1 Introduction

The problem of fitting an event distribution when the total expected number of events is not fixed, keeps appearing in experimental studies. Peelle’s Pertinent Puzzle (PPP) notes that in a $\chi^2$ fit, if overall normalization is one of the parameters to be fit, the fitted curve may be seriously low with respect to the data points, sometimes below all of them. This puzzle was the subject of a NIM article by G. D’Agostini (NIMA 346 (1994) 306). This problem and the solution for it are well known within the statistics community, but, apparently, not well known among some of the physics community. The purpose of this note is didactic, to explain the cause of the problem and the easy and elegant solution.

The solution is to use maximum likelihood (ML) instead of $\chi^2$. The essential difference between the two approaches is that ML uses the normalization of each term in the $\chi^2$ assuming it is a normal distribution, $1/\sqrt{2\pi\sigma^2}$. In addition, the normalization is applied to the theoretical expectation not to the data. In the present note we illustrate what goes wrong and how maximum likelihood fixes the problem in a very simple toy example which illustrates the problem clearly and is the appropriate physics model for event histograms. We then note how a simple modification to the $\chi^2$ method gives a result identical to the ML method. I will also discuss the models in G. d’Agostini’s article (p. 309) and add one more.

2 Toy Model–$\chi^2$

Consider a simple data set with only two bins. Theory predicts that the expected value of $N$, the number of events in the bin should be the same for each bin, and that the bins are uncorrelated. Let $x_1$ and $x_2$ be the number of events experimentally found in the two
bins. The variance ($\sigma^2$) is $N$ for each bin, ($\sigma = \sqrt{N}$).

$$\chi^2 = \frac{(N - x_1)^2}{\sigma^2} + \frac{(N - x_2)^2}{\sigma^2}. \quad (1)$$

We want to find the minimum, $\frac{\partial \chi^2}{\partial N} = 0$. Call term 1, the derivative with respect to the numerators of the $\chi^2$.

$$\text{Term 1} = 2 \frac{(N - x_1 + N - x_2)}{N} = 2(1 - \frac{x_1}{N}) + 2(1 - \frac{x_2}{N}). \quad (2)$$

If we ignore the derivative of the denominator, then Term 1 = 0, is solved by $N = \frac{x_1 + x_2}{2}$. Call this the naive solution.

Call Term 2 the derivative with respect to the denominator of the $\chi^2$

$$\text{Term 2} = -\frac{(N - x_1)^2 + (N - x_2)^2}{N^2}. \quad (3)$$

Term 2 is negative and $O(1/N)$. The only way that Term 1 + Term 2 = 0 is for Term 1 to be positive. This means that the $\chi^2$ solution must have $N$ greater than the naive value. Although Term 1 is $O(1)$, $x_1/N$ and $x_2/N$ are $O(1/N)$. $N$ is pulled up as the fit wants to make the fractional errors larger. (Had the normalization been put into the data not the theoretical value, the fitted curve would have been low.)

### 3 Toy Model--Maximum Likelihood

The likelihood ($L$) is the probability density function for the two bins assuming each bin has a normal distribution. (This requires $N$ is not too small).

$$L = \frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(N-x_1)^2/(2\sigma^2)} e^{-(N-x_2)^2/(2\sigma^2)}. \quad (4)$$

For $\sigma^2 = N$, the log of the likelihood is:

$$\ln L = -\ln(2\pi) - \ln N - \chi^2/2. \quad (5)$$

Let Term 3 be the derivative of the normalization.

$$\text{Term 3} = -\frac{1}{N}. \quad (6)$$

The derivative of the $\ln L$ is Term 3 $- (\text{Term 1})/2 - (\text{Term 2})/2$. 

$$\text{Term 3} - (\text{Term 2})/2 = -\frac{1}{N} + \frac{(N - x_1)^2 + (N - x_2)^2}{2N^2} = -\frac{2N + (N - x_1)^2 + (N - x_2)^2}{2N^2}. \quad (7)$$
Since the expectation value $E(N - x_1)^2 = E(N - x_2)^2 = N$, the expectation value of Term 3 - (Term 2)/2 = 0. For fitted values a modification is needed. Assume that there is only one overall normalization factor and assume now that there are $n_b$ bins. The expectation value for a $\chi^2$ with $n_b$ bins and $n_f$ fitted parameters is $n_b - n_f$. This occurs because, after fitting, the multidimensional normal distribution loses $n_f$ variables. This means, for $n_b = 2$, $n_f = 1$, the value of Term 2 is $2 \times 1/2 = 1$. The same loss in dimensions requires term 3, the normalization term of the multidimensional distribution to be multiplied by $(n_b - n_f)/n_b$ to match the change in $\chi^2$ since the fit has integrated over those variables. The change in expectation value occurs automatically in the fit, but the modification to Term 3 must be put in by hand.

There is an easy general way to handle this problem. The problem arises because the error matrix is a function of normalization. When the simple $\chi^2$ method is applied, the derivative of the $\chi^2$ is in error because the change in the normalization of the particle density function is not taken into account. Including this term in the ML approach eliminates the problem. This leads to a simple approach using a modified $\chi^2$ analysis. Consider $n_b$ bins and $g$ fitting parameters $p_j$. Let $n_i(p_1, p_2, \cdots, p_g)$ be the expected number of events in bin $i$. The distribution of experimental events in each bin is taken as approximately normal. The total number of events in the histogram is not fixed. Choose the set $n_i$ as the basis. The error matrix is diagonal in this basis. Ignoring the $2\pi$ constants:

$$\ln L = \sum_{i=1}^{n_b} -\frac{\ln n_i}{2} - \frac{(x_i - n_i)^2}{2n_i}. \quad (8)$$

$$\frac{d \ln L}{dn_i} = \frac{x_i - n_i}{n_i} + \frac{1}{2n_i} [(\frac{(x_i - n_i)^2}{n_i}) - 1]. \quad (9)$$

The expectation value for the term in square brackets is zero. Recall that the expectation refers to the average value over a number of repetitions of the experiment. It is $x_i$ that changes with each experiment not the theoretical expectation, $n_i$. The expectation value of the term in square brackets will remain zero even if it is multiplied by a complicated function of the $p_j$ fitting parameters. Ignoring this term leads to:

$$\frac{\partial \ln L}{\partial p_j} = \sum_{i=1}^{n_b} (\frac{x_i - n_i}{n_i}) \frac{\partial n_i}{\partial p_j}. \quad (10)$$

By expressing the $n_i$ as the appropriate functions of the $p_j$, the error matrix can be written in terms of the $p_j$. However, the derivative of the inverse error matrix does not appear in the transform of Equation 10. This result means that one can use a modified $\chi^2$ approach. Use the usual $\chi^2$, but, when derivatives are taken to find the $\chi^2$ minimum, omit the derivatives of the inverse error matrix. The result is identical to the result from ML. The modified $\chi^2$ method should be generally used in place of the regular $\chi^2$ method.
In practice, since the differences are not precisely the expectation values for a given experiment, there is a small residual higher order effect, which causes no bias on the average.

4 Review of G. D’Agostini’s models

The problem he discusses is a bit different than that treated in the toy model. He imagines that we have two measurements of the same physical quantity, but that there is a possible scale error $f$ and a best value $k$ of two measurements, $x_1$ and $x_2$ to be fit. The models presented by D’Agostini can be written in the form:

$$
\chi_n^2 = \frac{(fx_1 - k)^2}{f^n \sigma_1^2} + \frac{(fx_2 - k)^2}{f^n \sigma_2^2} + \frac{(f - 1)^2}{\sigma_f^2} = \frac{(x_1 - k/f)^2}{f^{n-2} \sigma_1^2} + \frac{(x_2 - k/f)^2}{f^{n-2} \sigma_2^2} + \frac{(f - 1)^2}{\sigma_f^2}. \tag{11}
$$

He treats the cases $n=2$ (Model A) and $n=0$ (Model B). We will also discuss the case $n = -1$. D’Agostini finds that $n = 2$ does not exhibit PPP, but $n = 0$ does exhibit it.

There are two errors in the method of D’Agostini, which we have already mentioned in the previous section.

- The use of the $\chi^2$ distribution incorrectly ignores the changes of normalization of the multidimensional density distribution as the normalization parameter is changed.

- The normalization parameter $N$ should be included in the theoretically expected value, not in the data value. The experimentally observed number of events is what it is. D’Agostini’s $f = 1/N$. This has two effects. The first effect is that the normalization dependence of the error matrix is changed. The second effect is that the average of $N$ is not the same as the average of $1/N$.

First consider the ML solution. Using $N$ as normalization,

$$
\chi^2 = \frac{(x_1 - Nk)^2}{N^{2-n} \sigma_1^2} + \frac{(x_2 - Nk)^2}{N^{2-n} \sigma_2^2} + \frac{(N - 1)^2}{\sigma_N^2}. \tag{12}
$$

It is assumed here that $\sigma_N^2$ is a fixed number, rather than having $\sigma_f^2$ fixed. Let

$$
\chi^{2*} = \chi^2 - \frac{(N - 1)^2}{\sigma_N^2}. \tag{13}
$$

The derivative of the numerator of $\chi^2$ with respect to $N$ is:

$$
\frac{2(Nk - x_1)}{N^{2-n} \sigma_1^2} + \frac{2(Nk - x_2)}{N^{2-n} \sigma_2^2} + \frac{2(N - 1)}{\sigma_N^2}. \tag{14}
$$
The derivative of the denominator is:

\[ \frac{n - 2}{N} \chi^2. \]  

(15)

For ML the \( N \) dependent part of the normalization term is \((1/\sqrt{N^2-n})^2\). The log of this term is \(-(2-n)\ln N\) and the derivative of the log with respect to \( N \) is \((n-2)/N\). For ML then:

\[
\frac{\partial \text{ML}}{\partial N} = \frac{n - 2}{N} - \frac{1}{2} \left( \frac{2(Nk - x_1)}{N^2 - n\sigma_1^2} + \frac{2(Nk - x_2)}{N^2 - n\sigma_2^2} + \frac{2(N - 1)}{\sigma_N^2} + \frac{(n - 2)}{N} \chi^2. \right)
\]

(16)

Here, the expectation value of the \( \chi^2 \) term is 1 after fitting and the normalization term is reduced to \((n - 2)/(2N)\) to account for the loss of a degree of freedom. For any \( n \), the ML normalization term cancels the expectation value of the denominator derivative.

Next look at this using D’Agostini’s calculation. For any \( n \) value, the derivative with respect to \( k \) is:

\[
\frac{\partial \chi^2}{\partial k} = \frac{2}{f^{n-1}} \left[ \frac{(k/f - x_1)}{\sigma_1^2} + \frac{(k/f - x_2)}{\sigma_2^2} \right] = 0.
\]

(17)

Hence,

\[
k = f \left( \frac{x_1}{\sigma_1^2} + \frac{x_2}{\sigma_2^2} \right) / \left( \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} \right),
\]

(18)

which is the expected result from combining two measurements of the same quantity, except for the factor \( f \). Define the result for \( f = 1 \) to be \( \overline{x} \).

\[
\overline{x} = \left( \frac{x_1}{\sigma_1^2} + \frac{x_2}{\sigma_2^2} \right) / \left( \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} \right).
\]

(19)

Note that for \( \frac{\partial \chi^2}{\partial f} \), the derivative of the numerators of the first two terms together (using \( \frac{(f x_1 - k)^2}{f^2 \sigma_1^2} + \frac{(f x_2 - k)^2}{f^2 \sigma_2^2} \)) has been determined to be zero from the \( \frac{\partial \chi^2}{\partial k} \) derivative.

4.1 \( n = 2 \), Model A

Using the result from the derivative with respect to \( k \), it is seen that for the derivative with respect to \( f \), (using the 2nd expression in Equation 11 with \( f^{n-2} = 1 \) in the denominator), the derivatives of the first two terms add to be zero from the result of the derivative with respect to \( k \) seen in Equation 17, and then \( f \) is forced to be 1. D’Agostini finds that this does not have a PPP problem as expected since the variance is independent of \( f \).
4.2 $n = 0$, Model B

$$\chi^2_B = \frac{(fx_1 - k)^2}{\sigma_1^2} + \frac{(fx_2 - k^2)^2}{\sigma_2^2} + \frac{(f - 1)^2}{\sigma_f^2} = \frac{(x_1 - k/f)^2}{\sigma_1^2} + \frac{(x_2 - k/f)^2}{\sigma_2^2} + \frac{(f - 1)^2}{\sigma_f^2}. \quad (20)$$

$$\frac{\partial \chi^2_B}{\partial k} = 2\left[ \frac{(f - kx_1)}{\sigma_1^2} + \frac{(k - fx_2)}{\sigma_2^2} \right]. \quad (21)$$

Here, $f$ will not be one. Using the result from the partial derivative with respect to $k$, $\chi^2_B$ can be written:

$$\frac{\partial \chi^2_B}{\partial f} = 2f^2\left[ \frac{(x_1 - \bar{x})^2}{\sigma_1^2} + \frac{(x_2 - \bar{x})^2}{\sigma_2^2} \right] + 2\frac{(f - 1)}{\sigma_f^2}. \quad (22)$$

$$\frac{1}{f} = \sigma_f^2\left[ \frac{1}{\sigma_1^2} + \frac{(x_1 - \bar{x})^2}{\sigma_1^2} + \frac{(x_2 - \bar{x})^2}{\sigma_2^2} \right]. \quad (23)$$

$$f = 1/\left[ 1 + \sigma_f^2\left( \frac{(x_1 - \bar{x})^2}{\sigma_1^2} + \frac{(x_2 - \bar{x})^2}{\sigma_2^2} \right) \right]. \quad (24)$$

$$x_1 - \bar{x} = x_1 - \frac{(x_1^2 + x_2^2)/(1/\sigma_1^2 + 1/\sigma_2^2) = \frac{x_1 - x_2}{\sigma_1^2(1/\sigma_1^2 + 1/\sigma_2^2)}}. \quad (25)$$

Similarly,

$$x_2 - \bar{x} = \frac{x_2 - x_1}{\sigma_1^2(1/\sigma_1^2 + 1/\sigma_2^2)}.$$  

To find $f$, consider:

$$\frac{(x_1 - \bar{x})^2}{\sigma_1^2} + \frac{(x_2 - \bar{x})^2}{\sigma_2^2} = \frac{(x_1 - x_2)^2}{\sigma_1^2\sigma_2^2(1/\sigma_1^2 + 1/\sigma_2^2)^2} + \frac{(x_1 - x_2)^2}{\sigma_1^2\sigma_2^2(1/\sigma_1^2 + 1/\sigma_2^2)^2} = \frac{(x_1 - x_2)^2}{\sigma_1^2 + \sigma_2^2}. \quad (26)$$

$$f = \frac{1}{1 + \sigma_f^2(x_1 - x_2)^2/(\sigma_1^2 + \sigma_2^2)^2}. \quad (27)$$

$f$ is always less than one. This is the result obtained by D’Agostini.

4.3 $n = -1$, the Toy Model

Use the notation of D’Agostini. Again the first two terms of $\frac{\partial \chi^2_{n=1}}{\partial f}$ are zero.

$$\frac{\partial \chi^2_{n=-1}}{\partial f} = \frac{1}{f}\left[ \frac{(fx_1 - k)^2}{f^{-1}\sigma_1^2} + \frac{(fx_2 - k)^2}{f^{-1}\sigma_2^2} \right] + 2\frac{(f - 1)}{\sigma_f^2}. \quad (28)$$

The expectation value of the first two terms is $\frac{2}{f}$.

$$\frac{\partial \chi^2_{n=-1}}{\partial f} \approx \frac{2}{f} + \frac{2(f - 1)}{\sigma_f^2}. \quad (29)$$
This will be far from $f = 1$, unless $\sigma_f << 1$. However, the ML term is $\frac{1}{f}$.

$$\frac{\partial \ln \mathcal{L}_{n=1}}{\partial f} = \frac{1}{f} - \frac{\chi^2_{n=1}}{2} \approx \frac{1}{f} - \frac{1}{f} - \frac{(f-1)}{\sigma_f^2}. \quad (30)$$

For the ML method, $f = 1$.

5 Summary

The PPP problem arises because the $\chi^2$ method incorrectly ignores the normalizations of the multidimensional probability density functions when the total expected number of events is not fixed. For an event histogram the maximum likelihood method is correct if:

- Errors are taken as the square root of the theory model; they are not to be taken as the square root of the number of events in the bin.
- The normalization factor is included with the theory model.
- The subtraction for noise is included with the theory model. The data is the number of events obtained experimentally. All corrections belong to the theory model.

This ML result is completely equivalent to a modified $\chi^2$ approach. Use the usual $\chi^2$, but, when derivatives are taken to find the $\chi^2$ minimum, omit the derivatives of the inverse error matrix.