Signal and Noise in Measurement

This Mathcad document shows how signal and noise levels effect the analytical signal. First the signal and noise are defined (signal amplitude, noise amplitude, and signal width). The signal peak appears at a random location in the simulated dataset. This document calculates the signal, the noise, and the observed signal.

Variables:

Number of data points: $I := 500$

The signal average (This randomizes the location of the signal):

$\mu := 10\cdot\%\cdot I + \mathrm{rnd}(1)\cdot 0.8\cdot I$ $\qquad \mu = 50.507$

Calculations

$i := 0, 1 .. I$ $\qquad j := 0 .. \mathrm{Sweep} - 1$ $\qquad k := 0, 1 .. (I - \mathrm{Filter})$ — Counting Indexes

$$\mathrm{Signal}_i := S\cdot\left[e^{-\frac{1}{2}\cdot\left(\frac{i-\mu}{\sigma}\right)^2}\right]$$

Defines the signal with amplitude S, average at μ, and standard deviation (peak width) of σ.

$$\mathrm{NORM}(\sigma_n) := \sigma_n\cdot\sqrt{-2\cdot\ln(\mathrm{rnd}(1))}\cdot\cos(2\cdot\pi\cdot\mathrm{rnd}(1))$$

Random normal distribution

$$\mathrm{Noise\_array}_{i,j} := \mathrm{NORM}(N)$$

Random noise array with a standard deviation of N for j sweeps.

$$\mathrm{Noise}_i := \left(\sum_j \mathrm{Noise\_array}_{i,j}\right)\cdot\mathrm{Sweep}^{-1}$$

Sum and normalize noise for each sweep.

$$\mathrm{Observed}_k := \left[\sum_{m=k}^{k+\mathrm{Filter}} \mathrm{Noise}_m + \mathrm{Signal}_m\right]\cdot(\mathrm{Filter}+1)^{-1}$$

Combine signal with noise and filter with moving average.

$$\mathrm{Noise}_{\mathrm{filter}_k} := \left(\sum_{m=k}^{k+\mathrm{Filter}} \mathrm{Noise}_m\right)\cdot(\mathrm{Filter}+1)^{-1}$$

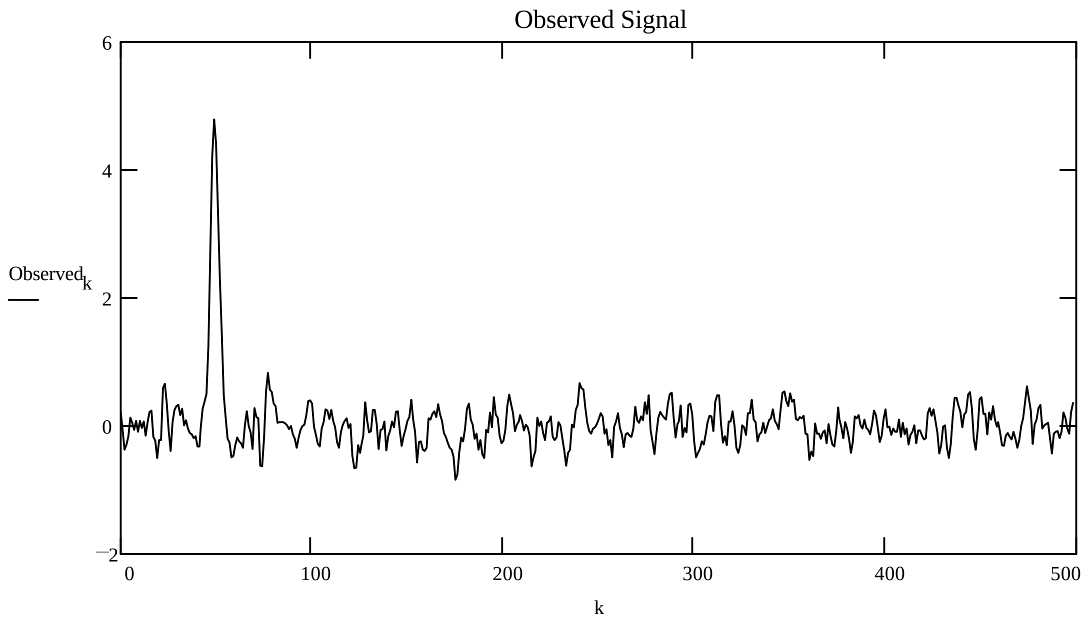
Calculate observed noise.

$S_{obs} := \max(\mathrm{Observed})$ $\qquad S_{obs} = 4.793$

Calculate maximum observed signal. Note: this is the max observed value, not the signal intensity (S).

$N_{obs} := \mathrm{stdev}(\mathrm{Noise}_{\mathrm{filter}})$ $\qquad N_{obs} = 0.26$

Calculate standard deviation of noise



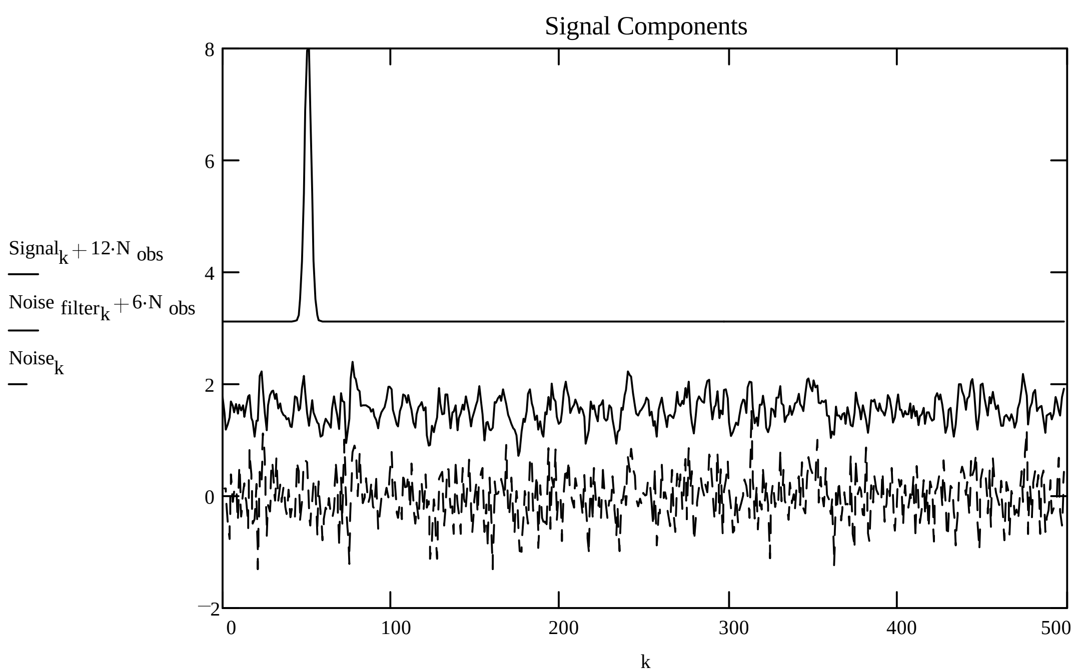
Settings:

Signal	$S \equiv 5$	Number of sweeps	$Sweep \equiv 5$
Peak Width	$\sigma \equiv 2$	Filter Setting	$Filter \equiv 2$
Noise	$N \equiv 1$		

Calculated S/N:

$$\frac{S_{obs}}{N_{obs}} = 18.419$$

Display Signal and Noise Separately:



Questions

Use the Mathcad document to change the following parameters and determine their effect on the observed signal. Pay attention to the graph of the observed signal and the S/N observed.

Note: when you make changes there are several different types of equals signs in mathcad. An = displays the current value of a variable. An := is used to define a variable from that point on. An equals with three lines is used to define a variable at all locations in a document.

1. Change the signal (S) and the noise (N).
   a. What is the minimum S/N where you can clearly identify the signal peak?
   b. Even with a signal of 0, what is the calculated S/N? Why?

2. Change the number of sweeps that are averaged (Sweep).
   a. How does the number of sweeps effect the S/N and the observed signal?
   b. What is the relationship between the number of sweeps and the S/N?
   c. Is it linear?
   d. Graph number of sweeps vs. S/N.
   e. Is there an optimal number of sweeps?
   f. Does the number of sweeps effect the peak shape?

3. Change the Filter setting (Filter). (NOTE: When the Filter is set at 0, NO filtering is used)
   a. Notice the effect on the noise and the signal.
   b. How does the Filter effect the S/N?
   c. Is there an optimal setting for the Filter?
   d. Does the filter effect the peak shape?
   e. How could you design the filter to reduce this effect?
   f. Change the Peak Width and repeat, is the filter optimum the same?

4. Construct a mathematical model of S/N Dependence on Averaging. Log - Log plots are often used to determine the order of an equation. In this exercise you will learn how these plots are used. This is an extremely valuable tool for analyzing experimental data. Use a spreadsheet to develop your model

   a. Start by preparing a spreadsheet that includes the following calculations.
      i. A column of X-axis values that covers a fairly large range. 10 points should show the effects you are looking for.
      ii. A cell for the order of the equation (Start with a value of 1)
      iii. A cell for the multiplier (Start with a value of 1)
      iv. Now calculate the Y-axis values with the following formula:
      Y = (multiplier * X)^order

      v. Next take the natural log of both the X and Y values
      vi. Plot X vs. Y. What does this look like?
      vii. Plot Ln(X) vs. Ln(Y). What does this look like?
      viii. Run a regression analysis on the ln(X) vs. ln(y) dataset.

b. Now use this spreadsheet to study the system when you make the following changes.
  i. Start with a first order reaction. Change the multiplier.
    a. What happens to both graphs?
    b. What happens to the calculated slope and intercept?

  ii. Now change the order of the reaction.
    a. What happens in both graphs?
    b. What happens to the calculated slope and intercept?

  iii. Change both the order of the reaction and the multiplier. Try to determine how these two values effect the slope and intercept of the ln - ln graph.

  iv. Write an equation to summarize your results.

c. You can verify your numerical model analytically as follows:

For a relationship that follows the general equation

$$y = m \cdot x^{a}$$

Take the natural log of both sides

$$\ln(y) = \ln\left(m \cdot x^{a}\right)$$

This rearranges to

$$\ln(y) = \ln(m) + a \cdot \ln(x)$$

So that a plot of ln(y) vs. ln(x) has the following properties

$$\text{Slope} = a$$

$$\text{Intercept} = \ln(m)$$

d. Use your spreadsheet to fit your S/N data and write an equation that relates S/N to the number of scans.

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