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Solving inverse problems with the unfolding program TRUEE: Examples in astroparticle physics

N. Milke [a,*], M. Doert [a,*], S. Klepser [b,1], D. Mazin [b,2], V. Blobel [c], W. Rhode [a]

[a] Experimentelle Physik 5, Technische Universität Dortmund, 44221 Dortmund, Germany
[b] IFAE, Edifici Cn., Campus UAB, E-08193 Bellaterra, Spain
[c] Institut für Experimentalphysik, Universität Hamburg, D-22761 Hamburg, Germany

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ABSTRACT

The unfolding program TRUEE is a software package for the numerical solution of inverse problems. The algorithm was first applied in the FORTRAN 77 program RUN. RUN is an event-based unfolding algorithm which makes use of the Tikhonov regularization. It has been tested and compared to different unfolding applications and stood out with notably stable results and reliable error estimation. TRUEE is a conversion of RUN to C++, which works within the powerful ROOT framework. The program has been extended for more user-friendliness and delivers unfolding results which are identical to RUN. Beside the simplicity of the installation of the software and the generation of graphics, there are new functions, which facilitate the choice of unfolding parameters and observables for the user.

In this paper, we introduce the new unfolding program and present its performance by applying it to two exemplary data sets from astroparticle physics, taken with the MAGIC telescopes and the IceCube neutrino detector, respectively.

0. Introduction

Solving inverse problems can be described as a method to find the cause of known consequences. Problems of this kind manifest themselves in a wide range of research fields such as natural sciences, economics and engineering. Looking at physics as an exemplary field, inverse problems are among the fundamental challenges in various areas, for instance particle physics, crystallography or medicine. The particular problems and solutions in this paper will be presented and described alongside the subject of astroparticle physics. The nomenclature used here is mainly following Ref. [1].

The structure of this paper comprises three main sections. First, the class of inverse problems and the general procedure of unfolding with regularization are outlined. In a second section, the new unfolding program TRUEE is introduced. Subsequently, the first applications of the program in astroparticle physics, namely in the data analysis of the experiments MAGIC and IceCube, are presented in the third section. We conclude with a summary of the obtained results and an outlook on further extensions and applications of the program.

1. Inverse problems and unfolding

In general, the distribution $f(x)$ of a variable x has to be determined. However, it is often not possible to measure the value x directly. Instead, the detector records x-correlated variables y. These signals can be seen as the mentioned consequences of the causation x. The goal is to get the best-possible estimate of the $f(x)$-distribution from the measured $g(y)$-distribution. As the measurement in a real experiment is distorted, this is not trivial. A direct allocation of a value x to a value y is not possible, because one x value causes different signals with different y values with certain probabilities. Furthermore, the probability to record a signal at all is usually less than one and depending on x, which causes a loss of events. Thus, the transformation of x to y is disturbed by a finite resolution and a limited acceptance of a real detector.

In mathematics, this problem can be described by the Fredholm integral equation [2]

$$g(y) = \int_c^d A(y,x) f(x)\, dx + b(y) \tag{1}$$

where $g(y)$ is the distribution of the measured observable y and can in general be multidimensional. The function $A(y,x)$ is called

* Corresponding authors.
E-mail addresses: natalie.milke@udo.edu (N. Milke), marlene.doert@tu-dortmund.de (M. Doert).
[1] Now at: Deutsches Elektronen-Synchrotron (DESY), D-15738 Zeuthen, Germany.
[2] Now at: Max-Planck-Institut fuer Physik, D-80805 München, Germany.

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the kernel or response function and includes all effects which occur in a real measurement process. In most cases, this function is not known exactly and has to be determined by Monte Carlo (MC) simulations, where the measured and the real distributions are known. The parameters c and d are the integration limits of the range where x is defined ($c \le x \le d$). The function $b(y)$ is the distribution of a possible background, which is assumed to be known.

In reality the measurement delivers discrete values. Furthermore the handling by the algorithm requires a numerical description of the distributions. Thus, a discretization of all functions is required. The distribution $f(x)$ can be parametrized with the Basis-spline (B-spline) functions $p_j(x)$ [3] and the corresponding coefficients a_j

$$f(x) = \sum_{j=1}^{m} a_j p_j(x). \tag{2}$$

The B-spline functions consist of several polynomials of a low degree. In the following cubic B-splines are used. They consist of four polynomials of the third degree each. The points where adjacent polynomials overlap are called knots. At the knot positions a B-spline is continuously differentiable up to the second derivative, which is important because the second derivative is used for the implemented regularization (see Eq. (8)). For equidistant knots, the cubic B-splines are bell-shaped. Because of the low degree of the polynomials, an interpolation with B-spline functions does not tend to oscillate. Using this parametrization, the B-spline functions can be included in the response function during the discretization:

$$\int_c^d A(y,x) f(x)\, dx = \sum_{j=1}^{m} a_j \left[\int_c^d A(y,x) p_j(x)\, dx \right] = \sum_{j=1}^{m} a_j A_j(y). \tag{3}$$

By integrating over the y-intervals, the kernel function becomes a response matrix

$$A_{ij} = \int_{y_{i-1}}^{y_i} A_j(y)\, dy. \tag{4}$$

The same integration can be carried out for the measured distribution $g(y)$ and the background distribution $b(y)$

$$g_i = \int_{y_{i-1}}^{y_i} g(y)\, dy \tag{5}$$

$$b_i = \int_{y_{i-1}}^{y_i} b(y)\, dy. \tag{6}$$

Consequentially, the Fredholm integral equation becomes the matrix equation

$$\mathbf{g} = \mathbf{A}\mathbf{a} + \mathbf{b} \tag{7}$$

with $\mathbf{g}$, $\mathbf{a}$ and $\mathbf{b}$ as vectors and $\mathbf{A}$ as the response matrix. To determine the sought distribution $f(x)$, the coefficients a_j need to be found.

Solving Eq. (7) is called unfolding and is generally not trivial. Due to the finite resolution a smoothing effect on the measured distribution $\mathbf{g}$ is introduced. After the rearrangement of the matrix equation this smoothing effect is inverted and results in implausible oscillations of the sought distribution $f(x)$. The most straightforward approach for the solution is the inversion of the response matrix $\mathbf{A}$, if $\mathbf{A}$ is quadratic and non-singular. The resulting inverse matrix $\mathbf{A}^{-1}$ contains negative non-diagonal elements and very large diagonal elements. This causes the mentioned oscillation, which appear in any approach of solving Eq. (7) if no additional corrections are applied. This is known as a so-called ill-posed problem and generally occurs in all measurement processes.

To suppress the oscillations in the unfolded distribution, so-called regularization methods are applied. In the presented realization the Tikhonov regularization [4] is implemented. The method, in its generalized form, requires the linear combination of the unfolding term with a regularization term (sometimes called penalty term), which contains a regularization factor. The regularization term contains an operator, which implies some a priori assumptions about the solution, such as smoothness. In the current case the smoothness of the solution is controlled by the curvature operator $\mathbf{C}$. A large curvature corresponds to large oscillations. Thus, reduction of curvature implies reduction of oscillations and that smoothes the resulting distribution. Since the parametrization of $f(x)$ is based on cubic B-spline functions, the curvature $r(\mathbf{a})$ takes the simple form of a matrix equation

$$r(\mathbf{a}) = \int \left(\frac{d^2 f(x)}{dx^2} \right)^2 dx = \mathbf{a}^T \mathbf{C} \mathbf{a} \tag{8}$$

with $\mathbf{C}$ as a known, symmetric, positive-semidefinite curvature matrix.

The actual unfolding is performed as follows. At first the response matrix $\mathbf{A}$ is calculated, based on the MC sample. To determine the coefficients $\mathbf{a}$ of the final result, the unfolding equation (Eq. (7)) is set up, where $\mathbf{g}$ is the real measured observable distribution. To fit the right hand side to the left hand side of this equation, a maximum likelihood fit is performed. For simplicity, a negative log-likelihood function

$$S(\mathbf{a}) = \sum_i (g_i(\mathbf{a}) - g_{i,m} \ln g_i(\mathbf{a})) \tag{9}$$

is formed and minimized. Here $g_{i,m}$ is the number of measured events in an interval i including the possible background contribution in this region. This number follows the Poisson distribution with mean value g_i. A Taylor expansion of the negative log-likelihood function can be written as

$$S(\mathbf{a}) = S(\tilde{\mathbf{a}}) + (\mathbf{a}-\tilde{\mathbf{a}})^T \mathbf{h} + \tfrac{1}{2}(\mathbf{a}-\tilde{\mathbf{a}})^T \mathbf{H} (\mathbf{a}-\tilde{\mathbf{a}}) + \cdots \tag{10}$$

with gradient $\mathbf{h}$, Hessian matrix $\mathbf{H}$ and $\tilde{\mathbf{a}}$ as a first estimation of coefficients, which have to be found.

After considering regularization (Eq. (8)), the final fit function

$$R(\mathbf{a}) = S(\tilde{\mathbf{a}}) + (\mathbf{a}-\tilde{\mathbf{a}})^T \mathbf{h} + \tfrac{1}{2}(\mathbf{a}-\tilde{\mathbf{a}})^T \mathbf{H} (\mathbf{a}-\tilde{\mathbf{a}}) + \tfrac{1}{2}\tau \mathbf{a}^T \mathbf{C} \mathbf{a} \tag{11}$$

has to be minimized to obtain the unfolded result. The regularization parameter τ controls the effect of the regularization. The challenge is to find a proper value for τ, to get an optimal estimation of the result as a balance between oscillations and the smoothing effect of the regularization.

One method to define a value for τ is to set up the relation between τ and the effective number of degrees of freedom ndf

$$ndf = \sum_{j=1}^{m} \frac{1}{1+\tau S_{jj}}. \tag{12}$$

Here S_{jj} are the eigenvalues of the diagonalized curvature matrix $\mathbf{C}$, arranged in increasing order. The summands in Eq. (12) can be considered as filter factors for the coefficients. These coefficients represent the transformed measurement and are arranged in decreasing order. The filter factors with values < 1 diminish the influence of insignificant coefficients. Accordingly an increasing value of τ cuts away smoothly the high order coefficients and reduces the number of degrees of freedom. In turn, the definition of number of degrees of freedom allows the specification of the number of filter factors and thus of the regularization strength.

To obtain Eq. (12), the Hesse and curvature matrices in Eq. (11) have to be diagonalized simultaneously. To do this, a common