

## Lecture 2: Introduction to Digital Signal Processing

Fourier transform spectroscopy, particularly NMR and ESR, can draw upon a large family of DSP techniques, which can often transform a noisy bump into a collection of beautifully resolved signals, or salvage a dataset that standard spectral processing software would deem completely corrupted. Before we start theorising about spin systems, it seems wise to get our datasets into the best shape possible.

### Sampling rate and digital resolution

*Sampling rate* is the number of points per unit time used to represent a time domain signal in a discrete form. Modern spectrometers always digitize the time domain signals at the highest rate their hardware is capable of (usually between 1 MHz and 1 GHz). The signal is then *downsampled* to the desired sampling rate by averaging nearby points – meaning that low sampling rates tend to yield a better signal-to-noise ratio.

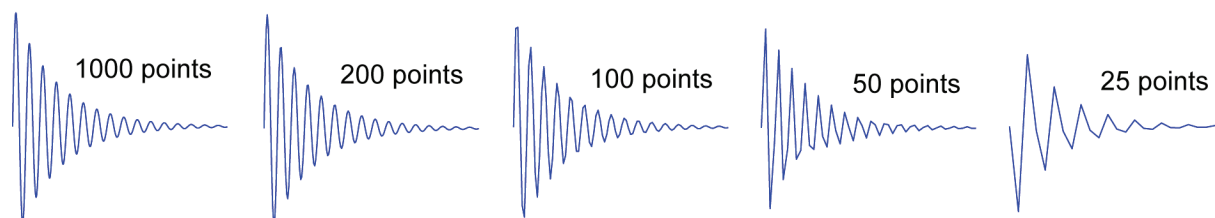


Figure 1. A decaying oscillation digitized at different sampling rates. Note the frequency distortion in the rightmost trace.

*Nyquist condition*: perfect reconstruction of the time domain signal from the samples is possible if and only if the sampling rate exceeds two points per period of the fastest oscillation found in the signal. For example, correct digitization of an NMR spectrum located between  $-7$  kHz and  $15$  kHz requires at least  $30$  kHz sampling rate.

In the NMR context, the consequences of *undersampling* a free induction decay are quite severe – the high-frequency signals end up in the wrong place. This phenomenon is known as *aliasing*.

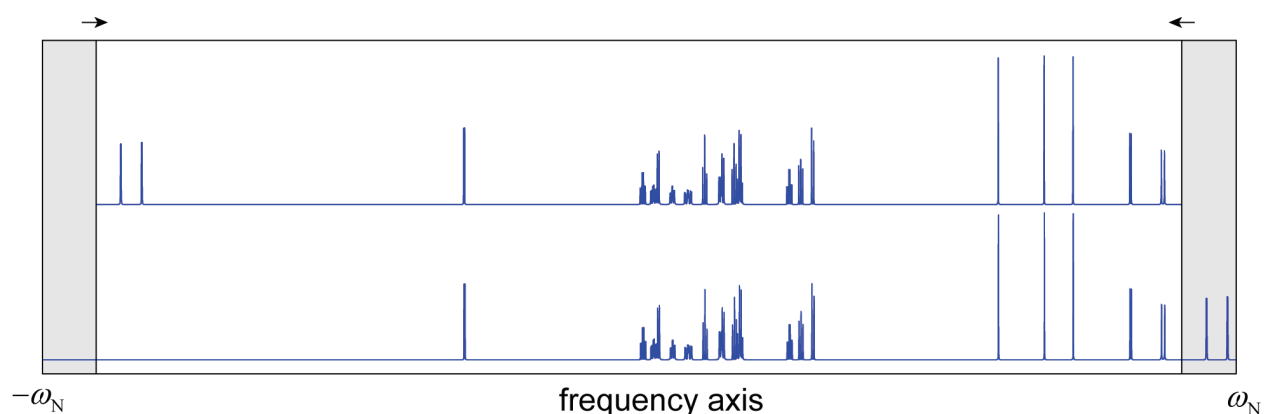


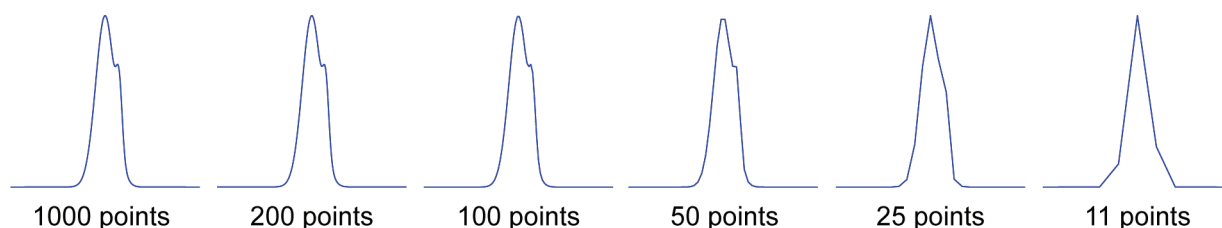
Figure 2. Frequency distortion caused by sub-Nyquist sampling. Note the two methyl peaks folding over the spectrum edge.

The DSP software in modern spectrometers would often cause such signals to be suppressed rather than aliased, in which case they are lost completely. If the free induction decay is *oversampled*, the serious practical consequence is increased noise level.

Conclusion: *the best sampling possible in almost any experiment is the Nyquist sampling.*

*Spin Dynamics, Lecture 2 – Dr Ilya Kuprov, University of Oxford, 2011.*

*Digital resolution* is the number of points per unit frequency used to represent a frequency domain signal in a discrete form.



**Figure 3.** A pair of overlapping peaks digitized with different resolution. Note the gradual loss of detail from left to right.

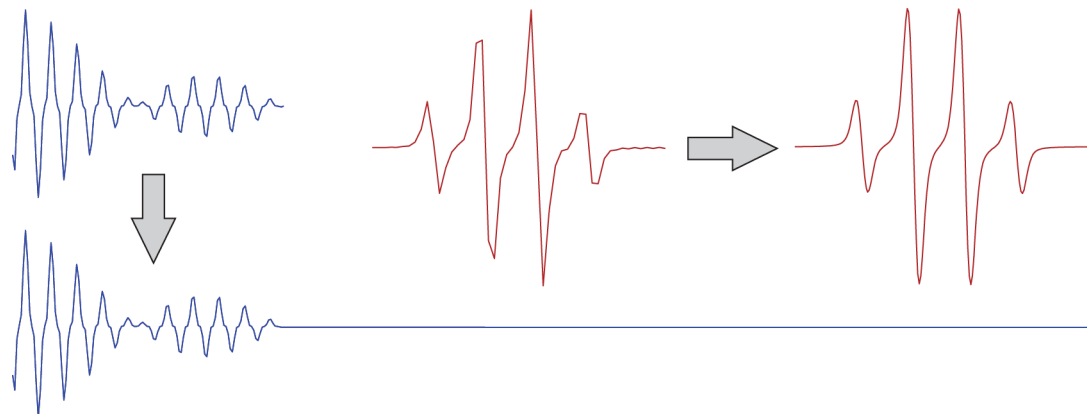
The accuracy of spectral quantification (peak picking, integration, *etc.*) is directly determined by the digital resolution available.

### Harmonic interpolation and zerofilling

Padding the time-domain signal with zeros amounts to harmonic interpolation in the frequency domain:

$$\begin{aligned} \text{original spectrum: } F_n &= \frac{1}{N\sqrt{2\pi}} \sum_{k=0}^{N-1} f_k e^{\frac{-ikn}{N}} \\ \text{after zerofilling: } F_n &= \frac{1}{2N\sqrt{2\pi}} \sum_{k=0}^{2N-1} f_k e^{\frac{-ikn}{2N}} = \frac{1}{2N\sqrt{2\pi}} \sum_{k=0}^{N-1} f_k e^{\frac{-ikn}{2N}} \end{aligned} \quad (1)$$

After zerofilling, the frequency sampling step (digital resolution) became finer, resulting in a more accurate quantification. Sharp signals often require zerofilling to be integrated accurately, particularly in multi-dimensional experiments.



**Figure 4.** Improvement in digital resolution of an ESR signal resulting from time-domain zerofilling.

### Band-pass filters

Imagine a time-domain chemical kinetics experiment with a large amount of signal integration noise. The frequency of the signal we are interested in is clearly much lower than that of the noise. Is it possible to remove the noise? The following transformation:

$$f^*(t) = F_- \left\{ M(\omega) F_+ \left\{ f(t) \right\} \right\}, \quad M(\omega) = \begin{cases} 0 & \text{for unwanted } \omega \\ 1 & \text{for wanted } \omega \end{cases} \quad (2)$$

is called a *band-pass filter* – it eliminates the undesired frequencies from the time-domain signal. The selection function  $M(\omega)$  is called a *magnitude transfer function*.

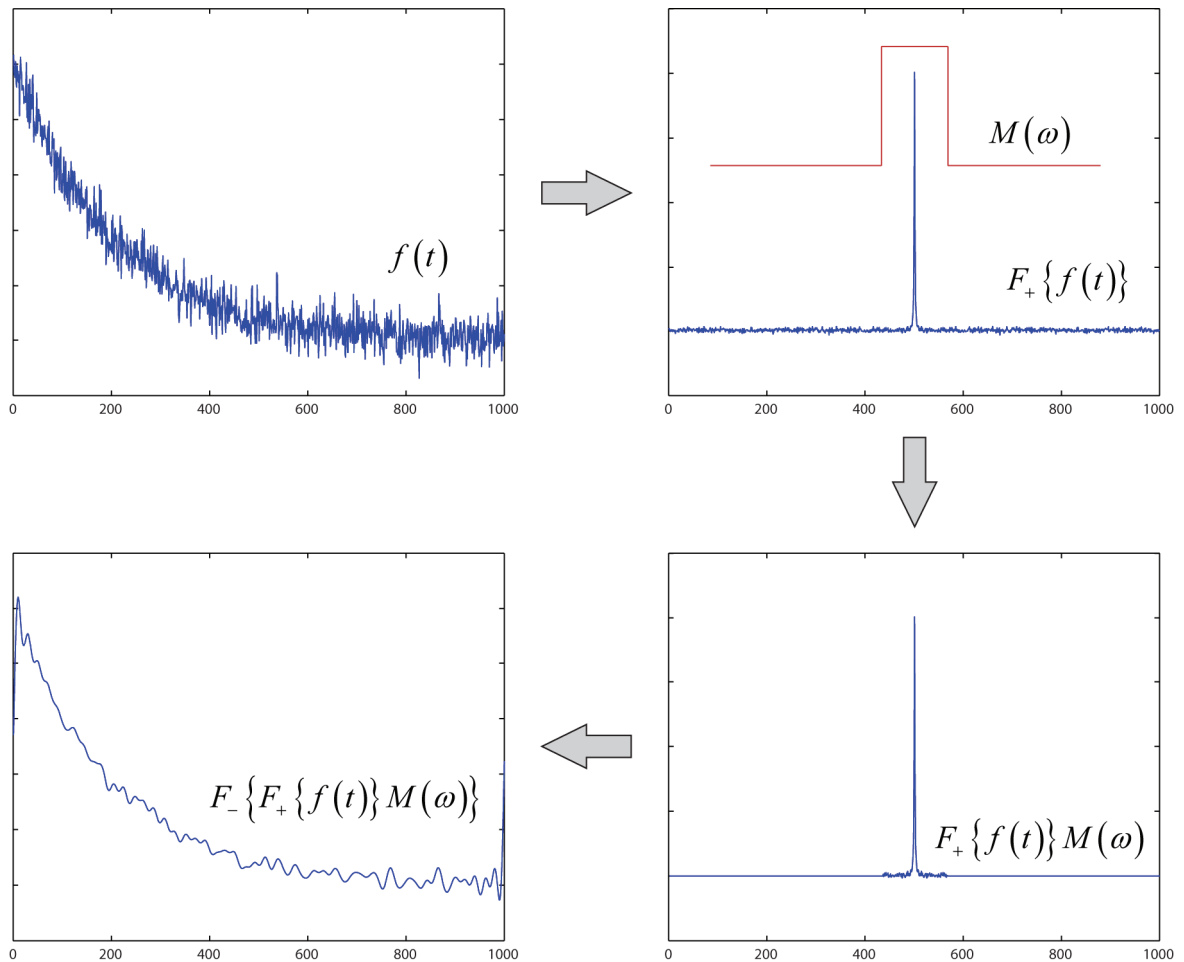


Figure 5. Band-pass filter applied to a noisy chemical kinetics decay trace.

- **Exercise:** find a way to prevent the edges of the filtered signal from jumping to the midpoint between the start and the end signal levels.

Despite their complicated appearance, the band-pass filters are linear, because the application of a discrete Fourier transform may be represented as an action by a matrix on a vector of digitized data values:

$$\left[ F_+ \{ f(t) \} \right]_n = \frac{1}{N\sqrt{2\pi}} \sum_{k=0}^{N-1} f_k e^{\frac{-ikn}{N}} = \sum_k A_{nk} f_k, \quad A_{nk} = \frac{1}{N\sqrt{2\pi}} e^{\frac{-ikn}{N}} \quad (3)$$

Magnitude transfer function zeroing unwanted frequencies may be represented by a diagonal matrix. Therefore,  $f^*(t) = \hat{A}^{-1} \hat{M} \hat{A} f(t)$ , which is linear in  $f(t)$ .

### Convolution filters (aka window functions)

Let us try to smooth our frequency domain signal using a local averaging filter to reduce the noise at the cost of some signal broadening. The filter (Figure 6) collects the data points from a certain interval in the original signal, applies Lorentzian weighting, calculates the average and places one point into the resulting “filtered” signal. Mathematically speaking, this is a convolution operation:

$$f^*(\omega) = \int_{-\infty}^{\infty} f(\nu) g(\omega - \nu) d\nu \quad \text{OR} \quad f^*(\omega) = f(\omega) * g(\omega) \quad (4)$$

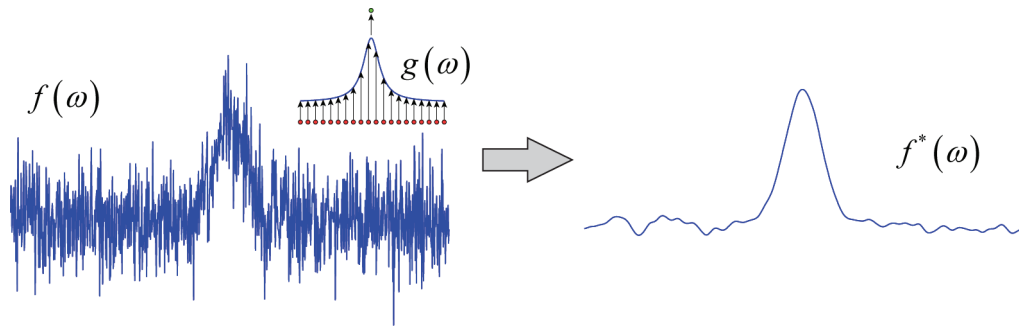


Figure 6. The result of the application of a Lorentzian local averaging filter to a noisy peak.

We do know however (Lecture 1) that we could also perform this procedure by computing inverse Fourier transforms of  $f(\omega)$  and  $g(\omega)$ , multiplying them together and performing a forward Fourier transform on the result (convolution in the frequency domain is equivalent to multiplication in the time domain). The inverse Fourier transform of  $f(\omega)$  is the free induction decay, and the inverse FT of a Lorentzian function is...

$$\int_{-\infty}^{\infty} \frac{1}{1+\omega^2} e^{i\omega t} d\omega = e^{-t} \quad (5)$$

...an exponential function. Therefore, the application of a Lorentzian smoothing convolution filter in the frequency domain is equivalent to exponential apodization in the time domain.

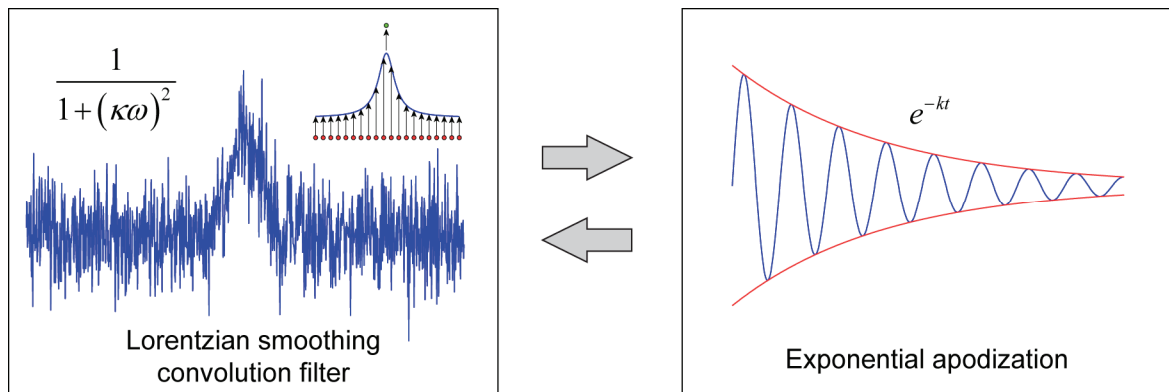


Figure 7. Illustration of the equivalence of Lorentzian convolution filtering in the frequency domain and exponential apodization in the time domain.

□ **Exercise:** demonstrate that any form of time domain apodization is equivalent to a convolution filter in the frequency domain. Show that the filter need not be a smoothing filter and suggest an apodization function that would perform signal sharpening.

□ **Exercise:** derive an equation relating the broadening parameter  $\kappa$  to the decay rate parameter  $k$ .

For illustration purposes, let us calculate the Fourier transform of a pure (without any sinusoidal modulation) exponential decay:

$$f(t) = e^{-kt}, \quad F(\omega) = \int_0^{\infty} e^{-kt} e^{-i\omega t} dt = \dots = \frac{1}{k+i\omega} = \left( \frac{k}{k^2 + \omega^2} \right) - i \left( \frac{\omega}{k^2 + \omega^2} \right) \quad (6)$$

The real part of the result is the familiar Lorentzian curve. The imaginary part is known as the *dispersion curve*. So the Fourier transform of an exponential yields a standard NMR line shape at zero frequency.

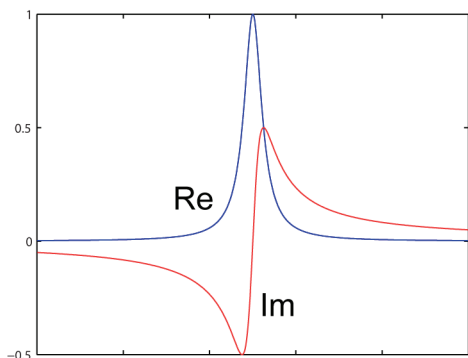


Figure 8. The real and the imaginary part of the Fourier transform of an exponential decay.

Now let us compute a Fourier transform of a pure non-decaying oscillation  $f(t) = e^{-i\omega_0 t}$  with a frequency  $\omega_0$ :

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{-i\omega_0 t} e^{-i\omega t} dt = \dots = \delta(\omega - \omega_0) \quad (7)$$

The result is a delta-function (an infinitely sharp peak) at the frequency of the oscillation. So, in the absence of decay, all lines in the Fourier transform are infinitely sharp – it is the decay of the time domain signal that gives frequency domain lines their shape.

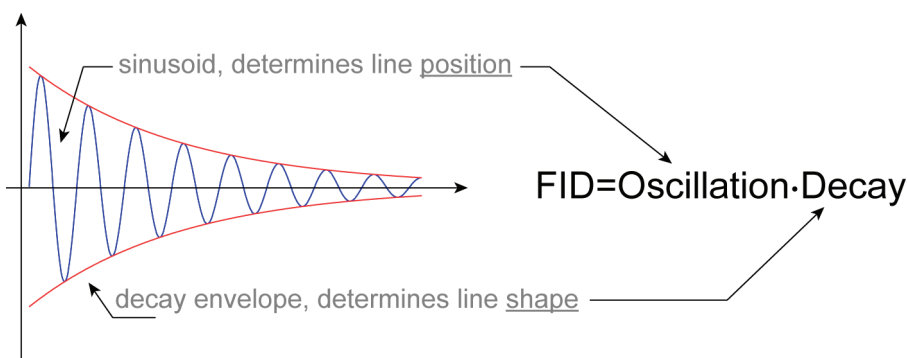


Figure 9. Schematic illustration of the factors affecting position and shape of a spectral line.

The free induction decay envelope is relatively easy to manipulate – we could divide one envelope away and multiply another one in. There is a large number of case-specific apodization functions.

- exponential weighting: aka soft low-pass filter – accelerates the decay and makes signals broader, but reduces noise.
- Lorentz-Gaussian transformation: replaces  $\exp(-kt)$  envelope with  $\exp(-kt^2)$ . This makes signals narrower (Gaussian curve has shorter wings), but enhances the noise.
- etc, etc (see NMR textbooks)

□ **Exercise:** demonstrate that the Fourier transform of a Gaussian function is another Gaussian function.

The window function choice is often determined by the signal-to-noise budget. Some S/N can be traded for some resolution and *vice versa*.

### Reference deconvolution

In a poorly shimmed NMR magnet, all spectral lines are distorted in *precisely* the same way:

$$S_{\text{exp}}(\omega) = \int_{-\infty}^{\infty} S_{\text{id}}(\omega') R(\omega - \omega') d\omega' \quad (8)$$

where  $S_{\text{exp}}(\omega)$  is the distorted “experimental” spectrum,  $S_{\text{id}}(\omega)$  is the “ideal” spectrum that we would like to recover and  $R(\omega)$  is the “distortion” – the shape that a perfectly sharp signal would have acquired in the current magnet. We know that the time domain version of Equation (8) is:

$$S_{\text{exp}}(t) = S_{\text{id}}(t)R(t) \quad (9)$$

from which we could easily recover  $S_{\text{id}}(t)$ , if we knew the envelope function of the distortion  $R(t)$ . This is where the “reference” comes in – if we have an *a priori* standalone signal (e.g. TMS)  $s(\omega - \omega_0)$ , then shifting it to zero and performing an inverse Fourier transform recovers the envelope:

$$R(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} s(\omega) e^{i\omega t} d\omega \quad (10)$$

If the desired FID envelope (e.g. an exponential decay) is  $P(t)$ , then the following transformation gets rid of the poor shimming:

$$S_{\text{id}}(\omega) = F_+ \left\{ F_- \left\{ S_{\text{exp}}(\omega) \right\} F_- \left\{ s(\omega) \right\}^{-1} P(t) \right\} \quad (11)$$

It should be noted that the signal-to-noise ratio cost of reference deconvolution is often huge.

An interesting philosophical question is about the extent to which such filtering may be applied to experimental data – as of 2005, strict guidelines are in place for digital image manipulation, for example. The community consensus at the moment is that *linear* signal processing can be applied freely, whereas *non-linear* methods (some of which we shall see in Lecture 3) must be declared and detailed in full.

### SVD de-noising of data arrays

The singular value decomposition (SVD) of a complex matrix  $M$  is defined as follows:

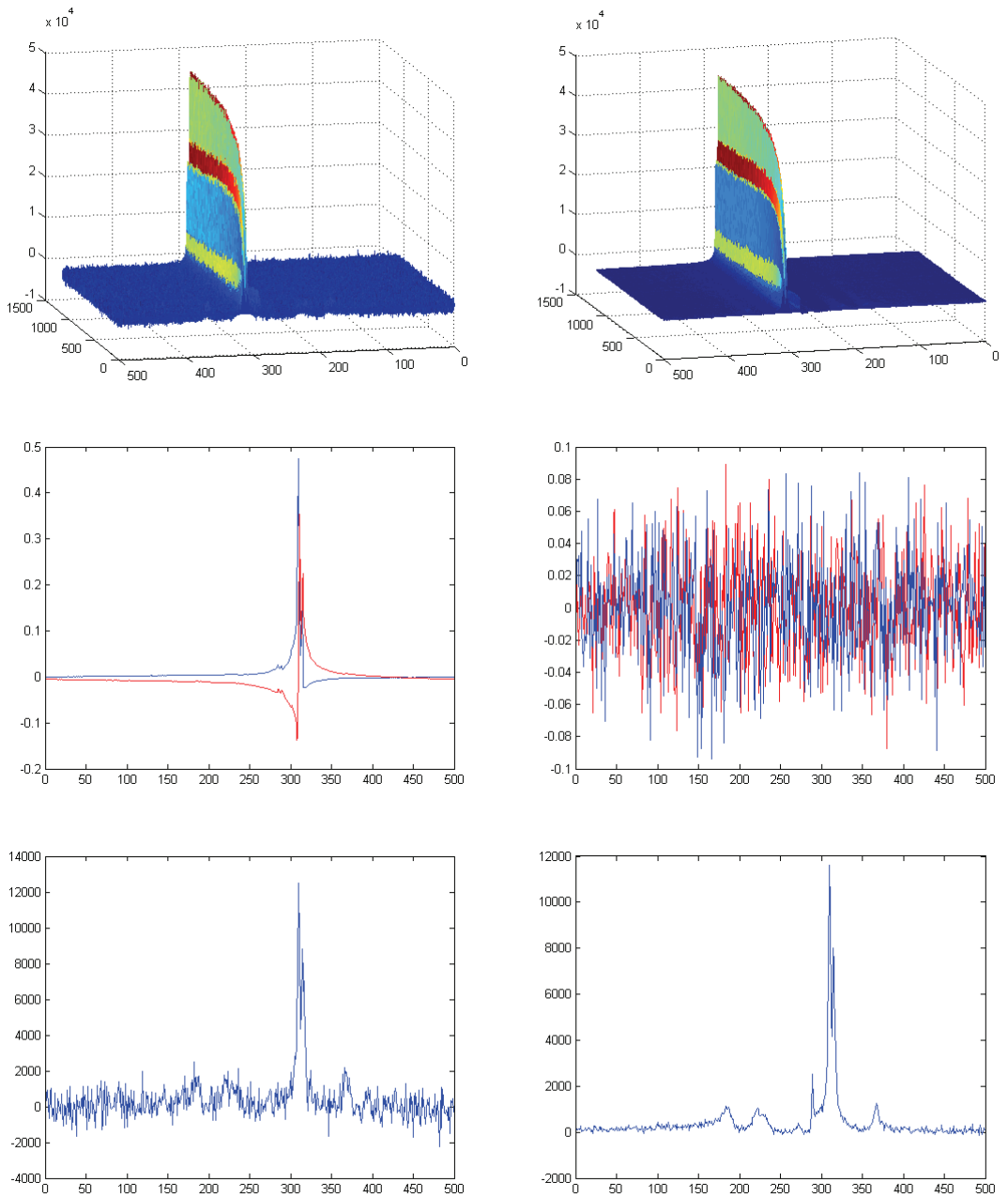
$$M = U \Sigma V^\dagger \quad (12)$$

where  $U = \{\vec{u}_1, \dots, \vec{u}_p\}$  is a complex matrix of left singular vectors,  $V = \{\vec{v}_1, \dots, \vec{v}_q\}$  is a complex matrix of right singular vectors and  $\Sigma$  is a  $p \times q$  diagonal matrix with positive real singular values  $\{\sigma_1, \dots, \sigma_n\}$  along the diagonal. All arrays are sorted in such a way as to put the singular values in decreasing order. A rank- $k$  approximation to the matrix  $M$  is then defined as:

$$M^{(k)} = \sum_{i=1}^k \sigma_i (\vec{u}_i \otimes \vec{v}_i^\dagger), \quad \|M - M^{(k)}\| = \sum_{i=k+1}^n \sigma_i^2 \quad (13)$$

where  $\|\cdot\|$  is a Frobenius norm. That is, to a good approximation, the contributions to Equation (12) from near-zero singular values may be dropped. In practice, the singular vectors associated with small singular values are often filled with random noise and the procedure improves the signal-to-noise ratio. Some components can correspond to undesired signals (such as the solvent) and may likewise be dropped.

The SVD de-noising recipe is therefore quite simple: run the SVD on the data matrix, drop the singular values and singular vectors associated with random noise (they correspond to the smallest singular values, the threshold is left to your discretion), re-construct the data using the remaining singular values and Equation (12). The result can be quite dramatic – this is illustrated below with a  $^{19}\text{F}$  NMR spectrum of an unfolding protein: (upper left) initial data array, (upper right) final data array, (middle left) real and imaginary part of the largest left singular vector, (middle right) real and imaginary part of the smallest singular vector, (lower left) one of the spectra from the original data array, (lower right) one of the spectra from the final data array.



**Figure 10.** An illustration to SVD de-noising of NMR data – see text for description.