Linear Prediction in 1D

NMR SPECTROSCOPY

(Xwinnmr for PC, version 3.5)

on

DPX 200, DPX 300and DRX 500

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Log in and start xwinnmr. You should also know how to zero fill before using this manual.

Linear prediction is a mathematical procedure where a missing part of a FID can be constructed. Most linear prediction procedures are based on "singular value decomposition" (LPSVD), a digital processing technique which presupposes that the signal is composed of exponentially damped sinusoid curves. The information (frequencies, phases, amplitudes) in the part of the FID that does exist is used to calculate the part that is missing. The calculated part is then added to the end of the original real existing FID and the new combined "FID" is then used in the Fourier transform process. This is a much better way of processing half good data than simply zero filling the missing portion of the FID. Linear prediction can be used forward in time (the last part of the FID is missing) or backwards in time (the first part of the FID is missing). Linear prediction is extremely useful in 2D NMR as a way of reducing experiment time and/or improving the quality of already existing data sets. In our laboratory the linear prediction is routinely used in for 2D spectra acquired at the DRX 500 instrument for the following types of 2D spectra: GS-HMQC, GS-HMBC, GS-COSY, COSY, TOCSY, NOESY, ROESY, COLOC and XHCORR (By Dirk Petersen for you).

In 1D spectra linear prediction is extremely useful for spectra where the FID has not decayed to zero when the acquisition time (AQ) is over. This often happens with slow relaxing nuclei (quaternary carbons for instance) and for experiments with extremely wide sweep widths (wide ppm area). If you do not have time to use long acquisition time (AQ) and long D1 (= 10 seconds or more for the relaxation delay) between the pulses you can use linear prediction as an alternative to increase the signal to noise (S/N) ratio for small intensity carbon resonances. The digital resolution is also increased whenever linear prediction is used.

1. To do this exercise you need a dataset with an **aq** of approx. 0.4 s. This is too short to get full T1 relaxation and the FID is cut (truncated) before it is down to zero. Click on the appropriate button (FID). If you have your own dataset with a non decayed FID use that. You can also make one yourself by setting **aq** to 0.4 s in the usual 1H setup.

2. If you want to use an existing dataset you should do as follows: Type **wrd↵** this is the command for copying the dataset which is on screen to another disk (home or other place) for permanent storage and at the same time **change the ownership** of the files.

Enter target data set **NAME:**   **LINEARPRE↵**   (use your own expname)

Enter target data set **EXPNO:**   **1↵**   (use the expno seen in the top part of the xwinnmr window).

Enter target data set **PROCNO:**   **1↵**   (use the procno seen in the top part of the xwinnmr window).

Enter target disk unit **DU**:   **D:↵**   (if you want to, you can choose **M**: and the dataset will go to your home directory)

Enter target user name **USER**:   **uio user name↵** (your own uio user name)

3. If you copied a dataset from another user you must now use **search** to find the **LINEARPRE** dataset which is now owned by you, then **append** and **apply** it to the xwinnmr window and **efp** to Fourier transform it. You can not work properly with a dataset not owned or not processed by yourself. If the computer you are using does have another plotter attached than the one used under acquisition use **edo** (edit output) to select the new plotter. The data set does regretfully remember the plotter name connected to the computer used to acquire the spectrum.

4. **apk** the spectrum. Expand a sensible part of the spectrum on the screen and look at the form of the spectrum, especially at the baseline.

5. Type **eda** to see acquisition parameters. Look for the parameter **TD**. TD is approximately 8k eda parameters can only be changed before the experiments starts.

6. Type **edp** to see processing parameters. Look for the parameter **SI** (size). SI is 4k. No zero filling is performed or other tricks is performed on this dataset.(When SI=TD/2 no zero filling has taken place.) If you want to simply zero fill use the manual for that purpose.

7. Use **edc** to increase the **procno** (processing numbers) to **2** for the following. Change **SI**, either by typing SI in the xwinnmr window or by changing SI in the edp window. Select SI to 32 k to make "space" for the rest of the missing FID. An 8 fold "elongation" of the FID is possible with increasing SI from 4k to 32k.

8. Click on **ME_mod** in the EDP window. A list of options comes up, LPfr (forward real), LPfc (forward complex), LPbr (backwards real), LPbc (backwards complex). Since we are adding the missing end of the FID LPfr and LPfc can be used. Select **LPfc** to use both the imaginary (**Im**) and real part (**Re**) of the FID in the calculations.

9. Find **NCOEF** (number of coefficients) in the edp window. The number to be put in for **NCOEF** must be larger than the number of resonances in the spectrum. In 1D 1H spectra this is often a high number. Select 256 for this experiment. Then try with higher and lower numbers to see the effects.

10. Do an **efp** for each individual **NCOEF** and/or TD change and watch the result on an expanded part of the spectrum on the screen. Plot if you like.

11. A **NCOEF** value of **512** and a **LB** (line broadening) of **0.3 Hz** with the **EM** (exponential multiplication **WDW** (window function) gives a good result with **SI = 32k**.