Unfolding problem clarification and solution validation

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Abstract

The unfolding problem formulation for correcting experimental data distortions due to finite resolution and limited detector acceptance is discussed. A novel validation of the problem solution is proposed. Attention is drawn to the fact that different unfolded distributions may satisfy the validation criteria, in which case a least informative approach using entropy is suggested. The importance of analysis of residuals is demonstrated.

Key words: deconvolution, inverse problem, maximum entropy, chi-square test, regularisation

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1. Introduction

The probability density function (PDF) $P(x')$ of an experimentally measured characteristic $x'$, differs in general, from the true physical PDF $p(x)$. Formally the relation between $P(x')$ and $p(x)$ is given by equation

$$P(x') \propto \int_{\Omega} p(x) A(x) R(x'|x) dx,$$  

(1)

where $A(x)$ is the probability of recording an event with a characteristic $x$ (the acceptance); $R(x'|x)$, is the probability of obtaining $x'$ instead of $x$ (the experimental resolution).

If a parametric (theoretical) model $p(x, a_1, a_2, \ldots, a_l)$ for the true PDF is known, then the unfolding can be done by determining the parameters,
e.g., by a least squares fit to the binned data \([1-4]\). Here, the model, that allows a description of the true distribution by a finite number of parameters, constitutes a priori information that is required for correcting the distortions by the experimental setup.

In contrast, model-independent unfolding, as considered in \([5-15]\), is an underspecified problem, and every approach to solve it requires a priori information about the solution. Smoothness, positiveness and shape of the solution are examples of this a priori information. Methods differ, directly or indirectly, in the way a priori information is incorporated into the result.

In this article we discuss problems of model-independent unfolding, namely what the solution of the unfolding problem is and how to validate it. This is especially important because it affects our interpretation of physical data to which unfolding methods have been applied.

2. Unfolding problem and solution validation

An unfolded distribution \(\hat{p}(x)\) can be defined as a distribution that satisfies the validation criteria. The only objective method for validation of the solution \(\hat{p}(x)\) is to compare the measured \(P(x')\) with Monte-Carlo reconstructed \(\hat{P}(x')\) distributions simulated with PDF \(\hat{p}(x)\).

In practical applications there is a sample of experimentally measured events with \(P(x')\) distribution and a sample of simulated Monte-Carlo events with \(\hat{P}(x')\) distribution. To compare the two distributions a homogeneity hypothesis test is used:

\[
H_0 : P(x') = \hat{P}(x').
\]  

(2)

There are several methods to test the hypothesis of homogeneity. Here we will use the chi-square test \([17]\) since it can be used for both one-dimensional and multidimensional cases.

Let us represent the distributions of events \(P(x')\) and \(\hat{P}(x')\) by two \(k\)-bins histograms with \(N\) and \(M\) the numbers of events respectively. The test statistic

\[
X^2 = \frac{1}{MN} \sum_{i=1}^{k} \frac{(Mn_i - Nm_i)^2}{n_i + m_i}
\]  

(3)

has approximately a \(\chi^2_{k-1}\) distribution, if hypothesis \(H_0\) is valid \([17]\). Here \(n_i\) and \(m_i\) are the numbers of events in the \(i\)th bin of the histograms.
The chi-square test p-value must be calculated according to the formula

\[ p\text{-value} = \int_{+\infty}^{x^l/2-1} \frac{x^l/2-1 e^{-x/2}}{2^{l/2}\Gamma(l/2)} dx, \]  

(4)

where \( l = k - 1 \), see Ref. [18]. Hypothesis of homogeneity must be rejected if \( p\)-value is lower than a predefined significance level. Significance levels 0.1, 0.05 and 0.01 are usually used in statistical analysis.

The validation procedure can include an analysis of the residuals \( r_i, i = 1, ..., k \) that is helpful for identification of the bins of the histograms responsible for a significant overall \( X^2 \) value. The adjusted (normalized) residuals [19] are the most convenient for the analysis:

\[ r_i = \frac{n_i - N\hat{p}_i}{\sqrt{N\hat{p}_i(1 - N/(N + M))(1 - (n_i + m_i)/(N + M))}}, \]  

(5)

where

\[ \hat{p}_i = \frac{n_i + m_i}{N + M}. \]  

(6)

If the hypotheses of homogeneity \( H_0 \) are valid then the residuals \( r_i \) are approximately independent and identically distributed random variables with standard normal PDF \( \mathcal{N}(0, 1) \). Analysis of the residuals increases the power of a validation procedure (see illustration Example 3 in Section 3).

Graphical methods are routinely used for analysis of residuals [20]. Graphs representing dependencies \( r_i(x') \) and \( r_i(P(x')) \) can be considered. Residuals for both plots must fluctuate near the line \( r = 0 \) with the same variability, since they are approximately independent and identically distributed random variables, if hypothesis of homogeneity is valid.

A quantile-quantile plot is used to test if residuals are random variables with the standard normal PDF \( \mathcal{N}(0, 1) \) [18].

To make a quantile-quantile plot:

- Order residuals from the smallest to the largest \( r_{(1)}, r_{(2)}, ..., r_{(k)} \), where \( r_{(i)} \) is the \( i\)-th smallest;
- Calculate data quantiles \( r_{(i)} = [(i - 0.5)/k] \)th data quantile;
- Calculate theoretical quantiles \( r^*_i = [(i - 0.5)/k] \)th theoretical quantile,
where \( r^*_i \) is the solution of the equation

\[
(i - 0.5)/k = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{r^*_i} e^{-\frac{x^2}{2}} dx;
\]  \hspace{1cm} (7)

- Plot the points \((r(i), r^*_i)\).

If the distribution of residuals is close to a standard normal one, the plotted points will lie close to a straight line with a slope equal to 1.

Use of the chi-square tests is inappropriate if any expected frequency is below 1 or if the expected frequency is less than 5 in more than 20% of bins \[18\]. Expected frequency for the bin \(i\) of the histogram representing \(P(x')\) is equal to \(\hat{p}_i N\) and for the histogram representing \(\hat{P}(x')\) is equal to \(\hat{p}_i M\).

As mentioned in the introduction, solution of the main equation (1) is an underspecified problem. It means that an infinite number of solutions satisfying the validation criteria exists. \textit{A priori} information must be used to choose a particular solution among an infinite number of them.

If reasonable \textit{a priori} information is absent then the least informative solution of the problem can be chosen. One of the ways is to choose an unfolded distribution with a maximal value of entropy \[21, 22\]

\[
H(\hat{p}(x)) = -\int \hat{p}(x) \ln \hat{p}(x),
\]  \hspace{1cm} (8)

which is the solution with the lowest information content. This approach can be helpful to avoid artifacts, such as false peaks.

An unfolded distribution can be considered as the result of measuring a probability density function by a hypothetical set-up with better resolution. A similar interpretation of an unfolded distribution can be found in \[5, 16\].

Comparison of different unfolding algorithms is only possible when the same \textit{a priori} information about the solution is applied. Blind tests of algorithms do not make any sense without a clearly defined \textit{a priori} information.

3. Numerical examples

Following Ref. \[5\] let us assume a true distribution that is described by a sum of two Breit-Wigner functions \[5\]

\[
p(x) \propto 2 \cdot \frac{1}{(x-10)^2 + 1} + \frac{1}{(x-14)^2 + 1}
\]  \hspace{1cm} (9)
from which the experimentally measured distribution is obtained by the function

\[ P(x') \propto \int p(x) A(x) R(x'|x) \, dx, \tag{10} \]

with the acceptance \( A(x) \):

\[ A(x) = 1 - \frac{(x - 10)^2}{36} \tag{11} \]

and the resolution function describing Gaussian smearing (Figure 1):

\[ R(x'|x) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{(x' - x)^2}{2\sigma^2} \right), \sigma = 1.5. \tag{12} \]

An example of the measured distribution obtained by simulating a sample of \( N = 10^4 \) events is also shown in Figure 1. A histogram with a number of bins \( k = 89 \) and an approximately equal number of events in each bin was used.

![Figure 1: Acceptance \( A(x) \) and resolution function \( R(x'|x) \) for \( x = 10 \) (left) and a histogram of the measured distribution \( P(x') \) based on a sample of \( 10^4 \) events generated for the true distribution (right). Bin contents of the histogram are normalised to the bin width. The true distribution \( p(x) \) is shown by the curve (right).](image)

### 3.1. Example 1

Here an application of the validation method is demonstrated for the “ideal” case when the unfolded distribution \( \hat{p}_1(x) \) coincide with the true distribution, i.e.

\[ \hat{p}_1(x) = p(x). \tag{13} \]
Ten thousand events were simulated by a random number generator with a seed different from the one used for the measured distribution $P(x')$.

The results of unfolding validation are shown in Figure 2. It demonstrates how the Monte-Carlo reconstructed distribution $\hat{P}_1(x')$ (solid line), corresponding to the unfolded distribution $\hat{p}_1(x)$, agrees with the measured distribution $P(x')$ (markers with error bars) (Figure 2a). Unfolded distribution $\hat{p}_1(x)$ (solid line), multiplied by $10^4$ for convenience, is shown at the same plot. Residuals and quantile-quantile plots are represented on Figures 2b,c,d. No structure is observed in any of the control plots. The homogeneity test $p$-value is equal to 0.576, and the entropy $H(p_1(x)) = 2.408$.

![Figure 2](image_url)

Figure 2: (a) $10^4 \cdot \hat{p}_1(x)$ and Monte-Carlo distribution $\hat{P}_1(x')$ (solid lines) compared to the measured distribution $P(x')$ (markers with error bars); (b) normalized residuals as a function of $\hat{P}$; (c) normalized residuals as a function of $x'$; (d) quantile-quantile plot for the normalized residuals.
3.2. Example 2

This example demonstrates that \( \hat{p}_1(x) \) is not the only unfolded distribution that satisfies the validation criteria.

Let us consider an unfolded distribution

\[
\hat{p}_2(x) \propto p(x)(1 + 0.4 \sin(5x)).
\]  

Figure 3: (a) \( 10^4 \cdot \hat{p}_2(x) \) and Monte-Carlo distribution \( \hat{P}_2(x') \) (solid lines) compared to the measured distribution \( P(x') \) (markers with error bars); (b) normalized residuals as a function of \( \hat{P} \); (c) normalized residuals as a function of \( x' \); (d) quantile-quantile plot for the normalized residuals.

The results of unfolding validation are shown in Figure 3. It demonstrates how the Monte-Carlo reconstructed distribution \( \hat{P}_2(x') \) (solid line), corresponding to the unfolded distribution \( \hat{p}_2(x) \), agrees with the measured distribution \( P(x') \) (markers with error bars) (Figure 3a). Unfolded distribution \( \hat{p}_2(x) \) (solid line), multiplied by \( 10^4 \) for convenience, is shown at the same
plot. Residuals and quantile-quantile plots are represented on Figures 3b,c,d. No structure is observed in any of the control plots. The homogeneity test $p$-value is equal to 0.444, and entropy $H(p_2(x)) = 2.367$.

All these results show that the proposed PDF $\hat{p}_2(x)$ is also an unfolded distribution. It can be explained in terms of signal processing.

Acceptance is a filter in a “time domain” and any continuation of the unfolded distribution $\hat{p}_2(x)$ outside the interval [4; 16] does not have an influence on the reconstructed distribution $\hat{P}_2(x)$.

A resolution function is an acceptance in a “frequency domain” and is a low pass frequency filter. A high frequency component in the unfolded distribution $\hat{p}_2(x)$ does not have any effect on the reconstructed distribution $\hat{P}_2(x)$. Increasing the statistics of events does not lead to rejection of the homogeneity hypothesis.

For the true distribution $\sim p(x)(1 + 0.4 \sin(5x))$ the least informative approach would lead us accept $\hat{p}_1(x)$ rather than $\hat{p}_2(x)$ as unfolded distribution because $H(\hat{p}_1(x)) > H(\hat{p}_2(x))$.

### 3.3. Example 3

The homogeneity hypothesis test and analyses of residuals were proposed as validation criteria. The example illustrates the importance of residual analysis.

Let us take an unfolded distribution as:

$$\hat{p}_3(x) \propto 2 \left\{ \frac{0.8^2}{(x - 10)^2 + 0.8^2} + \frac{0.8^2}{(x - 14)^2 + 0.8^2} \right\}. \quad (15)$$

The results of unfolding validation are shown in Figure 4. It demonstrates how the Monte-Carlo reconstructed distribution $\hat{P}_3(x')$ (solid line), corresponding to the unfolded distribution $\hat{p}_3(x)$, agrees with the measured distribution $P(x')$ (markers with error bars) (Figure 4a). Unfolded distribution $\hat{p}_3(x)$ (solid line), multiplied by $10^4$ for convenience, is shown at the same plot. Residuals and quantile-quantile plots are represented on Figures 3b,c,d. Figures 4b and 4c demonstrate deviation of residual fluctuation from the line $r = 0$. Figure 4d demonstrates deviation of points on the quantile-quantile plot from the straight line with slope equal to 1. The homogeneity test $p$-value is equal to 0.477. However, the distribution $\hat{p}_3(x)$ does not satisfy validation criteria because the analysis of residuals does not satisfy the hypothesis of homogeneity.
4. Summary and conclusions

A novel validation method for an unfolded distribution is proposed in this work. A solution of the unfolding problem is defined as a distribution that satisfies validation criteria. The unfolding problem does not have a unique solution and one of the ways to define a least informative solution to this problem is discussed here. A least informative approach to the unfolding problem can be recommended as a first step. Solid a priori information in an unfolding procedure can be used in a subsequent step as well as an indirect parametric fit of measured data \[1-4\]. In all the cases the proposed validation procedure should be applied. Numerical examples illustrate basic statements of this paper.
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