

Unfolding x-ray Spectra from a Multichannel Spectrometer

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Abstract:

Limitations exist on the amount of spectral detail that can be unfolded from multichannel spectrometer readings and their known filter response functions. These limitations exist because during the process of converting (“folding”) x ray spectra into channel voltage readings, a lot of spectral detail and information is inevitably lost. Thus the process of “unfolding,” inferring a spectrum from a set of channel readings and their known response functions, can only recover a limited amount of spectral information. The goal of this project was to find out what parameterized spectrum model, when used with weighted least squares fitting, recovers the most spectral information. Weighted least squares, the method used to unfold the spectra, is a parameter estimation technique that finds the model spectrum parameters that are most consistent with the readings of the multichannel spectrometer. The multigroup model spectrum, with bin widths based on filter function edges, is the most reliable parameterized spectrum model.

1.1 Introduction:

During a direct drive fusion experiment conducted at the Laboratory for Laser Energetics, multiple high power laser beams strike a very small deuterium/tritium target. As a result, this target implodes at an exceedingly high velocity and emits x rays of various wavelengths. It is very important to study the entire spectrum of x rays emitted. Currently, at the Laboratory, a multi-channel spectrometer called Dante is used to analyze the x ray spectrum emitted by the imploding target. Dante is able to accurately interpret spectral power. However, Dante provides only a limited amount of spectral information. In this report, various “unfolding” algorithms for converting Dante measurements into the x ray spectrum emitted by the imploding target will be analyzed.

Dante is an x ray spectrometer currently used at the Laboratory for Laser Energetics to measure the spectra emitted by imploding targets. Dante is comprised of 19 distinct channels. Each channel covers different spectral regions spanning from 50 eV to 20 keV with 20-ps resolution. Only 15 channels are used in the following models because these channels have

spectral regions pertaining to the photon energies in the simulated LILAC spectra. In each channel, x ray radiation passes through a spectrally distinct filter which is opaque to certain photons. The remaining photons pass through the filter into an x ray diode, which registers the total power of the x ray radiation incident on it as a voltage reading.¹ These voltage readings can be expressed with the equation: $V_i = \int_0^{\infty} k_i S(h\nu) f_i(h\nu) d h\nu$ [$i = 1, 2, \dots, M$], where the spectrum, $S(h\nu)$, is folded into the filter response function, $f_i(h\nu)$, to give V_i , the voltage reading. Here, k_i is the fraction of the total spectrum captured by the channel, and M is the number of channels on the spectrometer, h is Planck's constant, and ν is the frequency of a certain photon in the spectrum. A channel's sensitivity to certain photons can be characterized by its filter response function $f_i(h\nu)$.

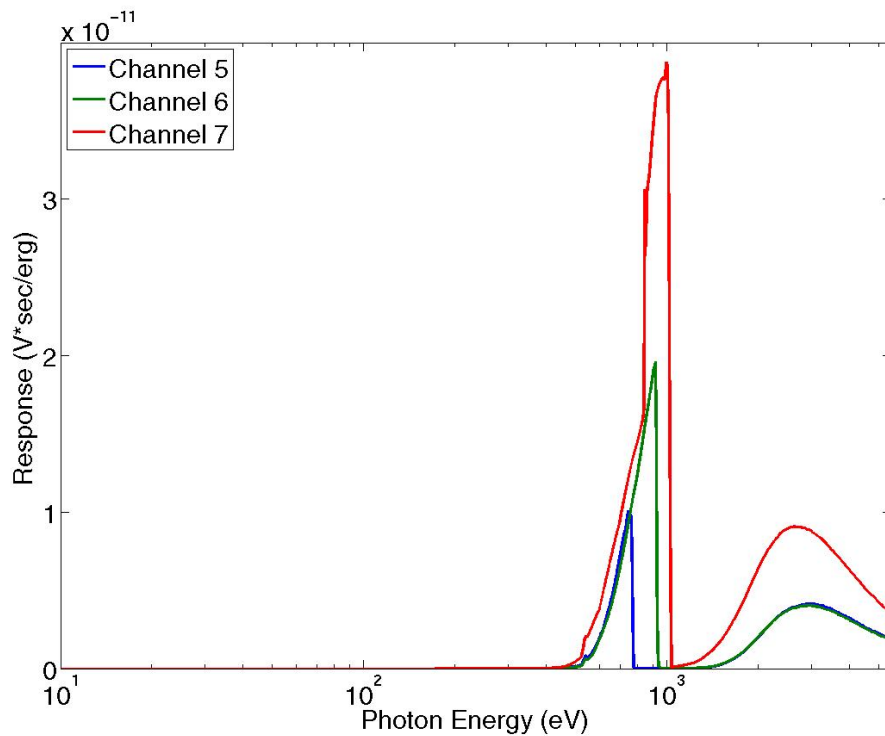


Fig. 1. Dante filter functions 5, 6, and 7 are plotted vs. photon energy. Each channel is sensitive to a specific range of photon energies. The location where the filter function turns suddenly opaque to certain photons corresponds to a photo-ionization “edge” of the filter material.

LILAC is a program used at the Laboratory for Laser Energetics that simulates an entire target implosion, including the x ray emission, at a series of time steps. The x ray emission is

divided into 48 spectral groups. The LILAC simulated x ray spectrum is then folded into the Dante channel response functions to obtain the voltage readings. These voltages are then unfolded into a spectrum that is compared with the original LILAC spectrum. Various algorithms are compared to see which one recovers the most spectral detail with the most accuracy.

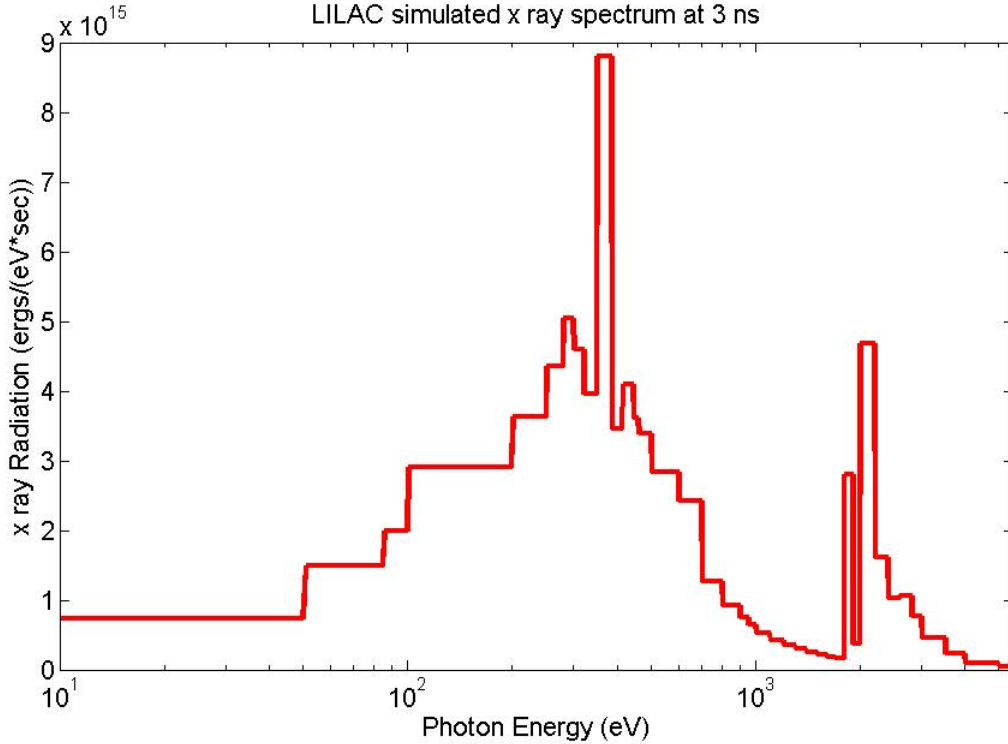


Fig. 2. A LILAC simulated spectrum of a target implosion at 3 ns is chosen as an example of hypothetical data. This simulated spectrum will be folded into Dante response functions and then unfolded as a fitted spectrum in order to illustrate the unfolding algorithm used.

2.1 Methodology:

The x ray spectra were unfolded using the weighted least squares method.³ In this method, the set of parameter estimates x_j , that minimizes $\chi^2 = \sum_{i=1}^M \frac{(V_i - Z_i)^2}{\sigma_i^2}$ is found, where V_i are measured voltage values, Z_i are the theoretical voltage values obtained from the model spectrum defined by the parameter estimates, and σ_i are the unavoidable random measurement errors in each channel associated with the experiment. The minimum of χ^2 is obtained when

$\frac{\partial \chi^2}{\partial x_j} = 0$ for all the parameters. This condition is satisfied by the solution to the set of M

equations and M unknowns,

$$\sum_{i=1}^M -\frac{2Z_i}{\sigma_i^2} \frac{\partial f(x_k; t_i)}{\partial x_j} + \frac{2f(x_k; t_i)}{\sigma_i^2} \frac{\partial f(x_k; t_i)}{\partial x_j} = 0.$$

Here, one assumes that the spectrum can be modeled as a function of the parameters x_k and t_i , where t_i is time. Time is a variable because a spectrum is time dependent, but it is not one of the fitting parameters. In other words, $f(x_k; t_i)$ is the function which models the spectrum. One can use Newton's method to solve the equations described by the equation above. In this method, one iteratively uses nominal parameter values as guesses, in order to obtain corrections to these guesses. This iterative process converges to the actual solution. When applying this methodology to solve for the zero, one will come up with a system of equations written in matrix notation as $\mathbf{J} * \Delta \mathbf{x} = \mathbf{r}$. Here, \mathbf{J} is a square matrix, also known as the coefficient matrix, with length and width equal to the number of parameters, and $\Delta \mathbf{x}$ and \mathbf{r} are both column vectors with lengths equal to the number of parameters. The quantities \mathbf{J} and \mathbf{r} are given by:

$$\mathbf{J}_{jk} = \sum_{i=1}^M \frac{1}{\sigma_i^2} \frac{\partial Z_i^0}{\partial x_j} \frac{\partial Z_i^0}{\partial x_k}, \text{ and}$$

$$\mathbf{r}_j = \sum_{i=1}^M \frac{1}{\sigma_i^2} \frac{\partial Z_i^0}{\partial x_j} (V_i - Z_i^0).$$

The superscript 0 in Z_i^0 is used to denote the fact that nominal parameter values were used to obtain the voltage values. The elements of $\Delta \mathbf{x}$ contain are the set of corrections that, when added to the set of parameter estimates, create a better set of parameter estimates. The set of corrections are obtained by multiplying each side of the equation by the matrix inverse of the coefficient matrix, $\Delta \mathbf{x} = \mathbf{J}^{-1} * \mathbf{r}$. The coefficient matrix is inverted using singular value decomposition as described by Press *et al.*⁴ This particular method is used in order to minimize the deleterious effect of the near singularity of the coefficient matrix. After $\Delta \mathbf{x}$ is found, new estimates for Z_i^0 are calculated, which are closer to the actual solution. These corrections become smaller with each iteration. This process is repeated until the corrections become negligible. At this

point, $\frac{\partial \chi^2}{\partial x_j} = 0$, and the parameter values are considered to have been solved for all practical purposes. This entire process is programmed in Matlab.

2.2 Formal Errors Estimates:

One of the benefits of using the weighted least squares method is that formal error estimates of the parameter estimates, based on the random errors of the experiment, can be found.³ The J^{-1} matrix is also known as the covariance matrix. Its elements are the covariances of the parameter estimates between parameter estimates x_j and x_i ; $J_{ij}^{-1} = \langle \delta x_j \delta x_i \rangle$. The angle brackets indicate the statistically expected value. The expected error is based on the assumption that the voltage errors, V_i , are normally distributed about 0. When $j=i$, $J_{ii}^{-1} = \langle \delta x_i^2 \rangle$. Thus, one can take the square root of the elements on the major diagonal of the covariance matrix to see the errors associated with all of the parameter estimates. This is the method used to place error bars on the parameter estimates.

Total spectral power, P , and error, δP , can also be calculated, as $P = \int_0^\infty S(h\nu) d h\nu$. Total spectral power error, δP , can be found with the equation:

$$\delta P = \sqrt{\sum_{k=1}^M \sum_{j=1}^M \frac{\partial P}{\partial x_k} \frac{\partial P}{\partial x_j} \langle \delta x_k \delta x_j \rangle}$$

where once again, M is the number of parameters, and $\langle \delta x_k \delta x_j \rangle$ is the variance of parameters k and j .

3.1 The Fits:

The weighted least squares method finds the set of parameter values that minimizes χ^2 for a particular spectral model. However, this method places no restrictions on the spectral model and its parameterization. Well-chosen models will give a more accurate representation of a spectrum than other models.

3.2 The Polynomial Fit:

A very popular fit used in many applications of curve fitting is the polynomial fit. In this fit, the spectrum is modeled with the equation

$$S(x) = a_1x^n + a_2x^{n-1} + a_3x^{n-2} + \dots + a_n,$$

where the fitting parameters are a_n .

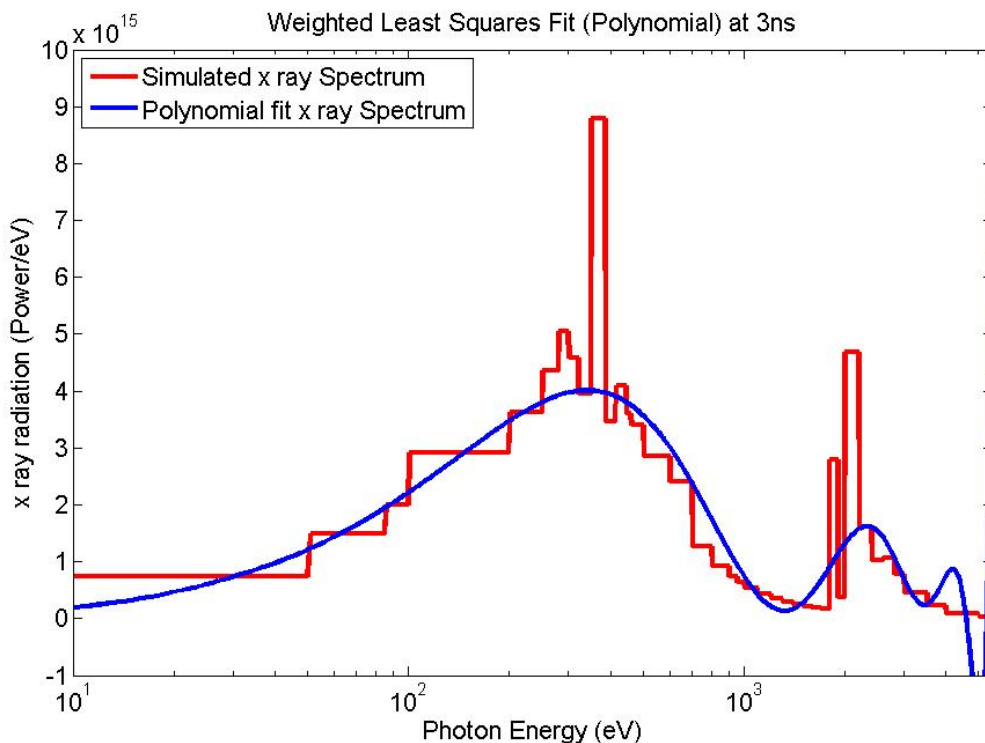


Fig. 3. The polynomial fit of the hypothetical spectrum obtained with a 10-parameter fit is shown. Fifteen Dante channels were used to unfold the spectrum.

A polynomial does not fit this spectrum well. The narrow spectral lines emitted by an imploding target are represented poorly by a smooth polynomial curve. In an attempt to match the peaks of the spectrum, artificial curves on the right side of the spectrum were generated. Furthermore, one of the major faults of a polynomial fit is the correlation between parameters. Correlation occurs when one parameter affects the value of another parameter. In this example, the adjustments in any one parameter (any one coefficient a_n) will strongly affect the fitted

values of some of the other parameter values. This correlation was evident in the resulting near-singular \mathbf{J} matrix. The condition number, a number which gives evidence of a near-singular matrix,⁴ was: 2.05×10^{-70} . A completely singular matrix has a condition number of 0. Therefore, the coefficient matrix in this example was very close to singular. The inverse was only approximated, the true solution could not be obtained, and the fit is not as unambiguous as it should be. A polynomial is obviously not a viable fit for this spectrum.

3.3 Spectral Point Fit:

In the spectral point method, the fitting parameters are the spectral points. Each point can move up and down to best fit the voltage readings. Neighboring spectral points are then connected with straight lines.

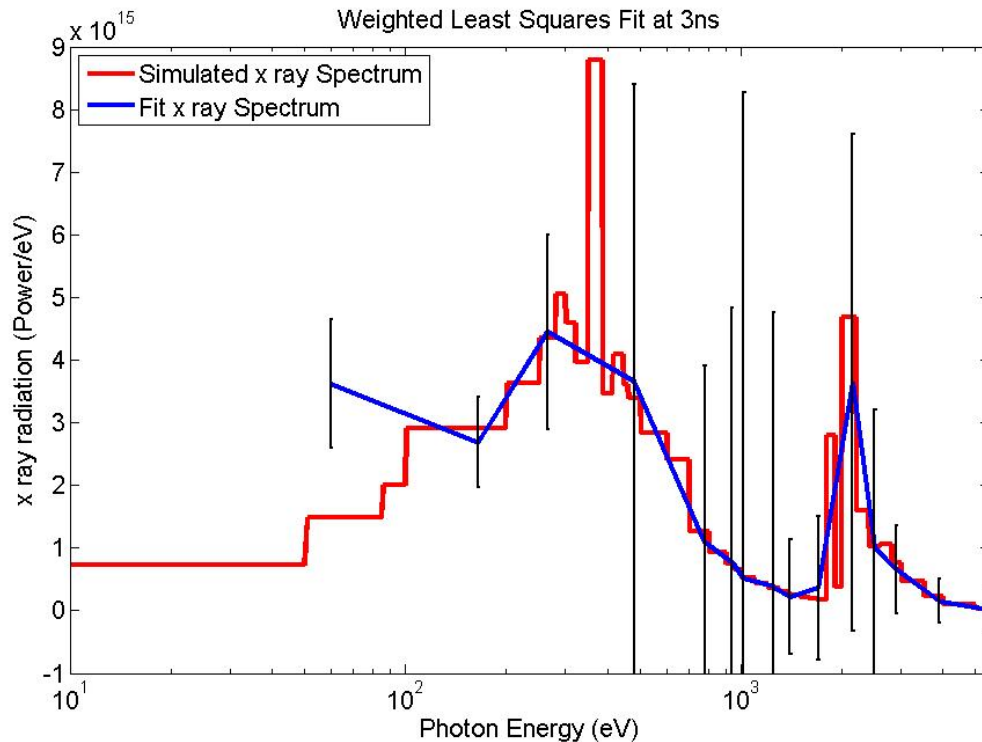


Fig. 4. A spectral point fit of the hypothetical spectrum is shown. Spectral points were placed in the middle of each filter function sensitivity range. Error bars were generated based on a 10% accuracy in Dante voltage readings.

Although the model spectrum is quite accurate, the error bars are very large. This is caused by the anti-correlation between the estimates of adjacent spectral points. If one point moves upward, re-optimizing the fit of the model spectrum to the voltage readings will push surrounding spectral points downward to maintain the quality of the fit of the model spectrum to the voltage reading data. Thus, the parameter estimates have some room to move, which translates into large error bars.

Despite the high relative uncertainties in the parameter estimates, the relative uncertainty in the power is still quite low. The total spectral power was $5.30 \cdot 10^{18}$ ergs/sec, with an estimated error of $6.18 \cdot 10^{17}$ ergs/sec. This is a relative uncertainty of 11.67%, which is much smaller than the error bars in Fig. 4 would suggest. This reflects the strong anti-correlation between the parameters. Although not much confidence can be placed on each parameter estimate individually, a lot of confidence can be placed on the total spectral power estimate.

3.4 Correlations:

The largest problem that exists in both the spectral point fit and the polynomial fit is the large correlations between the parameter estimates for both models. A large correlation implies that a change in any one parameter estimate will drastically affect a different parameter estimate. Strong correlations generally impair the quality of the fit by creating a near-singular \mathbf{J} matrix, which reduces the accuracy of the parameter estimates, which can be seen in the large error bars of the spectral point fit. The errors associated with the parameter estimates in this model were unacceptable. Finding a set of parameters which are not correlated with one another is vital.

3.5 The multigroup model spectrum:

One way to reduce the deleterious correlation between parameter estimates is to use a multigroup model spectrum, where one divides the entire spectrum into a number of intervals. A set of numbers n_k are the average spectrum values within each interval k . The different n_k numbers are the fitting parameters. The edges of the interval will be placed at the edges of the

filter functions.² It is very important to use filter function edges because if a filter has strong sensitivity in more than one parameter range, correlation will again present a problem. For example, when a filter function has sensitivity in two spectral intervals, the spectral values of the two intervals will be strongly anti-correlated with one another. If one parameter estimate increases, the other is able to decrease without affecting the overall voltage reading of the channel. By using filter function edges as interval boundaries, this anti-correlation will be minimized.

3.6 The “flat-top” multigroup model spectrum:

A “flat-top” multigroup model spectrum is the simplest multigroup spectrum. In each interval, there is only one spectrum value. Thus, each interval will have a “flat-top”.

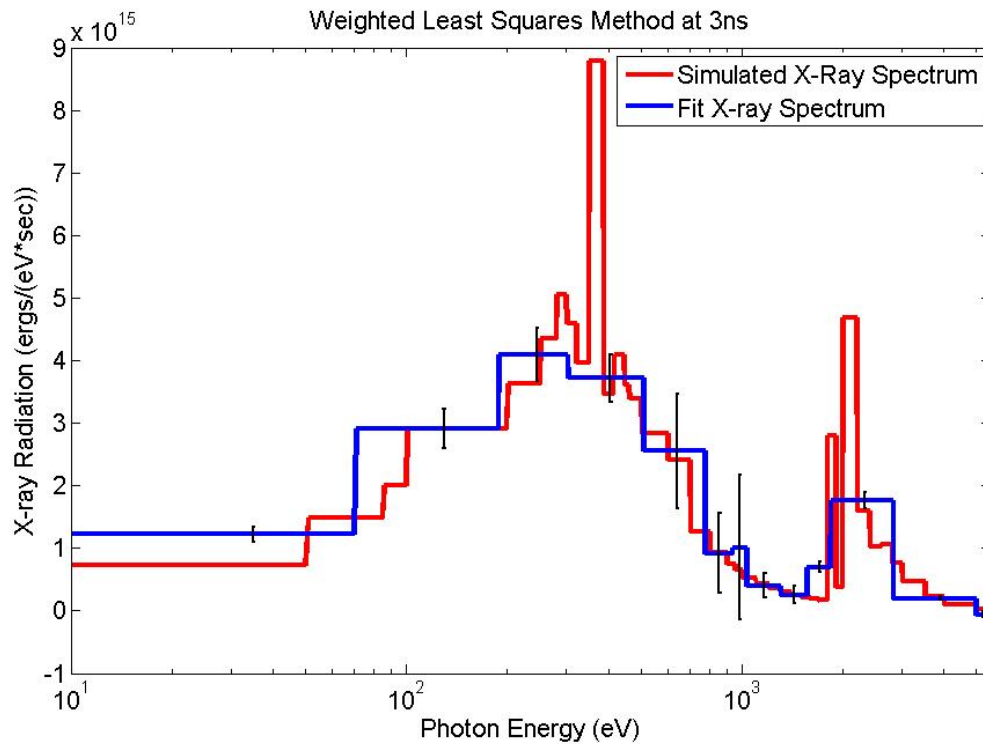


Fig. 5. A sample of the flat-top multigroup model spectrum with 13 intervals is shown. Error bars were generated based on a 10% accuracy in the voltage readings. Intervals were determined by the Dante filter function edges.

The “flat-top” multigroup model spectrum consistently models the general shape of the

actual spectrum. The error bars are also much smaller. However, almost no spectral detail is apparent in the model.

This model also minimizes spectral power uncertainty, which is estimated to be $5.07 \cdot 10^{18}$ ergs/sec, with a relative uncertainty in the spectral power of only 4.13%.

3.7 The “spectrum-top” multigroup model spectrum:

It is possible to use an expected spectrum as a guide when trying to fit Dante voltage readings. In this case, apparent detail in the fitted model spectrum that was not contained in the individual voltage readings is shown. This fit is an extension of the flat top model. Here, instead of using one average spectrum value in each interval as in the flat-top model, the form of the anticipated spectrum is retained within each interval. For this fit, an initial nominal guess of what the spectrum might possibly look like is needed. This nominal guess could be obtained from a LILAC simulation, for example, which has been done here. This nominal spectrum is broken up into several intervals and a multiplying factor n_k is added to the spectrum value in interval k as the adjustable model parameter.

This model spectrum fit shown in Fig. 6 is a very accurate representation of the spectrum. Almost all of the spectral detail has been artificially restored. This is not surprising, given that the shape of the model spectrum within each interval and the hypothetical voltage readings are obtained from the same LILAC-simulated spectrum. However, the relative uncertainties on each parameter are still quite large. This shows that errors are independent of how well the model spectrum fits the simulated spectrum.

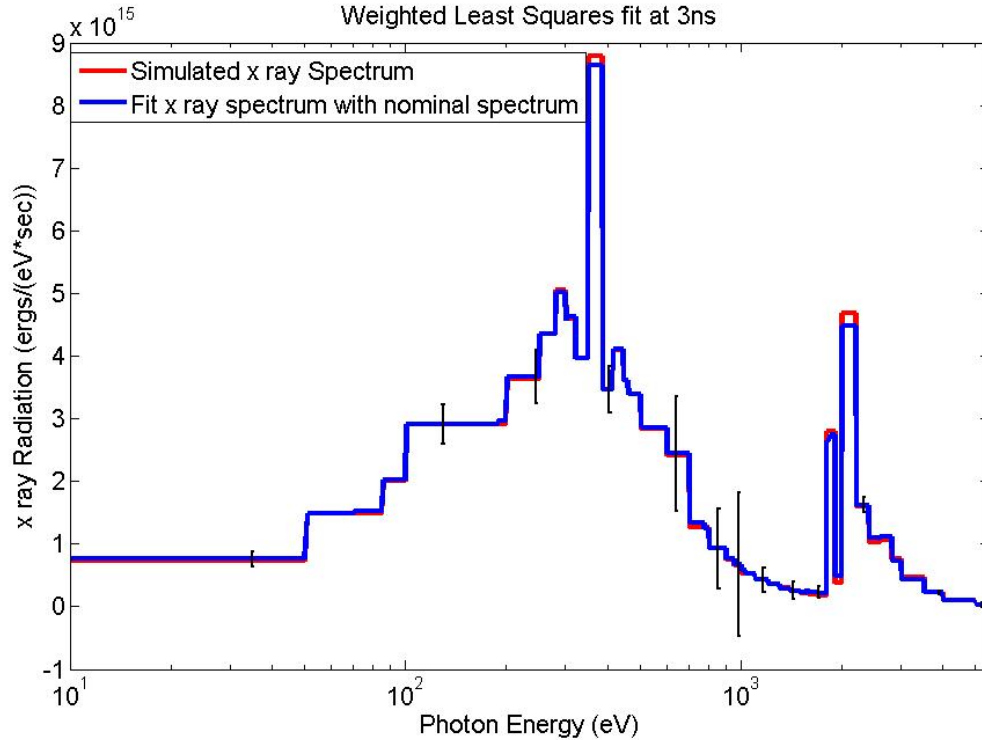


Fig. 6. A sample of a fit using the spectrum-top multigroup model spectrum with 13 intervals. Error bars were generated based on a 10% accuracy in the voltage readings. The LILAC simulation at 3 ns was folded into voltage readings and the simulated x ray spectrum at 2.98 ns was used as the nominal spectrum. Together, the voltages and the nominal spectrum were used to create the model.

The total model spectral power in this example was 5.42×10^{18} ergs/sec and the relative error was 3.87%. This small uncertainty in the estimate of the total power results from a 10% uncertainty in all of the voltage readings. Fifteen channels were used to estimate the total spectral power. According to the central limit theorem, one would expect $\sigma_y = \frac{\sigma_x}{\sqrt{n}}$ for n uncorrelated parameter estimates. Thus, the error in the total spectral power should approach $\frac{10\%}{\sqrt{15}}$ or 2.58% if the spectral model minimizes correlations, which it does. This verifies the methodology behind calculating the spectral power uncertainty.

4.1 Discussion

In the previous example of the spectrum-top multigroup model, the nominal spectrum happened to be very accurate. However, if the nominal spectrum is not accurate, it could force

the model spectrum to take a shape that does not resemble the actual spectrum. In this case, the “flat-top” multigroup model spectrum may be a better fit.

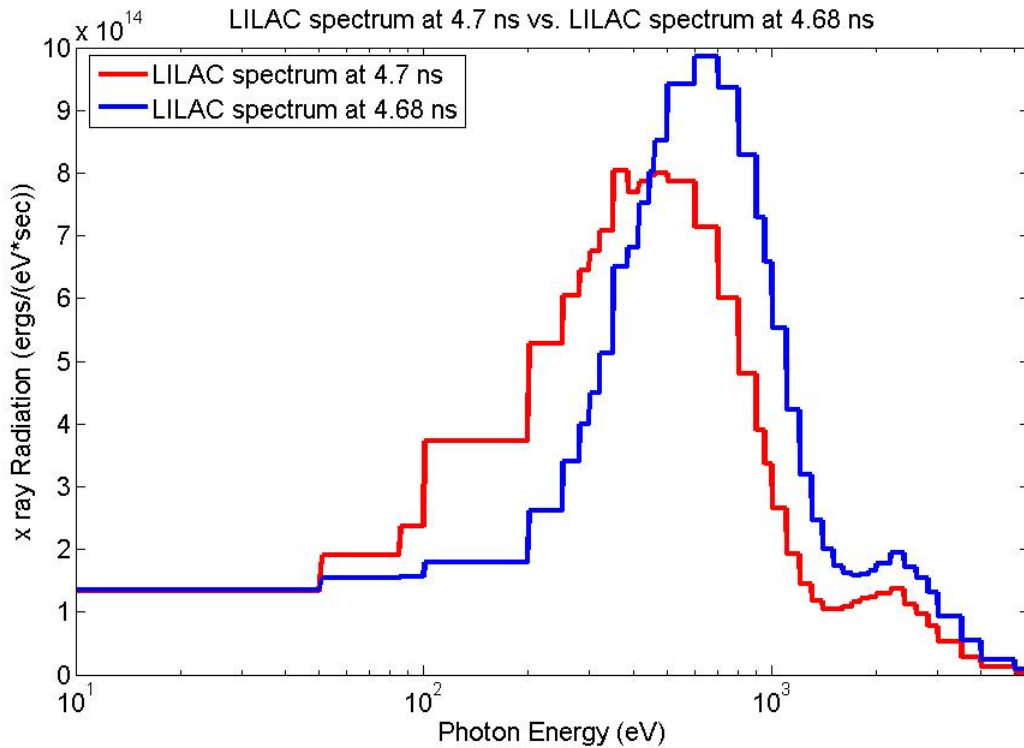


Fig. 7. LILAC spectra at 4.68 ns and 4.7 ns are shown. The spectrum at 4.7 ns is used as hypothetical data, and the spectrum at 4.68 ns is used to assign the shape of the fitting model spectrum within each spectral segment.

The spectrum at 4.68 ns is similar to the spectrum at 4.7 ns, but the peaks are shifted with respect to each other, as is shown in Fig. 7. The multigroup fitting process can only shift the model spectral values within their respective fixed spectral intervals, and the interval widths and positions are fixed. Thus, this model has a very difficult time predicting the shape of the spectrum.

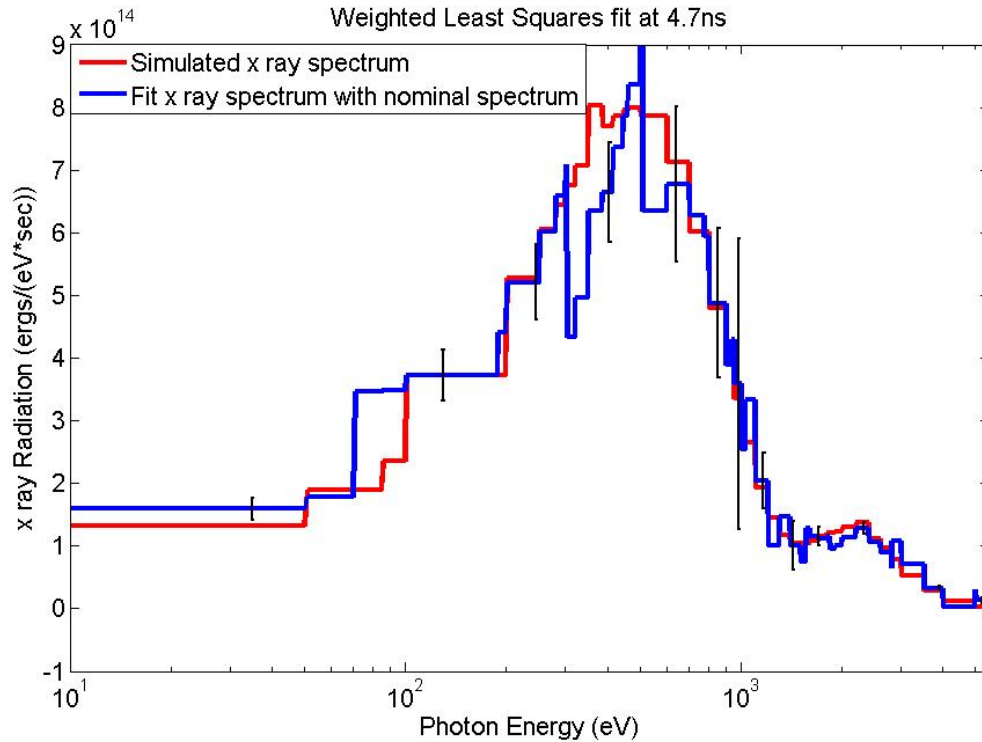


Fig. 8. A sample of the spectrum-top multigroup model spectrum fit with 13 intervals is shown. Error bars were generated based on a 10% accuracy in the voltage readings. The nominal spectrum was a LILAC simulated x-ray spectrum at 4.68 ns. Intervals were determined by Dante filter function edges.

In an attempt to fit the spectrum at 4.7 ns with the nominal spectrum at 4.68 ns, spurious spectral detail was created, as can be seen in Fig. 8. The program attempted to fit the behavior of the spectrum at higher photon energies with the nominal spectrum. As a result, the spectral peak at around 300 eV is mangled. In this example, the attempt to recover more spectral detail by anticipating it has reduced the reliability of the fit. A “flat top” model fit shown in Fig. 9 appears to recover less spectral detail, but is less vulnerable to the hazard of making poor nominal guesses. The “flat top” model is more reliable, in the sense that it does not create spectral information that does not exist in the first place. In addition, it still creates a fairly good representation of the spectrum.

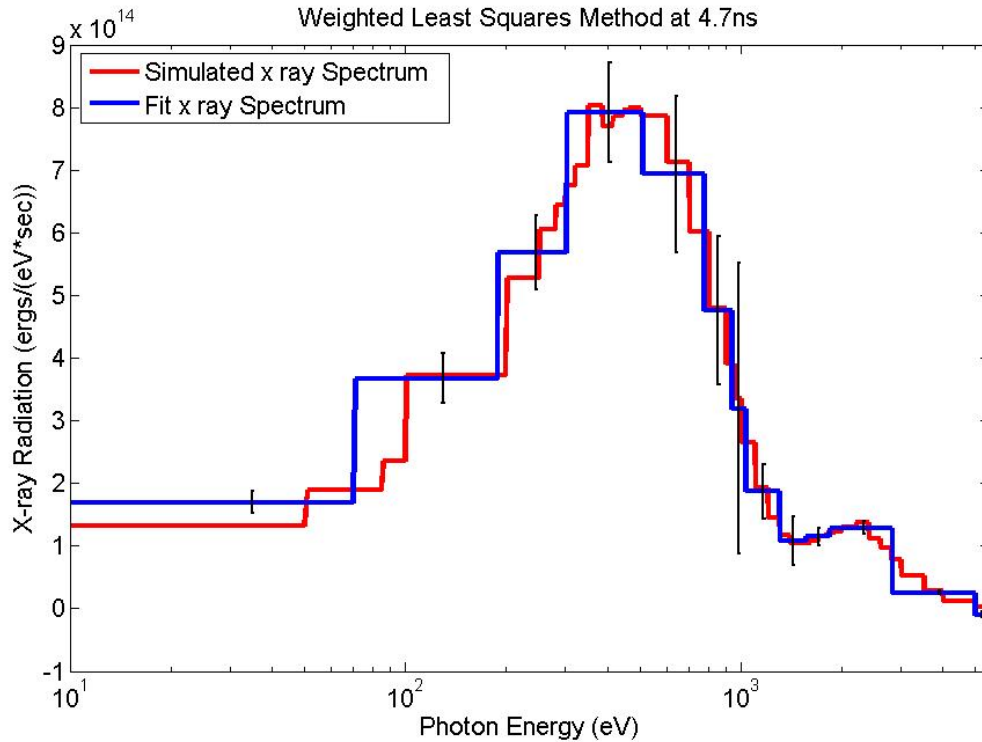


Fig. 9. A sample of the flat-top multigroup model spectrum fit with 13 intervals is shown. Error bars were generated based on a 10% accuracy in the voltage readings. Intervals were determined by Dante filter function edges.

When little confidence can be placed in the nominal spectrum, the “flat top” spectrum should be used because it is more reliable and will not create irrelevant spectral detail. However, if a lot of confidence can be placed in the “spectrum top” model, then the “spectrum top” model should be used because the spectral detail will be maintained.

5.1 Conclusion:

The weighted least squares method has been used to unfold x ray spectra obtained from simulated multi-channel spectrometer data using LILAC simulated spectra from laser-irradiated targets. The spectra emitted from these targets have been modeled with 15 parameters within 4 distinct modeling methods: the polynomial fit, the spectral point fit, the “flat top” multigroup model spectrum fit, and the “spectrum top” multigroup model spectrum fit. Each model utilizes the weighted least squares method to fit its parameters. The polynomial fit is able to capture the

basic curvature of the spectrum. However, this fit is crippled by correlation between parameter estimates. Furthermore, the shapes of polynomial functions are not characteristic of spectra. The spectral point model also introduces correlations that deleteriously affect the reliability of this fit. Formal estimates of the parameter variances reveal unreliability in the parameter estimates. The last two fits used multigroup models. This multigroup model divides the spectrum into groups based on filter function edges. These fits eliminate much of the correlation between parameter estimates. The “flat top” multigroup model is able to consistently capture the essential shape of the spectrum. The “spectrum top” multigroup model allows the user to enter a nominal spectrum and produces a good fit if the spectral detail can be anticipated with confidence. This model introduces artificial spectral detail if the first guess is not good enough. Only when confidence can be placed in the nominal spectrum can confidence be also placed in the “spectrum top” multigroup model. Otherwise, the more modest flat top multigroup model should be used.

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