Exploring Digital Signals and Noise in Instrumental Analysis©

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Goals: The purpose of this document is to allow the student to gain a familiarity with the concepts of signal-to-noise ratios and to explore the advantages of ensemble averaging and digital filtering analytical signals. The student is led through a series of individual exercises that culminate in a capstone experience where they simultaneously apply all of the concepts.

Prerequisites: This Mathcad document is designed to support the digital signals portion of a Junior or Senior level instrumental analysis course. Students should have a familiarity with the concept of random noise. While it is not necessary, it would be desirable if the student had an understanding of Fourier transforms [1]. A description of all of these subjects can be found in most analytical chemistry or instrumental analysis texts [2,3,4].

Requirements: This document was written using MathCad 8. It was successfully tested using MathCad versions 6 and 7. The version at the JCE web site requires Mathcad 6 of higher.

Performance Objectives:

After completing this document, you should ...

1. be able to determine the signal-to-noise ratio of an analytical signal.
2. be able to explain the relationship between ensemble averaging and signal-to-noise ratio.
3. be able to describe the effects of analog and digital filtering on an analytical signal.
4. be able to explain the relationship between the filter bandwidth, signal-to-noise ratio, and signal smoothing.
5. be able to explain the benefits of combining ensemble averaging with digital filtering of an analytical signal.

Noise

There are two components to every instrumental measurement. One is necessarily the analytical signal or quantity we are interested in measuring. The other is any unwanted component to the signal, which we classify as "noise." We can further classify noise into two general categories. One type of noise is called *systematic* or *instrumental* noise. This noise arises from the environment, the instrument, or the particular technique itself. This noise can usually be correlated as a function of time or with a particular event. Examples of this type of noise are AC current, mechanical vibrations, or temperature instability. Instrumental noise can usually be identified and mitigated with active measures. We will not be discussing this type of noise within the context of this document.

The other type of noise is essentially random and is always present. Random noise is independent of the analytical signal strength. Since it is statistical in origin, it cannot be completely eliminated; only minimized. Not only does the noise level in the analytical signal determine the precision of the measurement, but it ultimately establishes the smallest analytical signal that can be quantitatively measured with confidence.

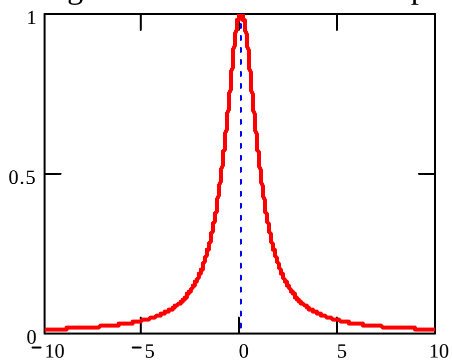
For most measurements, the random noise level is constant and independent of the strength of the analytical signal. So as the strength of an analytical signal decreases, the deleterious effects of noise on the measured signal become greater. The signal-to-noise ratio is a quantitative figure of merit used to determine the quality of a measurement and is given by:

$$\frac{S}{N} = \frac{\mathrm{mean}(\mathrm{Signal})}{\mathrm{stdev}(\mathrm{Noise})} .$$

You should notice that the signal-to-noise ratio is nothing but the inverse of the relative standard deviation of the measured signal.[5]

We are often interested in simultaneously measuring many analytical signals within a given laboratory experiment. An example of this would be an infrared or nuclear magnetic resonance (NMR) spectrum. Since most analytical signals themselves represent a statistical distribution around a given value, we will assume the best estimate of the true signal strength is the height of the band at its center (Figure 1). In the purest sense, we should define a signal-to-noise ratio for each measured signal. However, the best possible signal-to-noise ratio for a given measurement is obtained by using the strongest observed signal strength. We will follow this practice throughout the remainder of this document.

Figure 1: Lorentzian Band Shape



Lorentzian band shape showing the distribution of signal strength about a mean value.

Exercise 1: Shown in Figure 2 is a simulated analytical signal. It consists of a series of Lorentzian bands which could represent a typical signal recorded in any number of spectroscopic measurements.

1. Adjust the noise level (N1) and determine the point where the smallest signal is no longer distinguishable.
2. What is the signal-to-noise value at this point.
3. When calculating the signal-to-noise ratio, how was the amount of noise determined? Does it matter where in the array we measure the noise to make this determination?

Some Necessary Equations and Parameters:

$L \equiv 1024$ $x := 0..L-1$ **Data span and increment**

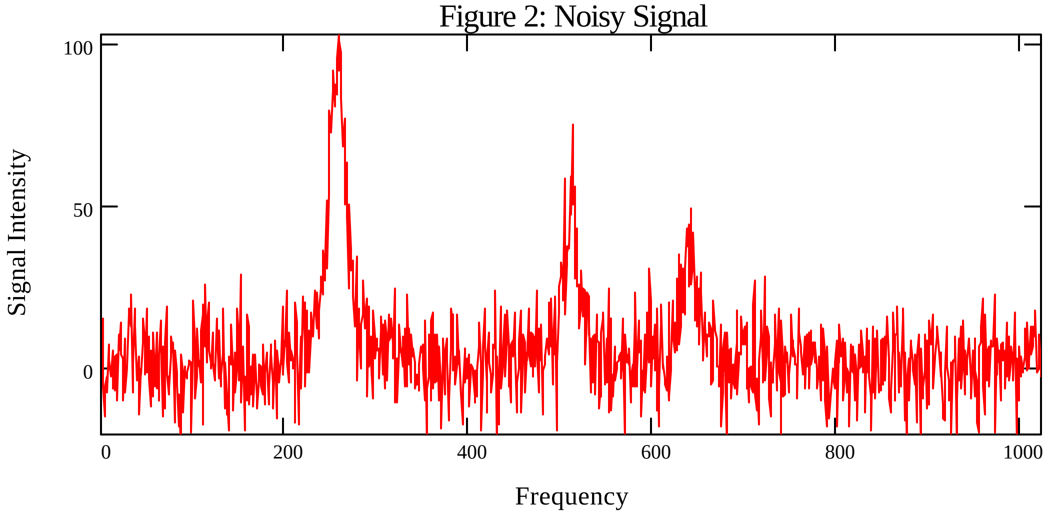
$A \equiv 100$ $W \equiv 20$ **Signal amplitude and bandwidth**

$$signal_x := \frac{A}{1+\frac{4\cdot\left(x-\frac{L}{4}\right)^2}{W^2}} + \frac{\frac{A}{2}}{1+\frac{4\cdot\left(x-2\cdot\frac{L}{4}\right)^2}{W^2}} + \frac{\frac{A}{3}}{1+\frac{4\cdot\left(x-2.5\cdot\frac{L}{4}\right)^2}{W^2}}$$ **Lorentzian signal**

$noise1 := rnorm(L, 0, N1)$ **Array of Random Noise**

$signal1_x := signal_x + noise1_x$ **Noisy Signal**

Figure 2: Noisy Signal



$N1 \equiv 10$ **Noise level**

$i := 0..199$ $noise\_sample_i := signal1_{800+i}$ **Sample of noisy signal**

$Signal := max(signal)$ $Noise := stdev(noise1)$

$\frac{Signal}{Noise} = 10.305$ **Signal-to-noise ratio**

Ensemble Averaging

Many types of laboratory instruments acquire multiple signals simultaneously as a data array. These multichannel signals have a highly reproducible and precise spacing between each data point. Multichannel measurements are important because they reduce the time required to collect the data, often called the "multiplex" advantage. They also allow successive arrays of data to be added together, then averaged. The process of averaging successive arrays of a signal is called *coaddition*. This process works in the following manner. As we add the arrays together the strength of the true signal remains constant. If we add *n* number of signal arrays together the sum is just $n \cdot \text{Signal}$. Since our measured signal contains noise, it too will get added along with the signal. However, because the noise is random it increases not as *n,* but as the square root of *n*.($\sqrt{n} \cdot \text{Noise}$) The expression for the signal-to-noise ratio then becomes:

$$\frac{S}{N} = \frac{n \cdot I_s}{\sqrt{n} \cdot I_n} = \sqrt{n} \cdot \frac{I_s}{I_n} \ ,$$

where I_s is the intensity of the signal and I_n is the intensity of the noise.

Exercise 2: Using Figure 3 below, investigate this relationship for yourself. In order to determine the signal-to-noise ratio of the averaged signal, we are going to sample the noise in a region where there is no true signal present.

1. Adjust the noise level (N2) to 10. Set the number of coadditions to 1. What is the signal-to-noise ratio? How many coadditions are required to make the signal-to-noise ratio equal to 50? Does the $\sqrt{n}$ relationship hold?
2. Reset the number of coadditions to 1. Adjust the noise to a point where the smallest signal is no longer recognizable. How many coadditions are required to obtain a signal-to-noise ratio of 50?
3. If each separate data array requires 10 seconds to acquire, how long will it take to obtain a signal-to-noise ratio of 1000 when coadding?
4. When acquiring very small signals, what becomes the limiting factor in obtaining measurements with acceptable signal-to-noise ratios?

$p := 0 .. EA2 - 1$ **Index variable**

$signal2_{p,x} := signal_x + rnorm(L, 0, N2)_x$ **Matrix of noisy signal arrays**

$$EA\_signal2_x := \frac{\sum_{p=0}^{EA2-1} signal2_{p,x}}{EA2}$$

Ensemble averaged signal array

$noise\_sample_i := signal2_{0,800+i}$ **Sample of noisy signal**

$eanoise\_sample_i := EA\_signal2_{800+i}$ **Sample of noise in ensemble averaged signal**

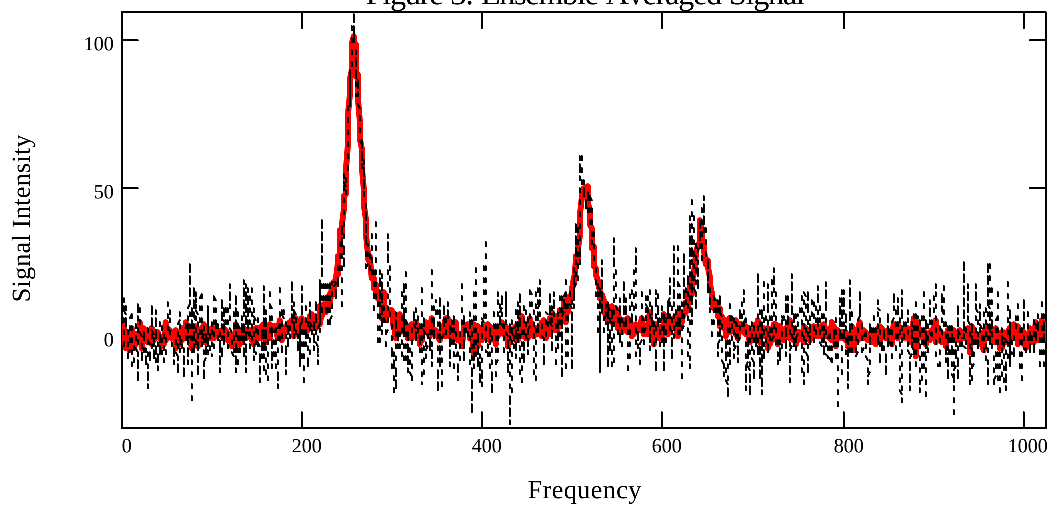
$Signal := max(signal2)$

$Noise := stdev(noise\_sample)$

$EA\_Signal := max(EA\_signal2)$

$EA\_Noise := stdev(eanoise\_sample)$

Figure 3: Ensemble Averaged Signal



$N2 \equiv 10$ **Noise level**

$EA2 \equiv 25$ **Number of coadditions**

$\frac{Signal}{Noise} = 12.473$ **Signal-to-noise ratio in original signal**

$\frac{EA\_Signal}{EA\_Noise} = 52.135$ **Signal-to-noise ratio in Ensemble Averaged signal**

Analog and Digital Filtering

Signal conditioning is an active means of improving the signal-to-noise ratio in a measurement. This technique often involves the use of analog filters to restrict certain frequencies from being measured. A low pass filter discriminates against high frequency signals. Since most analytical signals are either DC or slowly varying signals, these analog filters can remove the high frequency noise associated with electronic amplifiers. White or random noise has roughly an equal intensity across all frequencies. They can also help eliminate thermal and shot noise that occur in the high frequency region. When we apply a low pass filter we retain the signals at DC and low frequency and exclude the noise at high frequency. However, noise at low frequencies are passed by the filter the same as the signal. That is why we can never completely exclude noise by filtering. Analog filters have the advantages of being able to operate in real time and require no additional calculations to improve the signal-to-noise ratio. However, they offer only limited control over the measured signal. If the filter is not properly matched, it can also cause phase shifts or unnecessary band broadening to the signal.

Exercise 3: Shown below is a diagram of a typical low pass filter. The input voltage at, V_i, is the analytical signal and the output, V_o, across the capacitor is taken as the filtered signal.

1. Change the Resistance, R, or Capacitance, C, and look at the graphical output. Which provides the greatest control over the width of the pass band, resistance or capacitance?
2. What combinations of resistance and capacitance are necessary to restrict the signal frequencies between DC and 5 Hz?
3. What is the time constant and what information does it provide about the performance of the low pass filter?

$k := 1 .. 10000$ **Index variable**

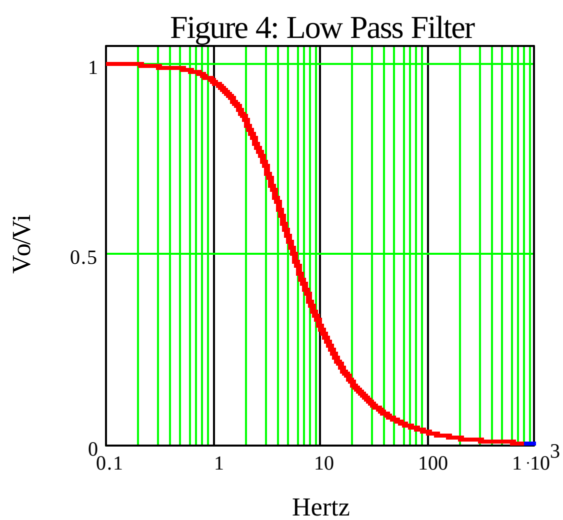
$f_k := \frac{k}{10} \cdot Hz$ **Frequency range**

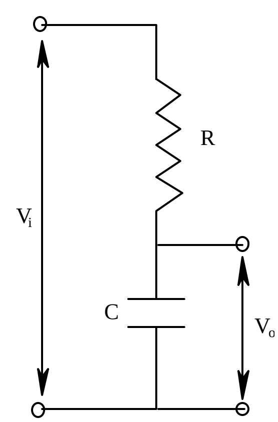
$$LP_k := \frac{1}{2 \cdot \pi \cdot f_k \cdot C \cdot \sqrt{R^2 + \left(\frac{1}{2 \cdot \pi \cdot f_k \cdot C}\right)^2}}$$

The ratio of the output voltage to the input voltage defines the behavior of the low pass filter.

$C \equiv .1 \cdot \mu F$ $R \equiv 500 \cdot k\Omega$ $\tau := R \cdot C$ $\tau = 0.05 \ s$ $\frac{1}{\tau} = 20 \ Hz$

Capacitance **Resistance** **Time Constant**





Digital filtering is a mathematical tool that produces the same smoothing effect on signals as analog filtering with a low pass filter. Digital filtering offers advantages over analog filtering in that it provides greater control on the output and it does not cause any phase shifts in the resulting signal. Because digital filtering is computationally based, the technique also allows for the use of alternative filters to generate more desirable line "shapes" in the final signal. To accomplish digital filtering, the data array is taken into an orthogonal domain through the use of the *Fourier transform*. The filter is then multiplied with the transform of the data, which removes the selected frequencies. The data is then reverse transformed to produce a smoothed signal.

The process just described is an example of *convolution*.[6] Because the function with the largest bandwidth dominates the convolution process, we must be careful to choose a filter function that removes most of the noise while not distorting the band shapes of the analytical signal.

Exercise 4: Shown below in Figure 6 is an example of an exponential filter function. It is superimposed on the Fourier transform of the noisy signal seen before in earlier exercises. Figure 5 shows the resulting filtered signal.
Set the noise level so that it is 10 times smaller than the largest signal strength.
Adjust the bandwidth of the exponential filter:

1. How does it affect the apparent signal-to-noise ratio?
2. How does it affect the band shape of the signal?
3. At which point does the bandwidth of the filter broaden the original peaks?

$j := 0 .. \frac{L}{2}$ **Time index**

$t_j := \frac{1}{e^{\left(\frac{j}{B4}\right)}}$ **Exponential filter function**

$noise4 := rnorm(L, 0, N4)$ **Random noise**

$signal4_x := signal_x + noise4_x$ **Noisy signal**

$FTsignal := \frac{1}{\sqrt{L}} \cdot fft(signal4)$ **Fourier transform of noisy signal**

$FTfsignal_j := FTsignal_j \cdot t_j$ **Application of digital filter**

$fsignal := \sqrt{L} \cdot ifft(FTfsignal)$ **Inverse transform of filtered signal**

$noise\_sample_i := signal4_{800+i}$ **Sample of noisy signal**

$F\_noise\_sample_i := fsignal_{800+i}$ **Sample of noise in filtered signal**

Noise := stdev(noise_sample)

F_Noise := stdev(F_noise_sample)

Signal := max(signal4)

F_Signal := max(fsignal)

Figure 5: Original and Filtered Signal

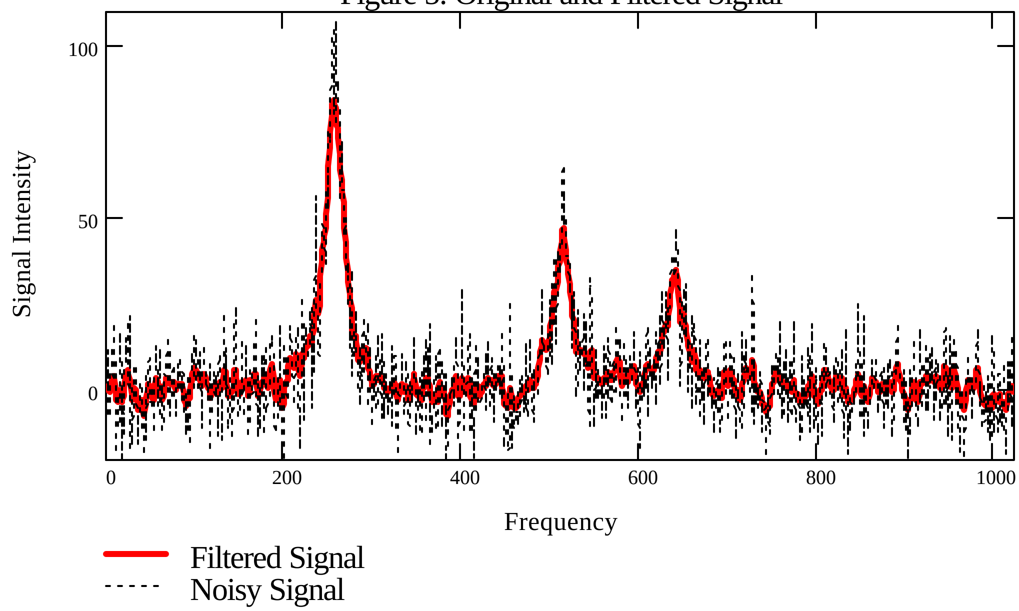
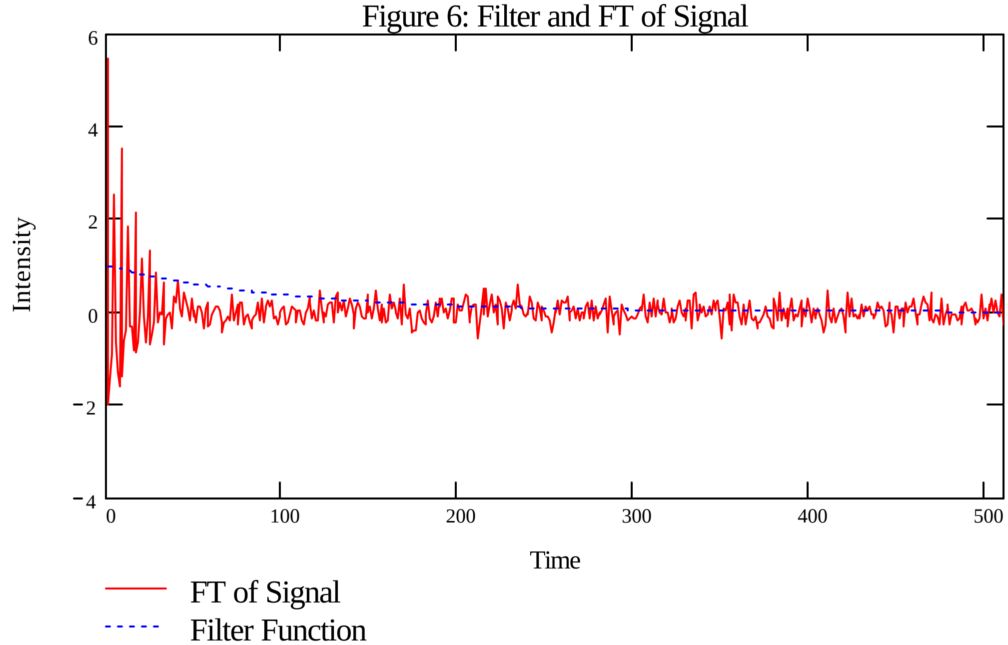


Figure 6: Filter and FT of Signal



$B4 \equiv 100$ **Filter bandwidth** $N4 \equiv 10$ **Noise level**

$$\frac{Signal}{Noise} = 11.926$$ **Signal-to-noise ratio in original signal**

$$\frac{F\_Signal}{F\_Noise} = 27.952$$ **Signal-to-noise ratio in filtered signal**

Notice the *rippling* effect produced by digitally filtering a noisy signal. During the process of convolution, the total area is conserved. While this helps to smooth the processed signal, it also can cause intensity reduction and band broadening if the filter width is not properly matched to the signal. Digital filtering can also introduce artifacts when working with a very noisy signal. Combining ensemble averaging and digital filtering allows us to utilize the advantages of both techniques, while minimizing the introduction of artifacts or errors.

Capstone Exercise: Shown below in Figure 7 is an example of ensemble averaging and digital filtering with a Gaussian function. The ensemble averaged signal is superimposed on the resulting filtered signal.

Set the noise level and the number of coadditions to 1. Then adjust the bandwidth of the Gaussian filter until the widths of the unfiltered and filtered signal match.

1. Increase the noise until it is at least 10 times smaller than the largest signal. How many coadditions does it require to achieve a signal-to-noise ration of 100?
2. How does that number compare to ensemble averaging alone?
3. How does the signal-to-noise ratio resulting from filtering and ensemble averaging compare to ensemble averaging alone?

$$t_j := \exp\left[-4 \cdot \ln(2) \cdot \frac{(j)^2}{B5^2}\right]$$ **Gaussian filter function**

$$noise5 := rnorm(L, 0, N5)$$ **Random noise**

$$signal5_x := signal_x + noise5_x$$ **Noisy Signal**

$$EA\_signal5_x := \frac{EA5 \cdot signal_x + \sqrt{EA5} \cdot noise5_x}{EA5}$$ **Ensemble Averaged Signal**

$$FTsignal := \frac{1}{\sqrt{L}} \cdot fft(EA\_signal5)$$ **Fourier transform of signal**

$FTfsignal_j := FTsignal_j \cdot t_j$ **Application of digital filter**

$fsignal := \sqrt{L} \cdot ifft(FTfsignal)$ **Inverse transform of filtered signal**

$EA\_noise\_sample_i := EA\_signal5_{800+i}$ **Sample of noise in ensemble averaged signal before filtering**

$F\_noise\_sample_i := fsignal_{800+i}$ **Sample of noise in ensemble averaged signal after filtering**

$Signal := max(signal5)$ $Noise := stdev(noise5)$

$EA\_Signal := max(EA\_signal5)$ $EA\_Noise := stdev(EA\_noise\_sample)$

$F\_Signal := max(fsignal)$ $F\_Noise := stdev(F\_noise\_sample)$

Figure 7: Coadded and Filtered Signal

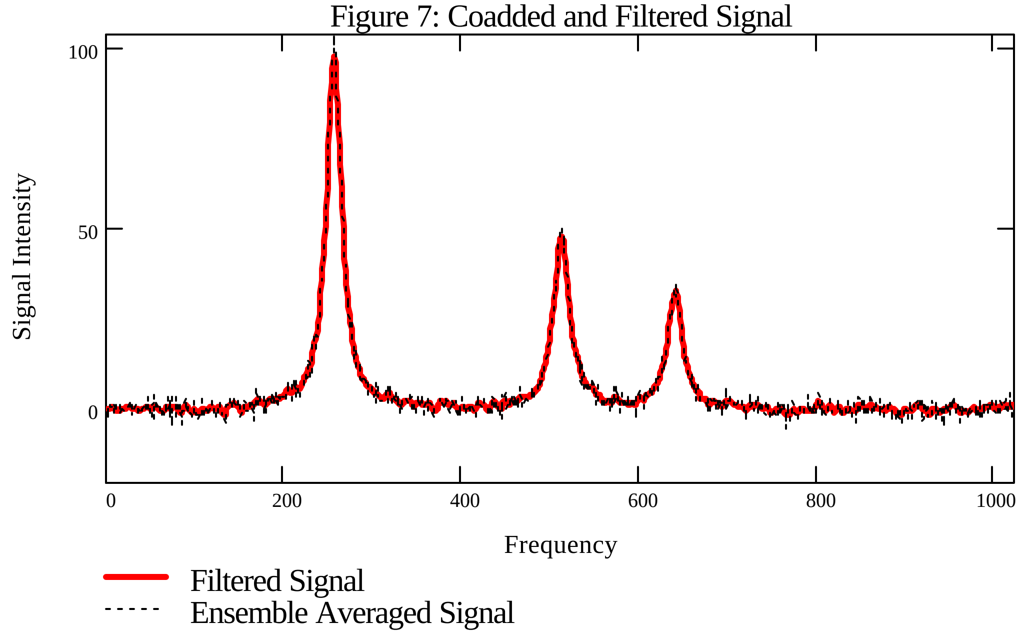
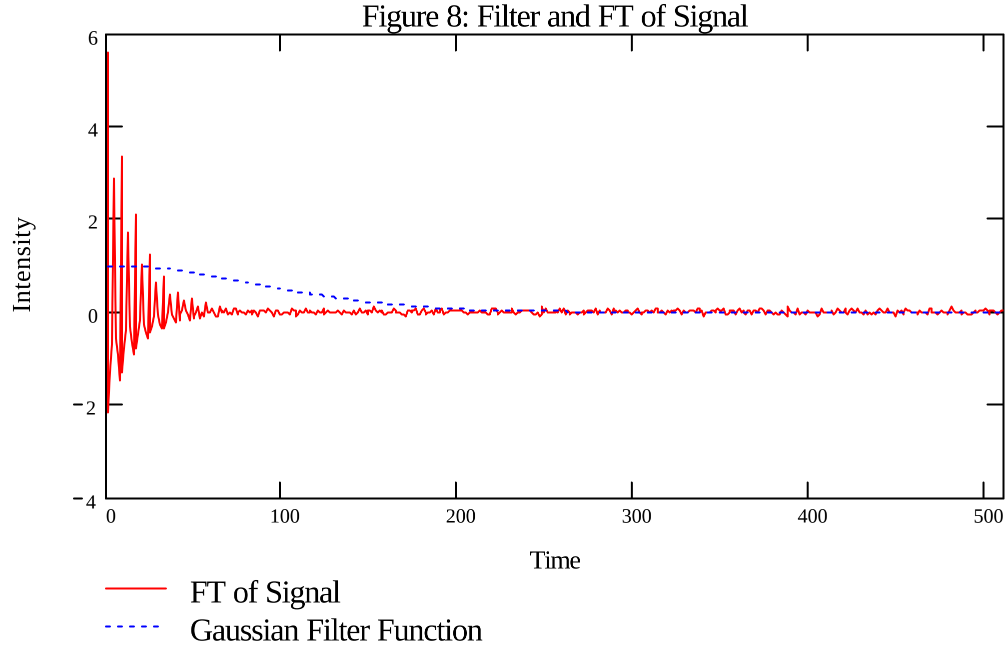


Figure 8: Filter and FT of Signal



$$\frac{Signal}{Noise} = 12.426$$ **Signal-to-noise ratio in original signal**

$B5 \equiv 200$ **Filter bandwidth**

$$\frac{EA\_Signal}{EA\_Noise} = 58.553$$ **Signal-to-noise ratio using ensemble averaging only**

$N5 \equiv 10$ **Noise level**

$EA5 \equiv 30$ **Coadditions**

$$\frac{F\_Signal}{F\_Noise} = 131.72$$ **Signal-to-noise ratio after filtering ensemble averaged signal**

Conclusion

The concepts of noise and signal-to-noise ratios are central themes in the discipline of analytical chemistry. Since chemical instrumentation dominates the modern laboratory, it is critical that students understand the role noise plays in limiting the precision of a measurement. It is equally important that they understand how to implement active and passive means to mitigate noise. Through the process of completing this Mathcad document the student should now be familiar with the concepts of noise and signal-to-noise ratios. They should also understand the advantages and limitations of both ensemble averaging and digital filtering analytical signals.

References:

van Bramer, S. An Introduction to the Fourier Transform *J. Chem. Educ.* 1999, 76, 286.
Rubinson, K. A.; Rubinson, J. F. *Contemporary Instrumental Analysis;* Prentice-Hall, Inc.: New York, 2000, pp. 740-787.
Skoog, D.A.; Leary, J. J. *Principals of Instrumental Analysis,* 4th Ed.; Harcourt Brace & Co.: Orlando, FL, 1992,pp. 47-57.
van Bramer, S. Using Mathcad to Teach Instrumental Analysis *J. Chem. Educ.* 1998, 75, 375.
Ingle, J. D. Jr.; Crouch, S. R. *Spectrochemical Analysis*; Prentice Hall, Inc.: Englewoods Cliffs, NJ, 1988, p. 138.
James, J.F *A Student's Guide to Fourier Transforms: with Applications in Physics and Engineering*; Cambridge University Press: Cambridge, UK,1998, pp. 24 - 33.