Parametric fitting of data obtained from detectors with finite resolution and limited acceptance

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Abstract

A goodness-of-fit test for the fitting of a parametric model to data obtained from a detector with finite resolution and limited acceptance is proposed. The parameters of the model are found by minimization of a statistic that is used for comparing experimental data and simulated reconstructed data. Numerical examples are presented to illustrate and validate the fitting procedure.

Keywords: fit Monte Carlo distribution to data, comparison experimental and simulated data, homogeneity test, weighted histogram, inverse problem, unfolding problem

1. Introduction

The probability density function (PDF) $P(x')$ of a reconstructed characteristic x' of an event obtained from a detector with finite resolution and limited acceptance can be represented as

$$P(x') = \frac{\int_{\Omega} p(x)A(x)R(x,x')\,dx}{\int_{\Omega'}\int_{\Omega} p(x)A(x)R(x,x')\,dx\,dx'}, \tag{1}$$

where $p(x)$ is the true PDF, $A(x)$ is the acceptance of the setup, i.e. the probability of recording an event with a characteristic x, and $R(x,x')$ is the experimental resolution, i.e. the probability of obtaining x' instead of x after the reconstruction of the event. The integration in (1) is carried out over the domain Ω of the variable x and the domain Ω' of the variable x'.

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There are two ways of fitting a parametric model $p(x, a_1, a_2, \ldots, a_l)$ of the true PDF to reconstructed data:

1. Find an estimate $p_u(x)$ of the true PDF $p(x)$ by solving an unfolding problem, and then fit a parametric model of the true PDF $p(x, a_1, a_2, \ldots, a_l)$ to the unfolded distribution $p_u(x)$.
2. Fit a parametric model of the reconstructed PDF, that is,

$$\frac{\int_\Omega p(x, a_1, a_2, \ldots, a_l) A(x) R(x, x')\, dx}{\int_{\Omega'} \int_\Omega p(x, a_1, a_2, \ldots, a_l) A(x) R(x, x')\, dx\, dx'}, \tag{2}$$

   directly to the reconstructed data.

These two possibilities have been discussed in [1, 2]. The acceptance $A(x)$ and the resolution function $R(x, x')$ must be defined for both methods. In the majority of cases, they cannot be found analytically, and a Monte Carlo method is used instead for that purpose. The unfolding (inverse) problem is known to be an ill-posed problem and cannot be solved without a priori information about the solution. Any solution of this problem has, in addition to statistical errors due to the finite statistics of the experimental data, also systematic errors related to the use of a priori information. These systematic errors have an influence on the choice of the parametric model and the estimation of the parameters in the first method. The second method avoids the use of an unfolding procedure and is preferable [1, 2].

After discretization of the problem, the authors of [1] found the acceptance function $A(x)$ and the resolution function $R(x, x')$, and then used these functions to fit the parameters of the true distribution. The main disadvantage of this approach is that the resolution function $R(x, x')$, which is a matrix after discretization, has rather noisy matrix elements because in real cases the size of the Monte Carlo sample of events is of the same order as the size of the experimental sample of events. Another source of uncertainty is the discretization. Also, the authors of [1] did not propose a statistic that could be used for a goodness-of-fit test.

In [2], a reweighting procedure for fitting a Monte Carlo reconstructed distribution to the reconstructed data was proposed. The procedure was 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 χ^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 parametric models.

Recently, a test for comparing a weighted histogram [3] that is a generalization of the classical chi-square test [4] has been proposed. In this paper, we apply the results obtained in [3] to develop a procedure for direct parametric fitting of data obtained from detectors with finite resolution and limited acceptance.

This paper is organized as follows. In Section 2, a method for fitting the parameters of the model of the true PDF to the data and a goodness-of-fit test are proposed. A statistic for comparing a histogram with unweighted entries and a histogram with weights that depend on the parameters is used for that purpose. In Section 3, a numerical example that demonstrates how one can estimate the parameters and the statistical errors in them practically is presented. A numerical experiment with 10 000 runs is described to validate the proposed method.

2. Parametric fitting of Monte Carlo results to data

We consider the PDF $P_1(x')$ of a reconstructed characteristic of experimental events and the PDF $P_2(x')$ of the corresponding reconstructed characteristic of the Monte Carlo events for the same detector.

A histogram with m bins for a given PDF $P_1(x')$ is used to estimate the probability P_{1i} that a random event belongs in bin i:

$$P_{1i} = \int_{S'_i} P_1(x')\,dx',\ i = 1, \ldots, m. \tag{3}$$

The integration in (3) is carried out over the bin S'_i, and $\sum_1^m P_{1i} = 1$. The histogram can be obtained as the result of a random experiment with the PDF $P_1(x')$. We denote the number of random events belonging to the ith bin of the histogram by n_{1i}. The total number of events in the histogram is equal to $n_1 = \sum_{i=1}^m n_{1i}$. The quantity $\hat{P}_i = n_{1i}/n_1$ is an estimator of P_{1i} with an expectation value $\mathrm{E}\,\hat{P}_{1i} = P_{1i}$.

A histogram of the Monte Carlo reconstructed PDF $P_2(x')$ can be obtained as the result of a random experiment (simulation) that has three steps [5]:

1. A random value x is chosen according to a PDF $g(x)$. The function $g(x)$ is some expected true (initial) distribution defined in the domain Ω.
2. We go back to step 1 again with probability $1 - A(x)$, and to step 3 with probability $A(x)$.
3. A random value x' is chosen according to the PDF $R(x, x')$.

The events x' are distributed according to the PDF $P_2^{in}(x')$, where

$$P_2^{in}(x') = \frac{\int_\Omega g(x)A(x)R(x,x')\,dx\,dx'}{\int_{\Omega'}\int_\Omega g(x)A(x)R(x,x')\,dx\,dx'}. \tag{4}$$

The quantity $\hat{P_{2i}^{in}} = n_{2i}/n_2$, where n_{2i} is the number of events belonging to the ith bin for a histogram with total number of events n_2, is an estimator of P_{2i}^{in},

$$P_{2i}^{in} = \int_{S_i'} P_2^{in}(x')\,dx',\ i = 1, \ldots, m, \tag{5}$$

with the expectation value of the estimator equal to

$$\mathrm{E}\,\hat{P_{2i}^{in}} = P_{2i}^{in}. \tag{6}$$

It is expected that $A(x)$ and the resolution function $R(x, x')$ for the real setup and for the Monte Carlo simulation will be the same. This is achieved by adjusting the Monte Carlo simulation program and by a suitable choice of the domains Ω and Ω' of the variables x and x'.

In experimental particle and nuclear physics, step 3 is the most time-consuming step of the Monte Carlo simulation. This step is related to the simulation of the process of transport of particles through a medium and the rather complex registration apparatus.

To use the results of the simulation with an initial PDF $g(x)$ to calculate a histogram of events distributed according to the PDF $P_2(x')$ with a true PDF $p(x)$, we write the equation for P_{2i} in the form

$$P_{2i} = \frac{\int_{S_i'}\int_\Omega p(x)A(x)R(x,x')\,dx\,dx'}{\int_{\Omega'}\int_\Omega p(x)A(x)R(x,x')\,dx\,dx'} = \int_{S_i'}\int_\Omega w(x)g(x)A(x)R(x,x')\,dx\,dx', \tag{7}$$

where

$$w(x) = p(x)/g(x)\int_{\Omega'}\int_\Omega p(x)A(x)R(x,x')\,dx\,dx' \tag{8}$$

is the weight function. Because of the condition $\sum_i P_{2i} = 1$, we shall call the weights defined above "normalized weights" from now on, as opposed to the unnormalized weights $\check{w}(x)$, which are given by $\check{w}(x) = \text{const} \cdot w(x)$.

The Monte Carlo reconstructed histogram for the PDF $P_2(x')$ can be obtained using reconstructed events for the PDF $P_{2i}^{in}(x')$ with weights calculated according to (8). In this way, we avoid step 3 of the simulation procedure, which is important in cases where one needs to calculate Monte Carlo reconstructed histograms for many different true PDFs.

We denote the sum of the weights of the events in the ith bin of the histogram with normalized weights by

$$W_i = \sum_{k=1}^{n_{2i}} w_i(k), \tag{9}$$

where n_{2i} is the number of events in bin i and $w_i(k)$ is the weight of the kth event in the ith bin. The quantity $\hat{P}_{2i} = W_i/n_2$ is an estimator of P_{2i} with expectation value $\mathrm{E}\,\hat{P}_{2i} = P_{2i}$.

A frequently used technique in data analysis is the comparison of a reconstructed PDF with a Monte Carlo reconstructed PDF through a comparison of histograms. The hypothesis of homogeneity [4] states that the two histograms represent random values with identical distributions. This is equivalent to assuming that there exist m constants $p_1, \ldots, p_m$ such that $\sum_{i=1}^{m} p_i = 1$ and that the probability of belonging to the ith bin for some measured value in the experiment and in the Monte Carlo simulation is equal to p_i.

From here onwards, we use the weighted histogram with *unnormalized* weights and $\check{W}_i$ denote the sum of the weights of the events in bin i. This is convenient because the calculation of normalization factors is quite problematic in many practical cases.

We introduce the statistics [3]

$$X_k^2 = \frac{1}{n_1} \sum_{i=1}^{m} \frac{n_{1i}^2}{p_i} - n_1 + \frac{s_k^2}{n_2} + 2s_k, \tag{10}$$

where

$$s_k = \sqrt{\sum_{i \neq k} r_i p_i \sum_{i \neq k} r_i \check{W}_i^2/p_i} - \sum_{i \neq k} r_i \check{W}_i \tag{11}$$

and

$$r_i = \sum_{k=1}^{n_{2i}} \check{w}_i(k) / \sum_{k=1}^{n_{2i}} \check{w}_i^2(k), \tag{12}$$

with the sums extending over all bins i except one bin k. In these equations, the probabilities p_i are unknown, and estimators of $\hat{p}_i$ can be found by minimization of (10). We denote by $\hat{X}_k^2$ the value of X_k^2 after substitution of the estimators $\hat{p}_i$ into (10). As shown in [3], the statistic

$$\hat{X}^2 = \mathrm{Med}\,\{\hat{X}_1^2, \hat{X}_2^2, \ldots, \hat{X}_m^2\} \tag{13}$$

has a χ^2_{m-2} distribution if the hypothesis of homogeneity is valid. The use of the chi-square test is inappropriate if any expected frequency is less than 1, or if the expected frequency is less than 5 in more than 20% of the bins for either histogram.

We substitute the PDF $p(x)$ by the parametric formula $p(x, a_1, a_2, \ldots, a_l)$; the weights of the Monte Carlo events and the statistic $\hat{X}^2(a_1, a_2, \ldots, a_l)$ are then dependent on the parameters. The estimators $\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_l$ of the parameters $a_1, a_2, \ldots, a_l$ can be found by minimization of this statistic. The statistic $\hat{X}^2(\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_l)$ has a χ^2_{m-2-l} distribution if the parametric model fits the data, because l parameters are estimated. It can be used for a goodness-of-fit test for selection of the best model from a set of alternative models.

3. Numerical example and test evaluation

We took the true PDF, as in [2], to be of the form

$$p(x) = (1 + x)/1.5, \tag{14}$$

defined on the interval [0,1]. The reconstructed PDF was defined as

$$P_1(x') = \frac{\int_\Omega p(x) A(x) R(x, x')\, dx}{\int_{\Omega'} \int_\Omega p(x) A(x) R(x, x')\, dx\, dx'}, \tag{15}$$

with an acceptance function $A(x) = 1$ and a resolution function of the form

$$R(x, x') = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x - x')^2}{2\sigma^2}\right), \tag{16}$$

with $\sigma = 0.3$. The domain of the variable x was taken as $\Omega = [0, 1]$ and that of x' as $\Omega' = [-0.3, 1.3]$. A simulation of events with a PDF $P_1(x')$ was done according to the algorithm described in the previous section.

For the Monte Carlo reconstructed PDF, we used the initial PDF $g(x) = 1$ and chose the parametrization for the true PDF in the form

$$p(x, a) \propto 1 + ax. \tag{17}$$

The Monte Carlo reconstructed PDF was defined as

$$P_2(x') = \frac{\int_\Omega p(x, a)A(x)R(x, x')\,dx}{\int_{\Omega'}\int_\Omega p(x, a)A(x)R(x, x')\,dx\,dx'}. \tag{18}$$

Monte Carlo events were simulated according to the algorithm described in the previous section with $g(x)$ as the initial PDF. Weights of events were calculated according to the formula $\breve{w}(x) = 1-ax$. Reconstructed and Monte Carlo reconstructed samples were simulated by generating $5 \cdot 10^2$, $5 \cdot 10^3$, and $5 \cdot 10^4$ events in the first step. We chose 5-bin and 20-bin histograms and used pairs of histograms with various numbers of events in the fitting procedure. 10 000 simulation runs were done for each case. To investigate the fitting procedure, the following quantities were calculated:

- Average values $\overline{a} = \sum_1^{1000} \hat{a}(i)/10\,000$ of the estimated parameter, where i is the run number.

- Average statistical errors $\overline{\Delta}$ of the estimated parameter. For this purpose, the various realizations of the estimator $\hat{a}$ were ordered, and then the positive error was defined as the minimal interval with lower bound $\overline{a}$ that contained 34.1345% of the realizations of $\hat{a}$ and the negative error was defined as the minimal interval with upper bound $\overline{a}$ that contained 34.1345%.

- The real sizes of the test α_s for a nominal test size $\alpha = 5\%$ were estimated as the fraction of runs that had a p-value lower than 5%.

The program MINUIT [6] was used for the minimization of $\hat{X}^2(\hat{a})$ and for error analysis.

The results of this calculation are presented in Table 1. We may notice that the estimators are biased in the cases where at least one histogram is the result of a simulation of $5 \cdot 10^2$ events. The bias is lower for 20-bin than for

5-bin histograms. The errors are asymmetric, and the asymmetry is reduced if the statistics of the generated events are reduced. The sizes of the tests α_s are close to the nominal value of $\alpha = 5\%$; see [3] for details of the method of comparison.

In the right part of Table 1, we present results of calculations for the case where "$\sigma = 0$", or $R(x, x') = \delta(x - x')$, which helps us to understand the effect of the resolution function. The results of calculations for "infinite" statistics of the Monte Carlo simulation are also presented. In this case, the data histograms were fitted by probabilities $p_i(a)$ that were calculated analytically:

$$p_i(a) = \int_{b_i}^{b_i+1/m} (1 + ax)\, dx \Big/ \int_0^1 (1 + ax)\, dx = \frac{1 + ab_i + a/2m}{m + ma/2}, \qquad (19)$$

where b_i is the lower bound of bin i. The statistic

$$\sum_{i=1}^{m} \frac{(n_{1i} - n_1 p_i(a))^2}{n_1 p_i(a)} \qquad (20)$$

was used to estimate the parameters and for goodness-of-fit tests. This case represents the best result that can be achieved for given statistics of the data, and is useful for comparison. The results presented in Table 1 show that a deterioration of the resolution leads to an increase in the statistical error of $\hat{a}$ and also a bias. We observe an asymmetry in the errors even in the case of an "infinite" Monte Carlo simulation. Note that the statistics (20) for the estimated values of the parameters $\hat{a}$ have a χ^2_{m-2} distribution if the experimental histogram is the result of a random experiment with probabilities $p_i(a), i = 1, \ldots, m$ [4].

For the purposes of illustration, we present the results of a parametric fit of the Monte Carlo results to the data for one of the cases described above. The numbers of generated events for the data and the Monte Carlo simulation were taken equal to $5 \cdot 10^3$, and we used histograms with 20 bins. The result of fitting with MINUIT was $\hat{a} = 1.11^{+0.30}_{-0.23}$, with $\hat{X}^2(\hat{a}) = 11.72$ and the p-value equal to 0.82. A comparison of the histograms of the true PDF with the weighted histogram of the Monte Carlo true PDF gave $\hat{X}^2(\hat{a}) = 18.03$, and the p-value was equal to 0.45. Figure 1a shows the histograms of the reconstructed PDF and of the Monte Carlo reconstructed PDF, calculated with the weights of the events equal to $1 + 1.11x$. Figure 1b shows the histograms of the true PDF and of the Monte Carlo true PDF.

Table 1: Mean values $\overline{a}$ of parameter estimates $\hat{a}$, mean values $\overline{\Delta}$ of errors of parameter estimates $\hat{a}$, and sizes of test α_s for a nominal size of test $\alpha = 5\%$. Calculations were done for histograms of the reconstructed PDF and Monte Carlo reconstructed PDF with various numbers of generated events n_{da} and n_{mc} for numbers of bins $m = 5$ and $m = 20$. The left part of the table presents calculations for a resolution function with $\sigma = 0.3$, and the right part for $\sigma = 0$.

$\sigma = 0.3$

n_{da}		$m=5$ n_{mc} $5{\cdot}10^2$	$5{\cdot}10^3$	$5{\cdot}10^4$	$m=20$ n_{mc} $5{\cdot}10^2$	$5{\cdot}10^3$	$5{\cdot}10^4$
$5{\cdot}10^2$	$\overline{a}$	1.29	1.16	1.13	1.17	1.07	1.07
	$\overline{\Delta}$	$^{+3.13}_{-0.66}$	$^{+1.16}_{-0.52}$	$^{+0.81}_{-0.54}$	$^{+1.84}_{-0.61}$	$^{+0.85}_{-0.46}$	$^{+0.79}_{-0.45}$
	α_s	5.2%	6.1%	6.3%	4.8%	5.2%	5.3%
$5{\cdot}10^3$	$\overline{a}$	1.12	1.02	1.01	1.11	1.02	1.00
	$\overline{\Delta}$	$^{+0.93}_{-0.52}$	$^{+0.30}_{-0.22}$	$^{+0.23}_{-0.17}$	$^{+0.91}_{-0.47}$	$^{+0.28}_{-0.22}$	$^{+0.20}_{-0.16}$
	α_s	6.1%	5.8%	5.5%	5.3%	5.2%	5.8%
$5{\cdot}10^4$	$\overline{a}$	1.10	1.01	1.00	l.10	1.01	1.00
	$\overline{\Delta}$	$^{+0.87}_{-0.49}$	$^{+0.22}_{-0.17}$	$^{+0.09}_{-0.08}$	$^{+0.83}_{-0.45}$	$^{+0.20}_{-0.16}$	$^{+0.08}_{-0.07}$
	α_s	5.4%	6.0%	5.7%	5.4%	5.7%	5.6%

$\sigma = 0$

n_{da}		$m=5$ n_{mc} $5{\cdot}10^2$	$5{\cdot}10^3$	$5{\cdot}10^4$	∞	$m=20$ n_{mc} $5{\cdot}10^2$	$5{\cdot}10^3$	$5{\cdot}10^4$	∞
$5{\cdot}10^2$	$\overline{a}$	1.08	1.05	1.04	1.04	1.04	1.02	1.01	1.01
	$\overline{\Delta}$	$^{+0.68}_{-0.44}$	$^{+0.48}_{-0.34}$	$^{+0.44}_{-0.33}$	$^{+0.43}_{-0.29}$	$^{+0.62}_{-0.39}$	$^{+0.44}_{-0.30}$	$^{+0.42}_{-0.28}$	$^{+0.40}_{-0.29}$
	α_s	6.0%	6.0%	6.4%	5.0%	5.1%	5.6%	5.4%	4.7%
$5{\cdot}10^3$	$\overline{a}$	1.03	1.01	1.00	1.00	1.02	1.01	1.00	1.00
	$\overline{\Delta}$	$^{+0.40}_{-0.34}$	$^{+0.17}_{-0.15}$	$^{+0.13}_{-0.11}$	$^{+0.12}_{-0.10}$	$^{+0.38}_{-0.31}$	$^{+0.16}_{-0.14}$	$^{+0.12}_{-0.10}$	$^{+0.11}_{-0.10}$
	α_s	6.0%	5.9%	5.8%	4.8%	5.5%	5.6%	5.6%	4.6%
$5{\cdot}10^4$	$\overline{a}$	1.04	1.00	1.00	1.00	l.02	1.00	1.00	1.00
	$\overline{\Delta}$	$^{+0.40}_{-0.32}$	$^{+0.12}_{-0.11}$	$^{+0.05}_{-0.05}$	$^{+0.03}_{-0.03}$	$^{+0.36}_{-0.32}$	$^{+0.11}_{-0.11}$	$^{+0.05}_{-0.05}$	$^{+0.03}_{-0.03}$
	α_s	5.7%	5.5%	5.8%	4.9%	5.5%	6.0%	5.6%	5.3%

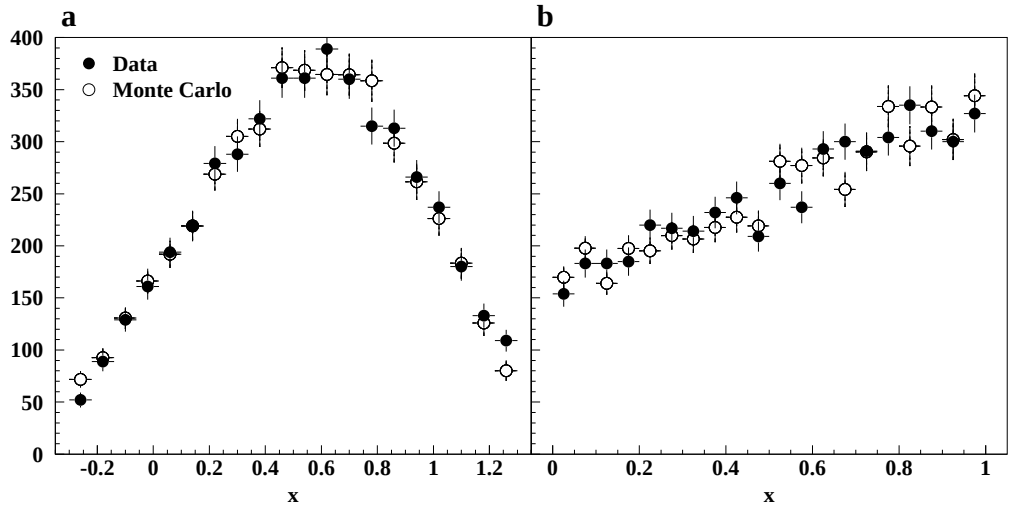

Figure 1: Results of parametric fit of Monte Carlo results to data: (a) histograms of reconstructed PDF and Monte Carlo reconstructed PDF; (b) histograms of true PDF and Monte Carlo true PDF.

For convenience of visual comparison, the Monte Carlo histograms have been divided by a factor $1 - \hat{a}/2 = 1 - 1.11/2$ in both figures.

4. Conclusions

A method of fitting a parametric model to data measured with a detector with finite resolution and limited acceptance has been developed. It was developed as an application of a test for comparing histograms with unweighted entries and histograms with unnormalized weights proposed in previous work by the present author. The method demonstrates a new approach to the direct parametric fitting of experimental data that permits one to decrease the systematic errors in the estimated parameters. It is a rather flexible tool for data analysis that can be used with multidimensional data, and does not have any restrictions on the configuration of the bins or the domain of the variables investigated. A goodness-of-fit test has been proposed that can be used for selection of the best parametric model from a set of alternative models for describing the data. An evaluation of the method has been done numerically for histograms with various numbers of bins and numbers of events. A numerical example has been given to demonstrate the use of the method in practice.

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