A linear iterative unfolding method

András László

Wigner RCP, P.O.Box 49, H-1525 Budapest, Hungary
CERN, CH-1211 Geneve 23, Switzerland

E-mail: `laszlo.andras@wigner.mta.hu`

Abstract. A frequently faced task in experimental physics is to measure the probability distribution of some quantity. Often this quantity to be measured is smeared by a non-ideal detector response or by some physical process. The procedure of removing this smearing effect from the measured distribution is called unfolding, and is a delicate problem in signal processing, due to the well-known numerical ill behavior of this task. Various methods were invented which, given some assumptions on the initial probability distribution, try to regularize the unfolding problem. Most of these methods definitely introduce bias into the estimate of the initial probability distribution. We propose a linear iterative method (motivated by the Neumann series / Landweber iteration known in functional analysis), which has the advantage that no assumptions on the initial probability distribution is needed, and the only regularization parameter is the stopping order of the iteration, which can be used to choose the best compromise between the introduced bias and the propagated statistical and systematic errors. The method is consistent: "binwise" convergence to the initial probability distribution is proved in absence of measurement errors under a quite general condition on the response function. This condition holds for practical applications such as convolutions, calorimeter response functions, momentum reconstruction response functions based on tracking in magnetic field etc. In presence of measurement errors, explicit formulae for the propagation of the three important error terms is provided: bias error (distance from the unknown to-be-reconstructed initial distribution at a finite iteration order), statistical error, and systematic error. A trade-off between these three error terms can be used to define an optimal iteration stopping criterion, and the errors can be estimated there. We provide a numerical C library for the implementation of the method, which incorporates automatic statistical error propagation as well. The proposed method is also discussed in the context of other known approaches.

1. Introduction

In data analysis one commonly faces the problem that the probability density function (pdf) of a given physical quantity of interest is to be measured, but some random physical process, such as the intrinsic behavior of the measurement apparatus, smears it. The reconstruction of the pertinent pdf based on the measured smeared pdf and on the response function of the measurement procedure is called unfolding. To be specific, let us have the original unknown pdf $x \mapsto f(x)$ of the undistorted physical quantity which we need to reconstruct, and assume that the actual measured pdf can be expressed of the form $y \mapsto g(y) = \int \rho(y|x) \, f(x) \, dx$, where $(y, x) \mapsto \rho(y|x)$ describes the smearing effect in a probabilistic manner.[1] Then, it is said that

---

[1] All pdfs are understood to be real valued non-negative Lebesgue integrable functions over some finite dimensional real vector space X.

the pdf g is the pdf f folded with the response function ρ.[2] Our mathematical task is to solve the above linear integral equation in order to obtain f, given g and ρ. This problem is known not to be a simple numerical task (ill-posed problem), and several methods are used by the data analysis communities in order to regularize the problem (for an overview on the most popular approaches, we refer to [1, 2]).

Let us denote by A_ρ the pertinent folding operator, which acts like $(A_\rho f)(y) = \int \rho(y|x) f(x)\,dx$ on a function f at a point y.[3] Given the measured pdf $g = A_\rho f$, the problem of unfolding can then be formalized as follows: the pdf $f = A_\rho^{-1}(g)$ is to be determined or approximated. The mathematical cause of the numerical ill-posedness of this unfolding problem can then be put forward as: the inverse A_ρ^{-1} of a generic folding operator can be shown not to be continuous despite the forward folding operator A_ρ always being continuous[4] (this phenomenon is discussed in detail e.g. in [9]). The non-continuity of the inverse folding operator A_ρ^{-1} may be also reformulated in a less abstract manner: initially distant functions can be mapped close by the folding operator A_ρ, as illustrated in Figure 1. I.e. one can lose discriminating power between pdfs upon a folding.
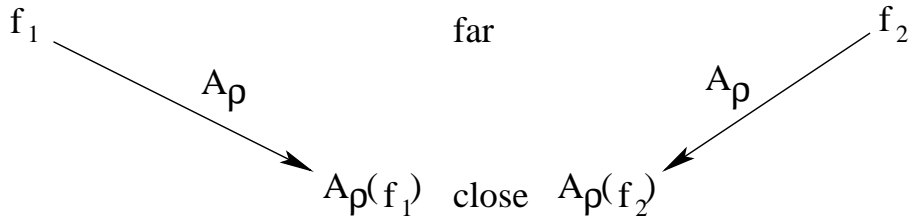
Figure 1. Illustration of the non-continuity of the inverse of a folding operator A_ρ: two distant functions f_1 and f_2 may be mapped close by the folding – distance of functions are here understood as probabilistic distance, i.e. in the $L^1(X)$ function norm.
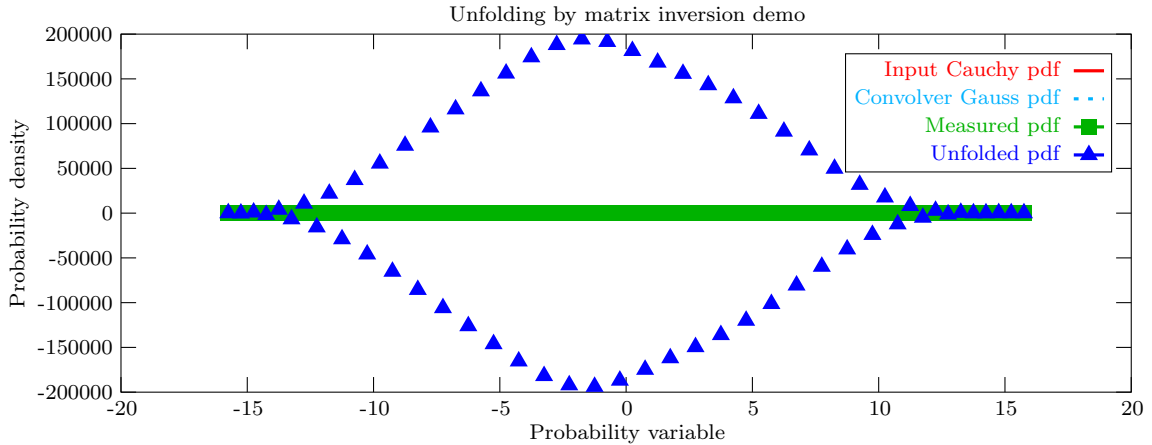
A further aspect of the numerical ill-posedness of the unfolding problem is that in practice the folded pdf g is often obtained via statistical measurements (e.g. histograming), and therefore is contaminated by statistical errors. I.e. in reality $g = A_\rho f + e$ holds instead of the idealized equation $g = A_\rho f$, where $e(x)$ is a random variable for each point x (or for each histogram bin – in the language of histograms). Thus, when estimating the unfolded pdf as $A_\rho^{-1}(g) = f + A_\rho^{-1}(e)$, the contribution of the second term is not guaranteed to remain small due to the non-continuity of the inverse folding operator A_ρ^{-1} even when e is initially known to be small. On top of this, the statistical error term e may contain modes not within the image of the folding operator A_ρ, on which the evaluation of the inverse operator A_ρ^{-1} is not meaningful if the problem is not initially discrete. These effects are demonstrated in Figure 2, which shows that simple inversion of the discretized folding operator on the measured pdf gives unphysical numerical result: a result very different from the initial pdf, having large negative and positive alternating amplitudes.

In order to regularize the numerical ill-posedness of the unfolding problem, various methods are used. These methods can be divided into three large classes.

---

[2] Whenever the response function ρ is translation invariant in the sense that for all $x, y, z \in X$ one has $\rho(y + z|x) = \rho(y|x - z)$, the folding is specially called convolution, and in that case ρ may be expressed by a single pdf: $\rho(y|x) = \rho(y - x|0)$.

[3] To be precise, A_ρ is a $L^1(X) \to L^1(X)$ continuous linear operator, where $L^1(X)$ denotes the normed space of complex valued integrable functions over the vector space X. The response function ρ is assumed to be $\rho(\cdot|x) \in L^1(X)$ for all $x \in X$.

[4] Continuous in the $L^1(X) \to L^1(X)$ sense.

Figure 2. (Color online) Demonstration of the numerical ill-posedness of the unfolding problem: a Cauchy distribution is convolved with a Gauss distribution with Monte Carlo method to generate the measured distribution contaminated with statistical errors. Clearly, the unfolded pdf, obtained by simple numerical inversion of the discretized folding operator on the measured pdf gives physically unreasonable numerical result: large alternating positive / negative amplitude pdf values.

(i) Using a parametric Ansatz for f, and fit parameters, so that $A_\rho f$ gets close to g. This method can be slightly insensitive to the details of the true f (as illustrated in Figure 1), and of course can introduce strong systematic bias on the result if the parametric Ansatz does not hold in an exact manner of the form that was assumed. Such methods are used in general for inclusive particle identification by specific ionization (see e.g. [10]).

(ii) Bin-by-bin fitting of the bin values of the histogramed f, so that $A_\rho f$ gets close to g. This is basically equivalent to the naive inversion of the discretized folding operator, and therefore produces similar oscillatory results, except when an artificial penalty function is added to the χ^2 in order to suppress large local gradients. In that case, the method can provide meaningful answers, but the introduced systematic bias is difficult to quantify. Similarly to the parametric Ansatz method, the fit can be slightly insensitive to the details of the true f. Most popular methods, such as SVD method [3], are based on this idea.

(iii) The iterative method of convergent weights (also known as iterative Bayesian unfolding) of Kondor-Mülthei-Schorr-d'Agostini [4, 5, 6, 7, 8]. This method is, as opposed to the previously mentioned methods, is non-linear. On the other hand, by construction it preserves positivity and integral of the initial pdf, and therefore maps a pdf exactly into a pdf, which does not hold for linear methods, thus, this approach is quite favorable for statistical applications. Regularization is achieved solely by stopping the iteration at a finite order. However, there is no known proof yet if the iterated pdfs converge[5] to the initial to-be-reconstructed pdf in a non-discrete scenario, even in the absence of measurement errors [6]. Also propagation of statistical and systematic errors of the measured pdf to the unfolded pdf has not been investigated, and consequently no generally applicable iteration stopping condition is known.

In a previous paper [9] we proposed a linear iterative unfolding method, for which under certain conditions convergence to the initial pdf was proved analytically for some unfolding problems

---

[5] In case of an iterative unfolding method it is an absolute must to show that the sequence of iterated unfolded pdfs converge to the initial one, in the absence of measurement errors (consistency of the method).

in probability theory (such as convolutions), and due to the linearity of the method, exact propagation of statistical errors of the measured (folded) pdf to the unfolded pdf was possible. In this paper we propose an improved version of that algorithm, which could be proved to be convergent in quite general cases for unfolding problems in a probability theory setting.[6] The key equality of the convergence proof leads to explicit error propagation formulae for the three important error terms: for the bias error (distance from the true unfolded pdf), for the propagated statistical error, and most notably for the propagated systematic error, which is of great importance in reporting experimental results. An implementation of the algorithm is written as C library, along with application examples [13]. The implementation also incorporates automatic statistical error propagation.

The paper is organized as follows: in Section 2 the algorithm and its convergence theorem shall be formulated, Section 3 is devoted to the corresponding error propagation formulae which help to formulate an optimal stopping criterion and error estimates therein, while in Section 4 we demonstrate our method on examples.

2. A linear iterative unfolding algorithm

We provide now a linear iterative solution for a probability theory unfolding problem of the form $g = A_\rho f$, where f is the initial (unknown) pdf, g is the folded (measured) pdf, and ρ is the response function. Given the response function ρ, one can also define along with the folding operator A_ρ the transpose folding operator A_ρ^T by swapping the variables of the response function.[7] Then, one can attempt to approximate the true unfolded pdf f in the following way: define the function sequence by setting the normalization factor

$$K_\rho = \max_x \int \int \rho(y|z)\,\rho(y|x)\,\mathrm{d}y\,\mathrm{d}z \tag{1}$$

and then taking the

$$
\begin{aligned}
f_0 &= K_\rho^{-1} A_\rho^T g, \\
f_{N+1} &= f_N + \left(f_0 - K_\rho^{-1} A_\rho^T A_\rho f_N \right)
\end{aligned}
\tag{2}
$$

iteration formula. We provide a convergence result on this iterative approximation below in absence of measurement errors on g (which is necessary for the consistency of the method).

Theorem 1. *(Convergence) The function sequence $N \mapsto f_N$ resulting from the above iteration scheme converges to the closest possible function to the true unfolded pdf f in the average over any compact region, whenever the normalization factor K_ρ is finite. I.e. for all compact sets $S \subset X$ one has*

$$\lim_{N \to \infty} \frac{1}{\mathrm{Volume}(S)} \int_S \left(f - P_{\mathrm{Ker}(A_\rho)} f - f_N \right)(x)\,\mathrm{d}x = 0. \tag{3}$$

Here, $P_{\mathrm{Ker}(A_\rho)}$ denotes the orthogonal projection operator to the kernel set of A_ρ, and thus $P_{\mathrm{Ker}(A_\rho)} = 0$ holds automatically whenever A_ρ is invertible. In addition, the convergence shall also hold in the space of square-integrable functions, i.e. one has also

$$\lim_{N \to \infty} \int \left| f - P_{\mathrm{Ker}(A_\rho)} f - f_N \right|^2 (x)\,\mathrm{d}x = 0. \tag{4}$$

---

[6] The detailed mathematical proof of convergence shall be published elsewhere: [11]. The proposed iteration scheme was motivated by the so called Neumann series and Landweber iteration [12] known in functional analysis, but the convergence of neither iterations hold, unfortunately, in a probability theory setting in their original form, as one can prove. Our improved iterative algorithm, however, is specially developed to be convergent for unfolding problems in probability theory.

[7] The transpose folding operator is defined by $(A_\rho^T f)(y) = \int \rho(x|y)\,f(x)\,\mathrm{d}x$ for all functions f and points y. Note, that this simply translates to matrix transposition whenever the folding is discretized.

Proof The proof is based on Riesz-Thorin theorem and on the spectral representation of positive operators in the space of complex square-integrable functions over X (to be published in a more mathematically specialized journal: [11]).

The following observations help to shed some further light on properties of the proposed unfolding algorithm.

(i) In case the pdfs are modeled with histograming, the setwise convergence of pdfs means binwise convergence of histograms, i.e. the probability of each histogram bin is restored in the limit of infinite iterations.

(ii) When the inverse of A_ρ exists, the original pdf f is completely restored. Whenever the pertinent inverse does not exist, still the maximum possible information about f is restored, namely the function $f - P_{\mathrm{Ker}(A_\rho)}f$.

(iii) Whenever A_ρ is a convolution, then $K_\rho = 1$ holds automatically, i.e. $K_\rho < \infty$ is satisfied.

(iv) The convergence condition $K_\rho < \infty$ holds provably for a wide class of practically relevant response functions, such as energy response function of calorimeters, momentum response function of track reconstruction in magnetic field etc.

(v) The iteration scheme of the theorem is motivated by the Neumann series known in functional analysis. A similar iterative solution, also referred to as Landweber iteration [12], is known in the theory of Fredholm operators. In probability theory unfolding problems, however, the necessary convergence criteria for Neumann series or for Landweber iteration do not hold in their original form.

(vi) The proposed iterative unfolding algorithm does not necessarily need an initial binning of pdfs. It may be implemented as well by different density estimators than histograms. However, when the pdfs are modeled by histograms, one may recognize that the binning and truncation of histograming domain can also be considered as folding operator. Therefore, the histogram binning and truncation effect may be included in the response function ρ, and then the effect of histograming can be unfolded (to the maximum possible extent) as well. If one wants to numerically implement this, the initial pdf f must be assumed to better approach the continuum pdf, i.e. must be assumed to be an unknown histogram over a larger domain with finer granulation than the folded one. The schematic of such possible rebinning trick is illustrated in Figure 3.
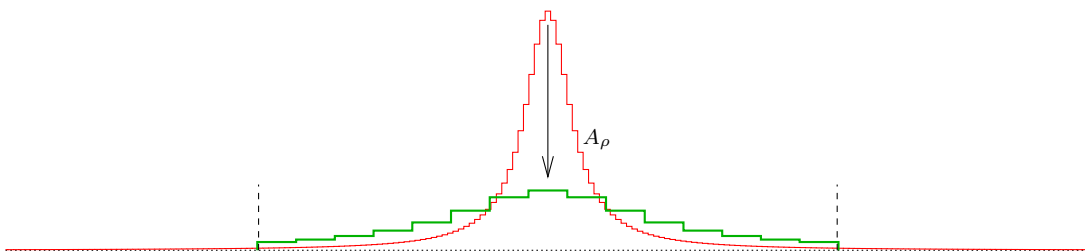
Figure 3. (Color online) Illustration the rebinning trick for unfolding the histogram binning and domain truncation as well (to the maximum possible extent) along with the smearing effect of the response function ρ. For this, the implementation of the folding operator A_ρ must map histograms over a larger domain and with finer graining to histograms with the binning scheme of the measured (folded) pdf.

3. Bias, statistical and systematic errors of the unfolded distribution

In real measurements, the folded pdf g also admits statistical and systematic errors, and the propagation of these terms into the unfolded pdf is necessary to quantify at each finite iteration step. The key equality of the proof of Theorem 1 leads to explicit error propagation formulae for bias error (distance from the true unfolded pdf), statistical error, and systematic error. First we present our result about bias error.

Theorem 2. *(Bias error) Take the iterative solution for the unfolding problem as in Section 2. Then, if the normalization factor K_ρ is finite, the distance of an N-th iterate f_N from the closest possible function to the true unfolded pdf f in the average over a compact region has the following upper bound: for any compact set $S \subset X$ one has*

$$\left| \frac{1}{\mathrm{Volume}(S)} \int_S \left(f - P_{\mathrm{Ker}(A_\rho)} f - f_N \right)(x)\,\mathrm{d}x \right| \leq \frac{1}{\sqrt{\mathrm{Volume}(S)}} \frac{1}{N+2} \sqrt{\int |f|^2(x)\,\mathrm{d}x}, \quad (5)$$

i.e. the residual deviation of f_N from the limit averaged to the set S decreases as $\frac{1}{\sqrt{\mathrm{Volume}(S)}}$ and as $\frac{1}{N+2}$.

The above result, translated to the language of histograms means that the bin-by-bin average deviation from the true unfolded pdf is bound by the right hand side of the inequality in Theorem 2., where $\mathrm{Volume}(S)$ is the histogram bin volume, N is the iteration order, and $\sqrt{\int |f|^2(x)\,\mathrm{d}x}$ is an unknown coefficient depending on the true unfolded pdf f. This unknown coefficient, however, may be substituted by the calculable expression $\sqrt{\int |f_N|^2(x)\,\mathrm{d}x}$ for large N. It is seen that the bias error tends to zero with increasing iteration order N.

In practical applications, the pdfs are often measured by statistical methods (e.g. histograming). In that case, the value of the folded pdf g in each histogram bin admits a statistical error. The below theorem states an exact formula for the propagation of this error into the unfolded pdf.

Theorem 3. *(Statistical error) Take the iterative solution for the unfolding problem as in Section 2. Let C be the covariance matrix of the measured pdf g, where g is assumed to be of the form of a histogram. Since a covariance matrix C is positive definite, it is always possible to decompose it – not uniquely – in the form $C = E\,E^T$ for some matrix E, $(\cdot)^T$ being the matrix transpose. (Whenever C is diagonal, construction of such an E is just trivial.) Then, the following iteration calculates the statistical error propagation:*

$$\begin{aligned} E_0 &= K_\rho^{-1} A_\rho^T E, \\ E_{N+1} &= E_N + \left(E_0 - K_\rho^{-1} A_\rho^T A_\rho E_N \right), \end{aligned} \quad (6)$$

where in each step the covariance matrix of f_N shall be $C_N = E_N\,E_N^T$.

Due to the linearity of the method, the contribution of the propagated statistical error term is exactly calculable by means of the above formulae, if it is known for the measured pdf g. This error term increases with increasing iteration order N. The statistical error of a given histogram bin of the N-th iterate f_N is nothing but the square-root of the corresponding diagonal element of C_N.

Whenever the folded pdf g is a result of an experiment, it may admit a systematic error δg. Also the systematic error $\delta\rho$ of the response function ρ may give a non-zero contribution to it: $A_{\delta\rho} f$. The effect of this initial systematic error on the unfolded pdf is quantified by the following theorem.

Theorem 4. *(Systematic error) Take the iterative solution for the unfolding problem as in Section 2. Assume that δg is the systematic error of g (possibly including contribution from systematic error of the response function). Then the systematic error for the N-th iterate f_N averaged over a compact region has the following upper bound: for any compact set $S \subset X$*

$$\left| \frac{1}{\text{Volume}(S)} \int_S \delta f_N(x)\, \mathrm{d}x \right| \leq \frac{1}{\sqrt{\text{Volume}(S)}} \left(\Psi(N+2) + \gamma \right) \sqrt{\int \left| K_\rho^{-1} A_\rho^T \delta g \right|^2 (x)\, \mathrm{d}x}, \qquad (7)$$

i.e. the systematic error of f_N averaged to the set S decreases as $\frac{1}{\sqrt{\text{Volume}(S)}}$ and increases as $\Psi(N+2) + \gamma \approx 1 + \ln(N+1)$. ($\Psi$ being the digamma function, γ being Euler's constant.)

The above result, translated to the language of histograms means that the bin-by-bin average systematic error of the N-th iterate f_N is bound by the formula in the right hand side of the inequality in Theorem 4., where $\text{Volume}(S)$ is the histogram bin volume, N is the iteration order, and the coefficient $\sqrt{\int \left| K_\rho^{-1} A_\rho^T \delta g \right|^2 (x)\, \mathrm{d}x}$ is calculable knowing the bin-by-bin systematic errors δg of the measured pdf g. Clearly, this contribution increases logarithmically with increasing iteration order N.

As the bias error decreases, while the statistical and systematic error of the N-th iterate f_N increases with the iteration order N, a trade-off between these error terms provides an optimal cutoff criterion[8] in the iteration order N, and error estimates therein. Consequently the true unfolded pdf f can be approximated optimally and the error of this approximation can be put under full control. Thus, the regularization of the numerically ill-posed unfolding problem is achieved, in case of the proposed approach, solely by using an iterative approximation and choosing an optimal iteration stop order taking into account the convergent terms (bias error) and the divergent terms (statistical and systematic errors).
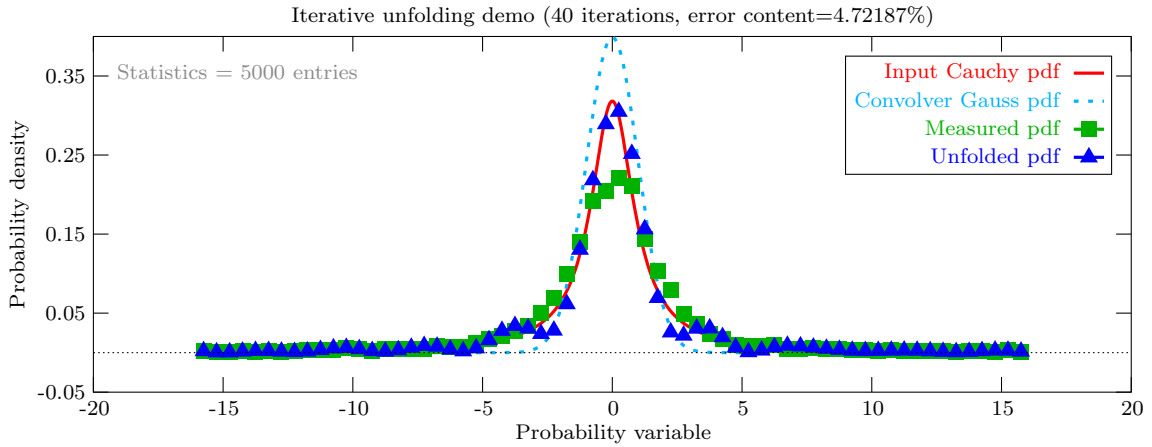
4. Examples

In this section we give two examples to demonstrate our method. In the first example, we take a Cauchy distribution, and convolve it with a Gaussian distribution with Monte Carlo method. The folded pdf is determined by histograming the sum of the Cauchy and Gaussian distribution random numbers, i.e. the measured pdf shall admit Poissonian statistical errors. In this example, a relatively modest statistics of 5000 entries was taken to be able to judge the method in the low statistics limit. The results is shown in Figure 4. It is seen that the original Cauchy pdf is restored, modulo the fluctuations arising from the propagated statistical errors – these are seen as "shoulders" of the unfolded pdf, the amplitude of which decrease with increased statistics. The iteration was stopped when the integral of the statistical error term reached about 5% level.

In the second Monte Carlo example, we generate the energy distribution of transversely emitted hadrons in 7 GeV p+p collisions [14], and we assume that this particle spectrum was measured by the CMS-HCAL calorimeter [15]. The unfolded spectrum, along with the true and measured distribution is shown in Figure 5.

5. Concluding remarks

We proposed a linear iterative spectrum unfolding method for application in data analysis. Convergence to the true unfolded pdf is proved under a quite general condition [11] in absence of measurement errors, and error propagation formulae are derived for bias error, statistical error, and systematic error in the presence of measurement errors. The method is demonstrated on physical examples. A numerical library in C is provided with the implementation of the method [13]. The algorithm could be included in the ROOUnfold package [16] in the future.

---

[8] E.g. one can take the sum of the three error terms, and stop the iteration when it reaches a minimum.

Figure 4. (Color online) Test example with unfolding a Cauchy distribution convolved with a Gaussian distribution. Iteration was stopped when the integral of the statistical error term reached about 5%.
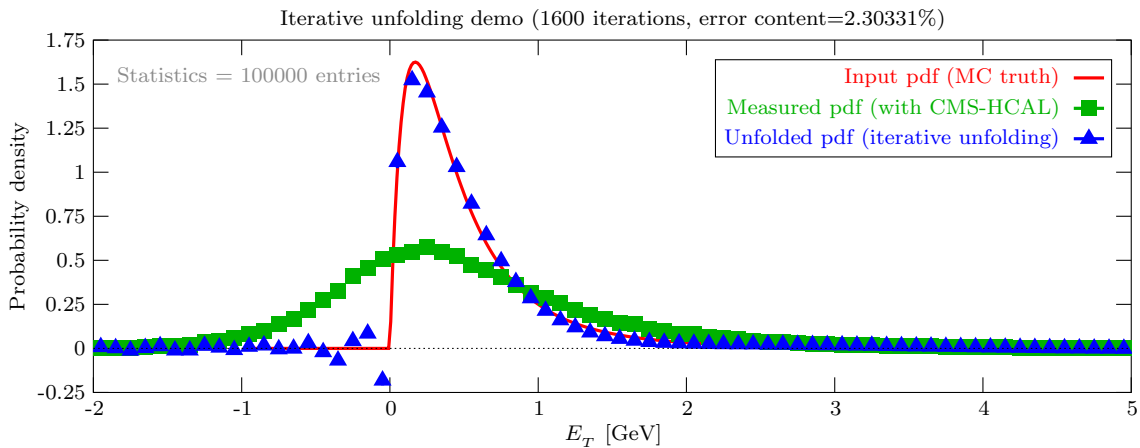
Figure 5. (Color online) A physical example with unfolding energy distribution of charged hadrons measured with hadronic calorimeter. Iteration was stopped when the integral of the statistical error term reached about 2.3%.

References

[1] Cowan G 2002 *Proceedings of Conference on Advanced Statistical Techniques in Particle Physics (18-22 March 2002, Durham, United Kingdom)* (IPPP/02/39, Durham) p 248
[2] Blobel V 2008 Unfolding for HEP Experiments (*Talk at DESY Computing Seminar*) http://www.desy.de/~blobel/DESYcompsem08.pdf
[3] Hoecker A and Kartvelishvili V 1996 *Nucl. Instr. Meth.* A **372** 469
[4] Shepp L A and Vardi Y 1982 *IEEE Trans. Med. Imag.* **1** 113
[5] Kondor A 1983 *Nucl. Instr. Meth.* **216** 177
[6] Mülthei H N and Schorr B 1987 *Mat. Meth. Appl. Sci.* **9** 137
[7] Mülthei H N and Schorr B 1987 *Nucl. Instr. Meth.* A **257** 371

[8] D'Agostini G 1995 *Nucl. Instr. Meth.* A **362** 487
[9] László A 2006 *J. Phys.* A **39** 13621
[10] László A 2008 *Phys. Rev.* C **77** 034906
[11] László A Convergence results on a linear iterative spectrum unfolding method (*in preparation*)
[12] Landweber L 1951 *Am. J. Math.* **73** 615
[13] László A 2011 The libunfold package (*Source code*)
       `http://www.rmki.kfki.hu/~laszloa/downloads/libunfold.tar.gz`
[14] Khachatryan V *et al* 2010 *Phys. Rev. Lett.* **105** 022002
[15] Yazgan E *et al* 2009 *J. Phys. Conf. Ser.* **160** 012056
[16] Adye T *et al* The ROOUnfold package
       `http://hepunx.rl.ac.uk/~adye/software/unfold/RooUnfold.html`