Comments to the article ”Parametric fitting of data obtained from detectors with finite resolution and limited acceptance” by Gagunashvili [1]

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Abstract

The publication [1] suffers from several caveats: i) The method is based upon the false assumption that the median of χ² distributed random variables is χ² distributed. ii) The information contained in the data is not fully used, iii) It is not clear how the uncertainties associated to the fitted parameters can be evaluated. A correct solution of the problem is presented and results of Ref. [1] are compared to results obtained using the approach described in our textbook [2]. Finally, we correct false statements in [1] about a section in our book.

1 Introduction

The determination of parameters of a theory from experimental data that are distorted by experimental effects is a relatively simple problem. This is why the solution of this problem had not been published in a referenced scientific journal so far, but last year Gagunashvili has submitted the cited paper.

The problem is solved in the following way: The experimental data are compared to a Monte Carlo simulation in form of histograms of the observed variable $x'$ which due to the finite experimental resolution differs from the true variable $x$. A χ² expression is formed that measures the statistical difference between the two histograms. The simulated histogram depends on the parameter $\theta$ of interest. ($\theta$ may also represent a set of parameters.) In a least square (LS) fit the parameters are estimated. The effect of changing the parameters is implemented by changing the weights of the simulated events, $w(x) = f(x|\theta)/f(x|\theta_0)$ where $x$ is the undistorted variable, $\theta$ the parameter of interest of the p.d.f. $f(x|\theta)$ and $\theta_0$ its value used in the simulation. This is explained in more detail in Ref. [2].

The purpose of this comment is twofold: i) We want to point out some caveats of the treatment in Ref. [1] which will lead in some applications to biased results and wrong error assignments. A correct solution is presented. ii) We want to correct several false statements in this article in respect to our textbook [2]. In a numerical example we compare our results to those published in Ref. [1].

2 The χ² approximation - multinomial versus Poisson distribution

To illustrate the problem, we look at a simple example: In an experiment the slope of a linear distribution is to be measured. A certain amount of data has been accumulated and distributed into histogram bins. The number of events in each bin follows a Poisson distribution the mean of which depends on the flux and the slope of the distribution. Usually the flux is not known and thus

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we have two unknown parameters, the slope and the normalization of our prediction to the data. The likelihood principle tells us that it does not matter whether the experiment has been stopped after a certain running time or after a certain amount of data had been collected. This follows from the likelihood principle and has been shown explicitly in Ref. \cite{3} for the maximum likelihood estimate (MLE). Asymptotically, in the Gaussian approximation which we use below, the least square (LS) expression coincides with half the negative log-likelihood function up to irrelevant terms and thus also the LS estimate is independent of the stopping condition. In Ref. \cite{1} it is assumed that the number of events is fixed and a multinomial approach is applied. This condition is rarely realized and does not require the multinomial treatment but the latter is correct, too.

For a Poisson distributed number of events \( d_i \) in a histogram bin \( i \) and predictions \( t_i \) which depend on parameters of interest, the distribution \( W(d_1,...,d_B) \) in the histogram with \( B \) bins is described by

\[
W = \prod_{i=1}^{B} P(d_i|t_i)
\]

(1)

where \( P(m|\lambda) \) is the Poisson distribution of \( m \) with mean \( \lambda \). It can also be written as

\[
W = P(d|t)M(d_1,...,d_B|p_1,...,p_B,d)
\]

(2)

with \( d = \sum_{i=1}^{B} d_i, t = \sum_{i=1}^{B} t_i, p_i = t_i/t \) and \( M \) the multinomial distribution for \( d \) events distributed into \( B \) bins with probabilities \( p_1,...,p_B \). Relations (1) and (2) describe the same distribution. We are free to use either form (see also Ref. \cite{4}), but (1) is to be preferred in our problem because the formulas become much simpler than with (2). In \cite{1} \( \chi^2 \) is evaluated based upon multinomial statistics, while in \cite{2} Poisson statistics has been applied. Both ways are correct, but the multinomial approach is involved because correlations have to be handled explicitly.

If only relative predictions are available, we have to normalize the predictions. From the factorization of (2) we find the maximum likelihood estimate \( t = d \) which is introduced into (1), \( \Sigma t_i = \Sigma d_i = d \).

To compare \( B \) Poisson distributed numbers \( d_i \) to a prediction \( t_i \), we form the statistic \( \chi^2 = \sum_{i=1}^{B} [(d_i - t_i)^2/t_i] \) which follows a \( \chi^2 \) distribution with \( B \) degrees of freedom (NDF) in the approximation where for each bin \( i \) the Poisson distribution of \( d_i \) with mean \( t_i \) can be approximated by a normal distribution with mean and variance \( t_i \). When the predictions \( t_i \) are normalized, i.e. \( \Sigma d_i = \Sigma t_i \), we loose one degree of freedom (1 parameter estimated) and have \( NDF = B - 1 \). If \( P \) parameters of interest have to be estimated, we have \( NDF = B - P - 1 \).

If we have a Monte Carlo prediction consisting of \( K_i \) events in bin \( i \) with weights \( w_{ik} \), we have \( t_i = c\Sigma_k w_{ik} \) where \( c \) is an overall normalization constant and we get:

\[
\chi^2 = \sum_{i=1}^{B} \chi_i^2 = \sum_{i=1}^{B} \left( \frac{d_i - c\Sigma_k w_{ik}}{c\Sigma_k w_{ik}} \right)^2.
\]

(3)

When we estimate the parameters hidden in the weights, also \( c \) is a free parameter in the fit and as above \( NDF = B - P - 1 \). In \cite{3} the relative statistical error of \( t_i \) is assumed to be small compared to \( d_i^{-1/2} \). This covers probably more than 90 % of all cases in particle physics applications.

If the statistical error of the simulation cannot be neglected, we consider the asymptotic case where not only the distributions of \( d_i \) but also that of \( \Sigma_k w_{ik} \) can be approximated by normal distributions. We form

\[
\chi^2 = \sum_{i=1}^{B} \left( \frac{d_i - c\Sigma_k w_{ik}}{\sigma_i^2} \right)^2.
\]

(4)

To obtain a \( \chi^2 \) expression, the quantity \( \sigma_i^2 \) per definition has to be the variance of \( d_i - c\Sigma_k w_{ik} \) under the assumption that the prediction is correct. A reasonable approximation is obtained from error propagation, \( \sigma_i^2 = d_i + c^2\Sigma_k w_{ik}^2 \). This approximation is adequate in most of the remaining cases. A correct treatment includes \( \sigma \) in the fit. A maximum likelihood estimate (see Appendix 13, subsection 13.8.1 and relation (13.32) of Ref. \cite{2} in different notation and Ref. \cite{5} is:
\[ \hat{\sigma}_i^2 = c(d_{ik} \frac{\Sigma_k w_{ik}^2}{\Sigma_k w_{ik}} + \Sigma_k w_{ik}) \].  

(5)

To derive (5) the expected values \( E(w_{ik}) \) and \( E(w_{ik}^2) \) have been replaced by the empirical values \( \Sigma_k w_{ik}/K_i \) and \( \Sigma_k w_{ik}^2/K_i \). For convenience, the derivation of (5) is given in the Appendix.

The normalization \( c \) is a free parameter in the fit. Asymptotically, the fitted normalization reproduces the number of observed events.

3 Caveats, restrictions and difficulties of the approach described in [1].

3.1 The choice of the median

The difficulties in the approach in [1] are related to the application of the multinomial distribution where the correlations have to be explicitly handled. There, \( \chi^2_i \) is evaluated excluding bin \( i \) for all \( B \) values of \( i \) and then the median is computed without any explanation and discussion of its properties.

The ad hoc solution to take the median instead of the mean of many incomplete evaluations is used because the median is a robust estimator - an indication that something is problematic with this approximation, but both choices are wrong: Neither the mean nor the median of the \( \chi^2_{N_{DF}} \) distributed values is described by a \( \chi^2_{N_{DF}} \) distribution as long as the values are not identical. For a typical example taken from [6] and using Relation (34) of [6], we find that the mean value of the medians of samples of partially correlated random variables following a \( \chi^2_{B-2} \) distribution is typically by half a unit off the nominal value of \( N_{DF} = B - 2 \). This bias does not disappear with increasing statistics. As a consequence the evaluation of parameter uncertainties from the curvature of the \( \chi^2 \) curve near its maximum is doubtful and p-values derived from a \( \chi^2 \) test are wrong. The fact that in specific examples the point estimate is sensible does not validate the proposed procedure.

3.2 The loss of a constraint

Comparing a prediction of a histogram to a histogram of observed events where the prediction is to be normalized to the data, we have \( N_{DF} = B - 1 - P \) degrees of freedom, where \( P \) is the number of additional parameters of interest. In [1] due to the difficulties created by the correlations, one additional degree of freedom is given away, \( N_{DF} = B - 2 - P \). As a consequence, precision is lost and, for example, an asymmetry in a two-bin histogram cannot be determined.

3.3 The weight restriction

The weights in [1] are restricted to functions of the histogrammed variable. This condition is violated in unfolding problems. The weight restriction seems not to be necessary for unnormalized weights but this point should be clarified officially by the author.

3.4 The error treatment

In [1] it is not explained how the parameter errors are obtained in the fitting procedure. A parameter fit without error assignment is useless. The reader will probably assume that the errors are obtained in the standard way from the variation of \( \chi^2 \) as a function of the parameter (at some point MINUIT errors are quoted). However, the standard error estimation can be wrong independent of the fact that in the evaluation of the \( \chi^2 \) statistic the errors are correctly implemented as a function of the parameter values. The reason is explained in our book: It is related to the fact that due to the weighting the denominators of the \( \chi^2 \) expression may have a sizable dependence of the parameters. The effect is small in most applications but can be large, if histograms with a large number of bins and large smearing are fitted. Therefore, in situations where the uncertainty of the simulated
numbers cannot be neglected, the validity of the error assignment has to be checked, for instance by changing the amount of Monte Carlo events.

In addition to the problems related to weighting, the error handling in least square fits where crude approximations of the $\chi^2$ statistic are used should have been discussed. The effects are especially important with low event numbers.

### 3.5 Problems with small event numbers

In many experiments the number of events is so small that the application of a least square fit is problematic. In [1] no solution for this situation is presented. However in this case enough Monte Carlo events can be generated such that their statistical error is negligible and a Poisson likelihood fit can be performed as explained in Ref. [2][5].

### 3.6 Technical difficulties

In the approach of [1] a parameter fit with a histogram of $B$ bins requires for each change of the parameter during the minimum search $B$ additional fits of an auxiliary parameter. For a two-dimensional histogram with $20 \times 20$ bins and 1000 minimum searching steps in the fit this means that 400,000 auxiliary parameters have to be estimated in LS fits.

### 4 Inflicting statements about the content of our book

In Section 1 of Ref. [1] figures the following paragraph:

“In [2], a re-weighting procedure for fitting a Monte Carlo reconstructed distribution to the reconstructed data was proposed. The procedure is presented rather sketchily, and cannot be repeated even for the example that was used in [2] for illustration. There is not a clear explanation of how the parameters and the errors in them were calculated. The authors of [2] stated without proof, that the statistic used for the fitting of the parameters had a $\chi^2$ distribution but did not define the number of degrees of freedom. This makes it impossible to use this statistic for choosing the best model from a set of alternative models.”

The reference was our book Ref. [2].

These statements are false:

- **Two methods are proposed. The likelihood ratio solution is not mentioned** in Ref. [1]. There are two examples. May be, the explanations were a bit short but certainly understandable in the context of preceding chapters of our textbook. We would have been glad to furnish further explanations to Gagunashvili. Our method is considerably simpler than that proposed in Ref. [1], certainly not less precise and we are convinced that it is easier to understand than that presented in Ref. [1].

- Contrary to the statement of Ref. [1], in the two examples **no parameter estimates and errors were quoted**. The section the author of Ref. [1] refers to is Section 6.5.9, “Comparison of Observations with a Monte Carlo Simulation”. It is part of a chapter on parameter inference in which it is explained in detail how parameters and their errors are estimated in least square and likelihood fits (see Sections 6.5.3 and 6.5.5, subsection $\chi^2$ approximation). A subsequent chapter on interval estimation discusses error assignments even in more detail.

- The author apparently refers to formula (6.17) in different notation of Section 6.5.9 of our textbook:

$$\chi^2 = \sum_{i=1}^{B} \frac{(d_i - cm_i)^2}{cm_i}$$

where $d_i$ was as the number of experimental events in bin $i$, $cm_i$ the Monte Carlo prediction with $c$ a Monte Carlo normalization constant and $m_i$ the corresponding sum of weights in bin $i$, $B$ was the number of bins. It was stated that the formula is valid if the statistical uncertainty of $m_i$ is negligible. The formula was derived and explained in the section “$\chi^2$ approximation” where $\chi^2$ for a histogram with Poisson distributed numbers was discussed. The NDF are irrelevant for
parameter estimation. (The NDF has to be known in goodness-of-fit tests which is a different subject and which is treated in a subsequent chapter of our book. Independent of this fact, the number of degrees of freedom (NDF) for $\chi^2$ statistics depending on fitted parameters were defined in Chapter 3 and therefore are known to the reader. The relation needed to apply a goodness-of-fit test for weighted histograms (13.32) is given in the Appendix 13 where also the NDF are defined. The relation needed for parameter estimation in the case that the uncertainty of the simulation has to be taken into account is given in the subsection 13.8.4 but the statements in Ref. [1] referred to the main text.)

5 Example

To perform a quantitative comparison of our approach to that of Ref. [1], we have applied our method to the first example given in Ref. [1] which was also used in our book to illustrate our method. The slope of a linear distribution is to be adjusted. The p.d.f. is $f(x|\alpha) = (1 + \alpha x)/(1 + \alpha/2)$, with $x \in [0, 1]$ and $\alpha > -1$. For the “experimental” events the slope parameter was $\alpha = 1$ and for the Monte Carlo events $\alpha_m = 0$. Events were generated in the interval $[0, 1]$. The variable $x$ was smeared with a Gaussian resolution of $\sigma = 0.3$. The smeared distribution was subdivided into 5 or 20 bins of equal width in the range between $-0.3$ and $1.3$. The number of experimental and simulated events was 500, 5000 and 50000. Each case was simulated 10,000 times. Some choices required to take the error of the simulation into account. We applied formula (13.32) of Ref. [2] which corresponds to Eq. (5). The slope parameter is hidden in the weights $w_k$. In the least square fit we included only bins with more than 5 events. Not all combinations quoted in Ref. [1] were repeated.

We compare our results to those of Ref. [1] in Table 1. The results of Ref. [1] are quoted in parenthesis. In the lines denoted by “+” and “−” some kind of estimates of the positive and negative errors as defined in Ref. [1] are given. In addition to the mean of the slope parameter which has the nominal value one, we quote the root mean square deviation (r.m.s.) of the distribution of the fitted slope parameter. For high statistics our and the results of Ref. [1] agree, for small event numbers we observe mostly a smaller bias and obtain smaller errors. The results for the specific case with 5 bins, 500 observed and 500 simulated events are unstable because arbitrarily large parameter values occur if the number of experiments is continuously increased. Also other cases with small observed or simulated event numbers may suffer from some rare cases where large slopes are found. Therefore we are not sure that all differences that we observe are really significant. Anyway, least square fits based on a $\chi^2$ approximation are problematic with such low event numbers. For physics applications only the last column of the table with 20 bins and 50000 simulated events is relevant.

We have also applied a maximum likelihood fit. The results were similar to those from the least square fit.

6 Conclusions

The comparison of histograms of statistical data with a Monte Carlo prediction should be treated in the framework of Poisson statistics. The correlation of the event numbers in the different bins can be taken into account by the normalization of the data to the prediction in the fit. This approach is considerably simpler than the method of Ref. [1] which starts from a multinomial distribution.

The treatment of Ref. [1] is based on the false assumption that the median of a sample of $\chi^2$ distributed random variables also follows a $\chi^2$ distribution with the same number of degrees of freedom. As a consequence, error estimates based on the corresponding statistic are wrong. Furthermore the result does not exploit the full information of the data in that it gives away one degree of freedom. Small event number cannot be handled and there is no error treatment. In the quantitative comparison of the point estimates of the two approaches in a special example published in Ref. [1], the results are found to be similar but they are slightly more precise in our method.
Table 1: Results from fitting the linear slope parameter $\alpha$ (with nominal value unity, see text) with our method compared with the results from [1] (in parenthesis) for various sample sizes and bin numbers. Besides mean and root mean square (rms) values some positive and negative $+$, − error estimates as defined in [1] are given.

| # data | 5 bins  | 5 bins  | 20 bins | 20 bins |
|--------|---------|---------|---------|---------|
|        | MC      |         |         |         |
| 500    | mean    | 1.25 (1.29) | 1.11 (1.13) | 1.10 (1.17) | 1.00 (1.07) |
|        | +       | 3.37 (3.13) | 0.91 (0.81) | 1.65 (1.84) | 0.72 (0.79) |
|        | −       | 0.60 (0.66) | 0.46 (0.54) | 0.59 (0.61) | 0.43 (0.45) |
|        | rms     | 1.15     | 0.65     | 1.14     | 0.55     |
| 5000   | mean    | 1.12 (1.12) | 1.01 (1.01) | 1.11 (1.11) | 1.01 (1.00) |
|        | +       | 0.87 (0.93) | 0.21 (0.23) | 0.89 (0.91) | 0.20 (0.20) |
|        | −       | 0.48 (0.52) | 0.16 (0.17) | 0.47 (0.47) | 0.15 (0.16) |
|        | rms     | 0.66     | 0.19     | 0.64     | 0.18     |
| 50000  | mean    | 1.10 (1.10) | 1.00 (1.00) | 1.11 (1.10) | 1.00 (1.00) |
|        | +       | 0.86 (0.87) | 0.08 (0.09) | 0.77 (0.83) | 0.08 (0.08) |
|        | −       | 0.46 (0.49) | 0.07 (0.08) | 0.46 (0.45) | 0.07 (0.07) |
|        | rms     | 0.63     | 0.08     | 0.62     | 0.07     |

We reject the false assertions made in Ref. [1] with respect to our book.

7 Appendix: Proof of the relation (5)

We prove relation (5) for a single bin and drop the bin index. We consider the quantity $d - cK\bar{w}$, where $d$ and $K$ are Poisson distributed, $\bar{w}$ is the mean value of $K$ weights and $c$ is a normalization constant common to all bins. In the limit where $d, K$ approach infinity, the statistic

$$
\chi^2 = \frac{(d - cK\bar{w})^2}{c(d\mathbb{E}(w^2)/\mathbb{E}(w) + \mathbb{E}(K)\mathbb{E}(w))}
$$

is $\chi^2$ distributed with one degree of freedom. Equivalently, $\sqrt{\chi^2}$ is normally distributed with variance equal to one.

**Proof:**

We set

$$
t = K\bar{w}, \quad \tilde{t} = t\mathbb{E}(w)/\mathbb{E}(w^2), \quad \tilde{c} = c\mathbb{E}(w^2)/\mathbb{E}(w).
$$

Relation (7) now reads

$$
\chi^2 = \frac{(d - \tilde{c}\tilde{t})^2}{c(d\mathbb{E}(w^2)/\mathbb{E}(w) + \mathbb{E}(t))}.
$$

According to the central limit theorem, $d, t$ and $\tilde{t}$ are asymptotically normally distributed. Furthermore we have $\text{Var}(\tilde{t}) = \mathbb{E}(\tilde{t})$ which is typical for the Poisson distribution. As asymptotically the Poisson distribution approaches the normal distribution, we are allowed to use in the following the Poisson approximation of the distribution of $\tilde{t}$ instead of the normal distribution. (Without proof we claim that the Poisson approximation is closer to the true distribution than the normal approximation. Examples can be found in Ref. [2].)

The variance $\sigma^2$ of $d - \tilde{c}\tilde{t}$ is

$$
\sigma^2 = \text{var}(d) + \tilde{c}^2\text{var}(\tilde{t}).
$$

Under the hypothesis that our description is correct, $d$ and $\tilde{t}$ should follow related Poisson distributions with mean $\lambda$ and $\lambda/\tilde{c}$, respectively and

$$
\sigma^2 = \lambda(1 + \tilde{c}).
$$
We fix $\lambda$ to its maximum likelihood estimate from the log-likelihood function derived from the product of the two Poisson likelihoods:

$$\ln L = d \ln \lambda - \lambda + \tilde{t} \ln \frac{\lambda}{\tilde{c}} - \frac{\lambda}{\tilde{c}}.$$ 

Determining $\hat{\lambda}$ as usual from the root of $\partial \ln L / \partial \lambda$ and re-substituting $c$ using (8) we get

$$\hat{\lambda} = \frac{\tilde{c}}{1 + \tilde{c}} (d + \tilde{t})$$

and with

$$\sigma^2 = \tilde{c} (d + \tilde{t}) = c (d \mathbb{E}(w^2)/\mathbb{E}(w) + \mathbb{E}(t))$$

the assertion (7).

We replace the expected values by their empirical estimates and obtain (5).

Remark 1: A different and more complicated estimate of $\sigma$ is obtained if we use the normal approximations for the distributions of $d$ and $t$, but in the asymptotic limit the different approximations coincide. Therefore our result does not depend on the use of the Poisson approximation for the distribution of the weighted sum.

Remark 2: If $t(\theta)$ depends on a parameter $\theta$ that has to be estimated, the parameter $\lambda$ and in principle also $\mathbb{E}(w), \mathbb{E}(w^2)$ are nuisance parameters. Estimating them out is correct for the point estimate of $\theta$. For the interval estimate the three nuisance estimates depend on $\theta$. Eliminating them with Rel. (9a) and taking the empirical means corresponds to a profile likelihood treatment of the error estimate of $\theta$.

References

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