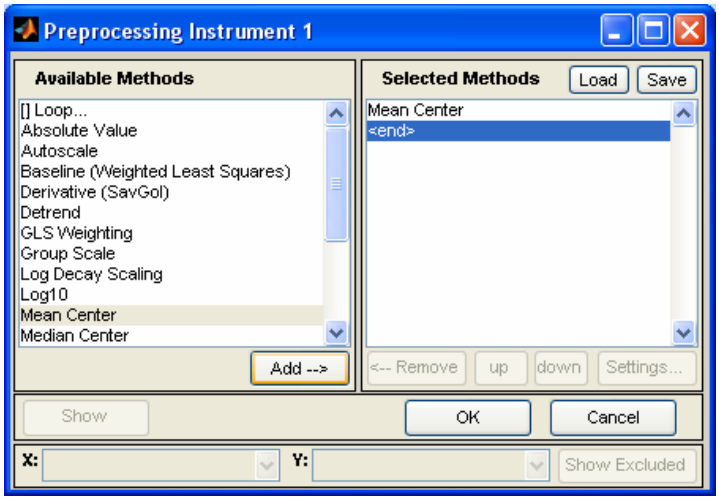
"dems" folder of PLS_Toolbox/Solo to find "nir_data.mat" and load 'spec1' and 'spec2' respectively:



Once both datasets are loaded, you'll notice the Diff Bar located between the Instrument 1/2 panels gives an indication of how different the two datasets are.

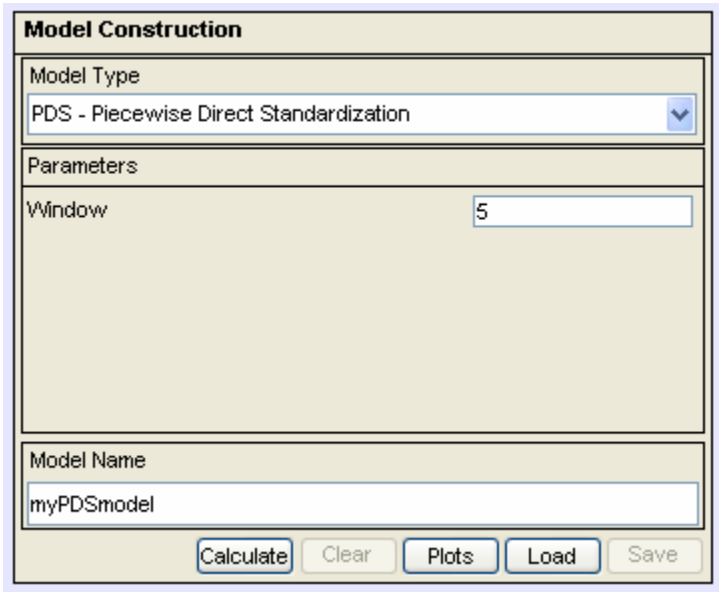


Next, select preprocessing for the data by clicking the **Pre Pro** button for Instrument 1 and add Mean Center. This data is quite "clean" so there's no need to consider more extensive preprocessing.



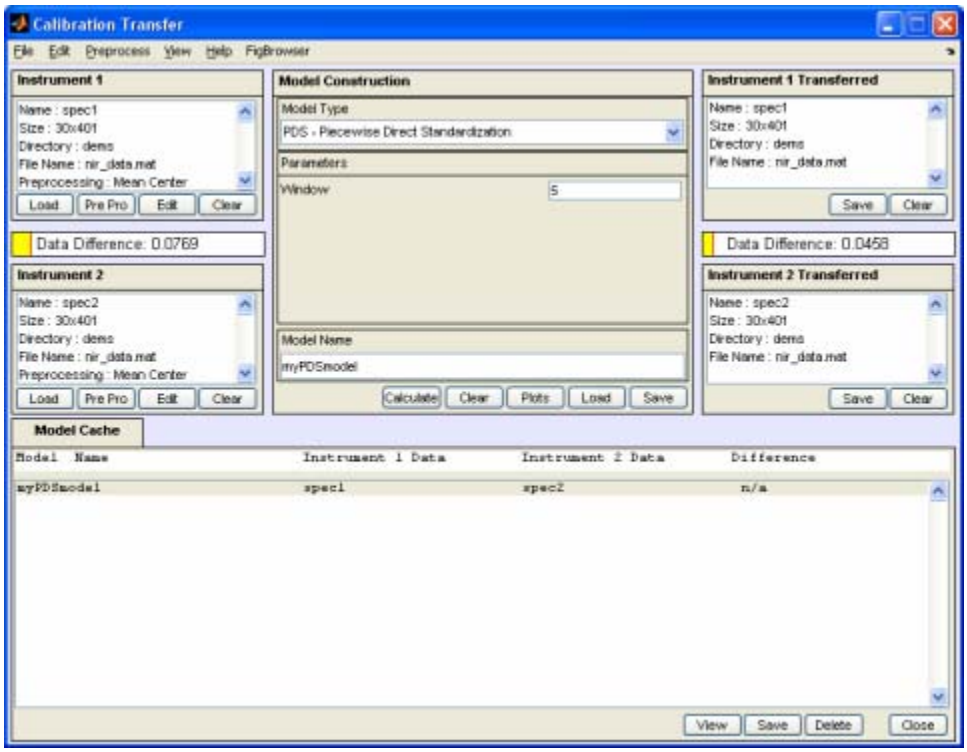
Notice that after Preprocessing has been selected for Instrument 1 it is automatically added to Instrument 2. In general it is recommended that the same preprocessing be used for each instrument but Instrument 2 preprocessing can be changed by clicking on its Pre Pro button.

Now that the data is ready, it's time to set up the model. In the Model Construction area select Piecewise Direct Standardization (PDS) from the **Model Type** dropdown menu. Notice that the **Window** parameter appeared in the **Parameters** panel with a default value already entered along with a unique default **Model Name**. Either of these values can be changed by directly editing the value in the text box. For this demonstration we'll try a value of 5 for the **Window** and change the **Model Name** to "myPDSmodel".



The **Plots** button is also enabled and will open a dialog box allowing you to select any available plots to open in PlotGUI. At this point it's possible to plot the raw datasets and the data difference. Click **Calculate** to create the model.

After a model has been calculated several things happen. The transferred data is added to its respective area, the model and all data (raw and transferred) are "cached" in the **Model Cache** panel, and additional plots are made available (via the **Plots** button).



From here you can explore the plots of your data and model, change parameters and create a new mode, or save your model and transferred data for further use. Clicking the **View** button will "reload" the selected cached model. Clicking the **Save** button will save the cached items (model, raw data, and transferred data) as a Matlab structure.

Applying a Model

If you have a need to automate model application this can be done using the 'caltransfer' function. The I/O looks similar to:

```
x2t = caltransfer(x2,transfermodel,options);
```

Where x2 is the Instrument 2 data and x2t is the Instrument 2 transferred data.