

Analysis of Noise

Part XIV

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This column is a continuation of the set (1–13) dealing with the rigorous derivation of the expressions relating the effect of instrument (and other) noise to their effects on the spectra we observe.

As we do in each column in this series-within-a-series, we again take this opportunity to remind readers that we are dealing with a continuous series of columns, and so we resume our discussion by continuing our equation numbering, figure numbering, use of symbols, and so forth, as though there were no break, except that when we repeat an equation or series of equations that were derived and presented previously, we retain the original number(s) for those equation(s).

In the previous column (13), we analyzed the effect of *scintillation noise*; that is, noise that is proportional to the signal, for the case of *low noise* — noise that is small compared to the signal level. Now we wish to analyze, as we have done previously, the situation when the noise is no longer negligible compared with the signal level. Here again we enter territory where extra care is

needed. In the previous cases, we could assume that all conditions of the measurement were constant except that the reference energy was reduced until it was of comparable magnitude to the noise level. In the case of scintillation noise, however, that is not an option. As we noted earlier, as the signal level is reduced (in either channel), the noise is reduced correspondingly, leaving the N/S (that is, the inverse of the S/N, in our notation $SD[E_r]/E_r$) ratio constant. Therefore, we cannot consider reducing the S/N by reducing the reference signal level. The only way we can change the signal-to-noise ratio is by changing the proportionality parameter k , which expresses the noise as a fraction of the signal. As we did for the low-noise case, we will introduce this parameter as the appropriate point in the derivation.

Following our usual sequence, our next step here, as it was for the previous two cases we treated (constant detector noise and Poisson-distributed noise), is to ascertain the effect of this noise on the expected value of computed transmittance. To do this we start with equation 5 (2):

$$T + \Delta T = \frac{E_s + \Delta E_s}{E_r + \Delta E_r} \quad [5]$$

In the low-noise case we justified separating equation 5 into two terms and setting T equal to $E_s/(E_r + \Delta E_r)$. Here we cannot do that for several reasons:

- In the large-noise case, ΔE_r in the denominator of equation 5 is nonnegligible and therefore induces an asymmetry that will prevent it from vanishing upon integration.
- An even larger asymmetry is introduced by a fact we have discussed previously: the physical causes of the error source under consideration preclude both the numerator and the denomina-



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tor from becoming negative. Thus when we evaluate equation 5 to ascertain the expected values, we cannot continue integration below zero; the integration must be truncated at that point.

For a physical picture to describe the situation, we can imagine an optical beam and some opaque component vibrating randomly into and out of the beam. A schematic picture of this is shown in Figure 31a. Clearly, the farther into the beam the obstruction intrudes, the more the beam is blocked and the less energy reaches the detector. The instantaneous blockage depends mainly on two factors: the average position of the obstruction and the magnitude of the vibration. For our purposes we will assume that the position of the obstruction varies around its central location in such a manner that the distribution of energy in the optical beam varies according to a normal distribution. Anyone who wants to calculate the actual distribution for an optical beam of interest to them is certainly free to do so and to follow through on the calculation of the distribution of noise that actual optical geometry will cause. We would certainly appreciate hearing about any efforts in that direction, and the results obtained. For our purposes, however, we simply wish to point out that as the center of the obstruction's motions moves closer to the center of the beam, more and more of the beam is blocked. Also, if the vibrational amplitude of the obstruction's motion is constant, then the blockage will represent larger and larger fractions of the beam's energy. However, there is a limit to that: if the obstruction moves so that it completely blocks the beam, then the instantaneous energy transmitted will be zero. As the obstruction continues to move closer to the optical beam, then complete blockage can occur more and more often, or equivalently, for larger and larger fractions of the time, but at no time can the energy transmitted become less than zero.

From Figure 31a we can also see a corollary: if the amplitude of the obstruction's vibration is large enough, it will move completely out of the optical beam, resulting in truncation of the normal distribution due to the fact that there will also be a maximum possible value for the energy, corresponding to the situation when the beam is completely unblocked. For our current analysis, however, we will consider only the case where the average position of the obstruction is within the beam and so the beam is always at least partially blocked. Then the vibrations of the obstruction cause it to block varying amounts of energy, down to complete blockage, but not to complete passage.

The effect of this on the beam energy is indicated in Figure 31b. If the distribution of energies is normal, then the part below the lower limiting edge is truncated, because it is not possible to have less than zero energy.

As we did in the analysis of Poisson-distributed noise, we compute the expected value of T as the weighted sum of the transmittance described by equation 5 (10):

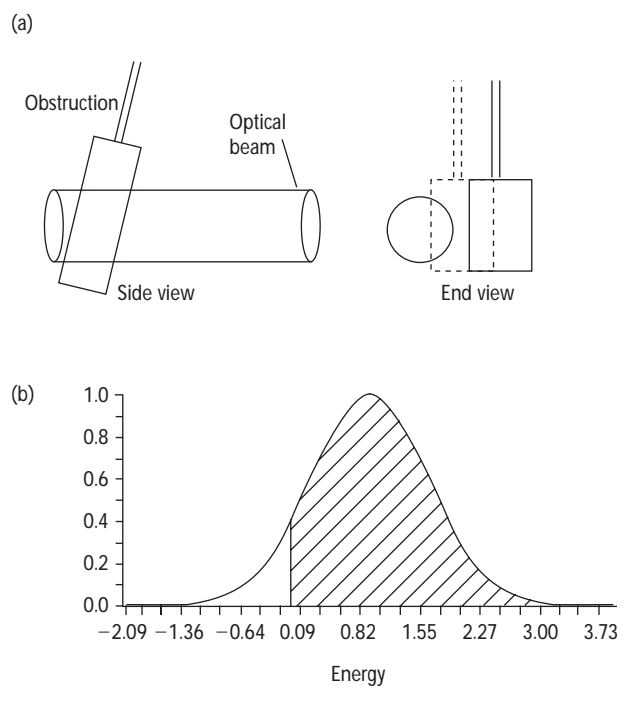


Figure 31. (a) An obstruction vignetting the beam randomly can affect the signal level, but cannot do more than block the entire beam, reducing the energy to zero. Once the optical beam is completely blocked, no less light can pass through the optical system. (b) The average light that then can pass is the integral of the shaded area.

$$\bar{T}_w = \frac{\sum_i W_i F(X_i)}{\sum_i W_i} \quad [59]$$

The evaluation of equation 59 for the current case of scintillation noise carries with it its own set of difficulties and cautions, just as the previous cases did. Some of them, caused by the physical limitation of not allowing the energy to go below zero, were mentioned above. Others mirror the two cases we have previously discussed in the past several columns; the case of scintillation noise seems to combine some of the more difficult aspects of the two previous cases. Like the Poisson distribution, the value of the function and therefore of the integration does not go below zero, mirroring the physical effect that the actual optical energy cannot go below zero. Unlike the Poisson distribution (which was discrete), the values of the energy form a continuum, as does the normal distribution we are assuming that the noise follows. Therefore, we cannot simply add together the relatively small number of discrete values that the function can assume but must perform a numerical integration over the range of values that will make appreciable contributions to the result. Another consequence of not following the Poisson distribution is that the noise level is not

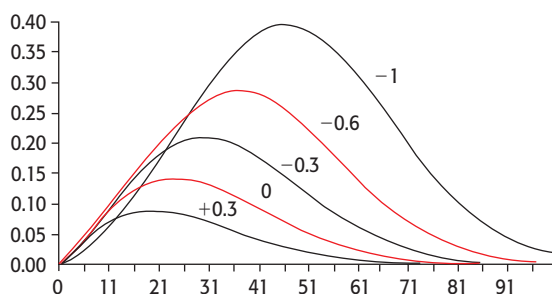
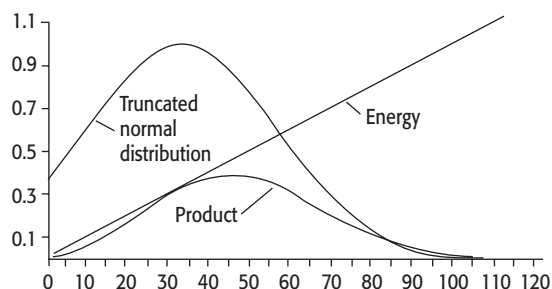
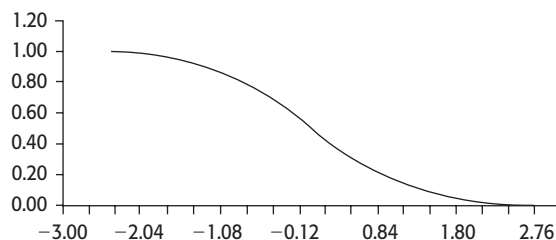


Figure 32 (top). The integral of the truncated normal distribution for values of the point of truncation between -3 and $+3$ SDs. In all cases the integration was continued to $+4$ SDs.

Figure 33 (middle). The relation between the normal distribution (truncated at -1 SD), the energy variation, and the product of the two curves.

Figure 34 (bottom). Family of curves of the energy-distribution product, corresponding to various truncation points. The numbers indicate the truncation point of the normal distribution as the number of standard deviations from the peak of the normal distribution.

locked to the energy level. Rather, the value of k , which determines N/S , is independent of the energy. This precludes any simplification of the equations such as we applied to the Poisson-distributed noise case.

On the other hand, neither can we apply some of the simplifications we used in the case of constant detector noise, particularly the fact that the integral of the normal distribution is unity. Because in the case we deal with now the distribution is truncated, we must perform numerical integrations of the distribution corresponding to the amount of truncation, to ascertain the behavior of this situation. This creates

Table V. Accuracy of the integral of the truncated normal curve for different values of the integration interval.

Integration interval	Error of integral
0.1	0.019
0.01	0.0019
0.001	0.00017
0.0001	0.000019

another complication in the analysis. Although at first glance this limitation of not allowing the signal to go below zero seems like a benefit because it gives us a hard limit for the computation of the integrals, we also have to consider the effect of this limitation on the denominator of equation 59 as well as on the numerator. In the previous cases we've considered, the weighting function was a well-behaved mathematical probability function, either the normal or the Poisson distribution. Both of these distributions evaluated to unity over the range of interest, and therefore, we could replace the denominator with unity and ignore it thereafter. Now we wish to use the normal distribution to describe the behavior of the error contribution we are evaluating, but we cannot consider evaluating the integral from $-\infty$ to $+\infty$, because we have seen that there is a lower limit to the integral. Furthermore, the lower limiting value remains at zero regardless of the value corresponding to the maximum of the distribution.

Preliminary Steps

The evaluation of equation 59, therefore, starts with the evaluation of the truncated normal distribution. This is the value of the normal distribution obtained by integrating the normal distribution not between $-\infty$ and $+\infty$, but between the lower cutoff value, whatever that is, and $+\infty$. The normal distribution, being simply another name for the error function, is well-known to not be analytically integrable; therefore, numeric approximations are needed to ascertain the value. Indeed, it has been computed to high accuracy and the values are available in tables (for example, see reference 14, page 3). It is necessary, however, for us to be able to perform these computations ourselves, so that we can also use them in evaluating the weighted averages specified by equation 59. This is similar to the computations we performed previously for the case of constant (detector) noise, but differs from that computation in that the previous computation was done over the full significant range of the normal distribution, instead of the truncated distribution. As a test, then, the computation was written in MATLAB (Mathworks, Natick, MA). The result of the computation, for a continuum of values of the point of truncation, is shown in Figure 32.

The accuracy of the integration was evaluated by comparing the values computed from the MATLAB program to the tables available (see reference 14, page 3) at several selected values of X (where X represents the number of standard deviations at

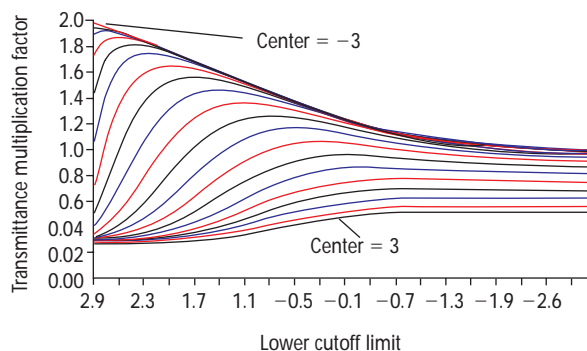


Figure 35. Transmittance multiplication factor as a function of the lower cutoff limit of the normal distribution, for varying values of the center of the distribution.

which the truncated SD was evaluated) as a function of the integration interval. The results are presented in Table V.

We also inspect the nature of the function that we will be integrating. In the picture corresponding to the small-noise case, the underlying energy of the optical beam is effectively constant over the range of variation of energy; indeed, this is the definition of “small noise.” For a normally distributed vibration, the energy would thus also be normally distributed. For the large-noise case, however, the energy varies appreciably over the range of vibration, and the variation increases with k , distorting the shape of the curve. This behavior, which is shown in Figure 33, corresponds to the plot in Figure 5 for the case of constant detector noise (4). Because the nature of the curve will vary as the degree of truncation varies, this also represents a family of curves. Figure 34 presents this family of curves, for various values of the point of truncation with respect to the normal distribution curve.

There’s a point that we’ve implied in the foregoing discussion but have not made explicitly, so let’s correct that oversight now: in the previous discussions of the mathematics behind the analysis of scintillation noise, we pointed out that, because the noise decreases with the signal, changes in S/N cannot be accomplished by changing the reference signal energy (or, for that matter, the sample energy) because the noise will be reduced proportionately. Therefore, the noise level must be expressed as a multiplier, which we called k , times the signal level. This parameter, k , expresses the standard deviation of the noise as a fraction of the signal energy. Thus, the value at which the normal distribution becomes truncated can be expressed as a function of k . Thus, for example, if $k = 1$ (the standard deviation of the energy due to movement of the obstruction equals the energy at the average position of the obstruction), then 95% of the time, more energy will be present than the value $\bar{E} - 2k$ and the cutoff will be at $-2k$ (strictly speaking, at $-1.98k$, but we will use the common approximation of 2 because it will be simpler to deal with in other cases; anyone concerned about the dis-

crepancy can adjust the probability levels to compensate). If $k = 2$, then the corresponding cutoff value will be at $-1k$. This relates the mathematical quantity k to the properties of the normal distribution that we will be working with in the evaluations of the integrals.

Indeed, there is a “gotcha” to watch out for. In the picture of Figure 31a, we show an obstruction obscuring part of the optical beam. If the physical amplitude of the vibrations of the obscuration are small, then k will increase as the average position of the obstruction moves closer and closer to the center of the beam, thus obscuring more of it, and reducing the energy by leaving a smaller and smaller crescent of the beam available. This movement of the obstruction corresponds to larger and larger values of k . Assuming that the distribution of positions of the obstruction is normal, then the value of k varies inversely with the average size of the crescent left available. When the average position of the obstruction corresponds to being just at the edge of the beam, then truncation occurs at zero SD from the maximum of the normal distribution. But there is nothing to prevent the obstruction from moving even farther into obscuring the beam; in such a case, light would be passing less than half the time, and the truncation point will have passed the center of the normal distribution. This behavior is indicated in Figure 34, shown as the change in sign of the number of standard deviations corresponding to the point of truncation of the SD in that figure. The “gotcha” is that it would require k to assume an infinite value to express the situation where the average position of the obstruction coincided with the edge of the optical beam, a situation which is physically reasonable but mathematically intractable. Therefore, our evaluations of the integrals will be based on specifying the truncation point in terms of the standard deviation of the position of the obstruction, rather than in terms of the obscuration of the optical beam.

Evaluation of the Function

We are now ready to evaluate the expressions in equation 59 and substitute them into equation 5. We will use the same value of k for both sample and reference beams. By having k the same, the results will be independent of the transmittance of the sample, as discussed previously. It also eases our task because we will not have to compute a family of curves, but only one curve representing the change in computed transmittance as k varies. Evaluating it this way also eliminates the need to perform a double integration; we can simply keep the sample transmittance constant at unity and plot the variation in computed transmittance.

As described above, we do not compute the integral as a function of k directly. Rather, we compute it as a function of the point of truncation of the normal distribution, which we allow to vary from $+3$ SDs to -3 SDs as the parameter. Figure 35 shows how the multiplication factor varies for the various places where the center of the obstruction is.

When the noise is small, the multiplication factor approaches unity, as we would expect. As we have seen for the

previous two types of noise we considered, the nonlinearity in the computation of transmittance causes the expected value of the computed transmittance to increase as the energy approaches zero, and then decrease again. For the type of noise we are currently considering, however, the situation is complicated by the truncation of the distribution, as we have discussed, so that when only the tail of the distribution is available (that is, when the distribution is cut off at +3 standard deviations), the character changes from that seen when most of the distribution is used.

Noise

To derive the transmittance noise for the case of large scintillation noise, we begin at a somewhat earlier point than we did for the low-noise case, with equation 14 (2):

$$\text{Var}(\Delta T) = \text{Var}\left(\frac{E_r \Delta E_s}{E_r(E_r + \Delta E_r)}\right) + \text{Var}\left(\frac{-E_s \Delta E_r}{E_r(E_r + \Delta E_r)}\right) \quad [14]$$

Attempting to solve this equation for the scintillation noise situation raises the same difficulties as the previous investigations of noise in the low-signal (high-noise) regime: the inseparability of the ΔE_r and ΔE_s terms in the denominator, and the generation of infinities in the integrals when attempting to evaluate it. In this case, however, we cannot make the infinities go away or ignore their existence. In the case of constant detector noise, we assumed the infinity away by making the assumption that no measurement would ever coincide with an exact zero value of the noise, because the probability of that would be infinitesimally small. In the case of Poisson noise, we could assume the infinity away by making the assumption that because the Poisson distribution represented a discrete distribution, then even though it could in fact take the value of exactly zero, if this occurred in the denominator of the transmittance computation, the user would reject that reading, and it would not be included with the data. Therefore, we were justified in rejecting readings with zero in the denominator from our calculations.

In the case of scintillation noise, however, we cannot do either of those things. By the physical picture we set up to describe the situation, the situation can in fact occur that the obstruction would completely block the optical beam and allow zero energy through, yet since it represents a continuum of values, we do not see a justification to arbitrarily reject those readings. Therefore, we cannot see a clear path to trying to determine the noise performance of such a system because it will inevitably come out as infinite in all cases.

This is a good stopping point. The title of this column is "Chemometrics in Spectroscopy," and for the past several columns we have departed somewhat from that general topic to discuss in some detail the very specialized question of noise in spectra. Although not outside the range of interest covered by the column's intent, it is somewhat near the edges

of what might be considered the mainstream purview of the column, and it is time to return to a more mainstream discussion, or at least one closer to the center of the topic. Hence, in our next few columns we will be discussing some of the pitfalls of multivariate calibration.

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