Comparison of unfolding methods using RooFitUnfold

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Abstract

In this paper we describe RooFitUnfold, an extension of the RooFit statistical software package to treat unfolding problems, and which includes most of the unfolding methods that commonly used in particle physics. The package provides a common interface to these algorithms as well as common uniform methods to evaluate their performance in terms of bias, variance and coverage. In this paper we exploit this common interface of RooFitUnfold to compare the performance of unfolding with the Richardson-Lucy, Iterative Dynamically Stabilized, Tikhonov, Gaussian Process, Bin-by-bin and inversion methods on several example problems.

1 Introduction

In High Energy Physics (HEP) and in many other fields one often measures distributions of quantities such as particle energies or other characteristics of observed events. Because the experimental apparatus (the "detector") inevitably has a limited resolution, the measured (or "reconstructed") value of the quantity in question will differ in general from its true value. This results in a distortion or smearing of the measured distribution relative to what would be obtained if the detector had perfect resolution. The statistical procedure of estimating the true distribution from the directly measured one is usually called unfolding in HEP, or deconvolution in many other fields. Unfolding algorithms and their implementation in software have been widely discussed in HEP (see, e.g., Refs. [5, 23, 6, 11, 19, 2, 3]).

In this paper we describe an extension of the statistical software RooFit [22] to treat unfolding problems called RooFitUnfold. The unfolding algorithms implemented in the package and studied here include: the Richardson-Lucy algorithm [17, 14, 7], Iterative Dynamically Stabilized [15] and Tikhonov [21, 10, 20] unfolding, as well as unregularised and bin-by-bin unfolding. RooFitUnfold provides a common interface to the algorithms and to methods for evaluating their performance.

In Sec. 2 we provide a mathematical description of the unfolding problem and discuss various concepts that enter into the algorithms that are studied. Section 3 then presents the specific algorithms implemented in RooFitUnfold and also describes how a number of important quantities of interest (bias, variance, coverage probability) are found using the software. In Sec. 4 we illustrate use of the different algorithms by means of several examples that compare properties of the unfolded distributions. Conclusions are given in Sec. 5.

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2 Mathematics of the unfolding problem

A brief description is provided here of the mathematics behind the unfolding algorithms studied in this paper. A definition of the unfolding problem is presented in Sec. 2.1 and some methods for its solution are described in Sec. 2.2. These methods require one to choose the degree of smoothness imposed on the solution, as discussed in Sec. 2.3.

2.1 Definition of the unfolding problem

The unfolding problem is formulated here largely following the notation and terminology of Ref. [5] (Ch. 11). Consider a counting experiment where a histogram of some variable x is used to construct a histogram. Let $\vec{\mu} = (\mu_1, \ldots, \mu_M)$ be the expected number of events in M bins that would be found if the variable x could be measured exactly for each event. We will call this the "true histogram", and the goal of unfolding is to estimate these M parameters. We will use hats to denote the estimators, i.e., $\hat{\vec{\mu}} = (\hat{\mu}_1, \ldots, \hat{\mu}_M)$.

Alternatively one may wish to estimate the probabilities

$$p_i = \frac{\mu_i}{\mu_{\text{tot}}} \, , \tag{1}$$

where $\mu_{\text{tot}} = \sum_{i=1}^{M} \mu_i$ is the total expected number of events. Below we will focus on the case where the goal is to estimate the M components of the true histogram $\vec{\mu}$.

Suppose that for each event the measured value of the variable x differs in general from the true value by some random amount owing to the limited resolution of the detector. Let us suppose that the measured values are used to construct a histogram $\vec{n} = (n_1, \ldots, n_N)$, whose bins may in general differ in their boundaries and total number N relative to the M bins of the true histogram. These data values follow some probability distribution, often taken to be Poisson or approximately Gaussian, and have expectation values $\vec{\nu} = E[\vec{n}] = (\nu_1, \ldots, \nu_N)$. We will refer to $\vec{n}$ as the data histogram (or simply "the data") and $\vec{\nu}$ as the "expected data histogram".

The expected data histogram $\vec{\nu}$ has a form that differs from what would be obtained with perfect resolution since events with a true value of the variable x in a given bin may be measured in a different one. This migration of events may be expressed as (see, e.g., Ref. [5])

$$\nu_i = \sum_{j=1}^{M} R_{ij} \mu_j \, , \tag{2}$$

where $i = 1, \ldots, N$ and the response matrix,

$$R_{ij} = P(\text{measured value in bin } i | \text{true value in bin } j) \, , \tag{3}$$

gives the conditional probability for an event to be reconstructed in bin i of the data histogram given that its true was in bin j of the true histogram. The response matrix can be determined using simulated events combined with Monte Carlo modelling of the detector's response. It is to first approximation dependent only on the properties of the measurement device, but it can depend at some level on the physics model used to generate the simulated events. For purposes of the studies presented in this paper we will suppose that the response matrix is known with negligible error, and we focus here on the uncertainties that result as a consequence of the unfolding procedure itself.

The effect of migration between bins is to smear out peaks or fine structure in $\vec{\mu}$ resulting in a flatter histogram for $\vec{\nu}$. The goal of unfolding is to estimate the true histogram, i.e., the parameters $\vec{\mu} = (\mu_1, \ldots, \mu_M)$ using the data values $\vec{n} = (n_1, \ldots, n_N)$ combined with the knowledge of the detector's response through the matrix R. The data are described with a given probability model that determines the likelihood function $L(\vec{\mu}) = P(\vec{n}|\vec{\mu})$. Often the n_i are modelled as independent and Poisson distributed, so that the likelihood is

$$L(\vec{\mu}) = \prod_{i=1}^{N} \frac{\nu_i^{n_i}}{n_i!} e^{-\nu_i} , \qquad (4)$$

where $\nu_i = \sum_{j=1}^{M} R_{ij}\mu_j$. Alternatively, the observed number of events may be modelled as following a Gaussian distribution with mean ν_i and standard deviation σ_{n_i}. In this case the log-likelihood is (up to an additive constant) a sum of squares,

$$\ln L(\vec{\mu}) = -\frac{1}{2} \sum_{i=1}^{N} \frac{(n_i - \nu_i)^2}{\sigma_{n_i}^2} . \qquad (5)$$

If the $N \times M$ response matrix R is in fact square, i.e., equal numbers of bins for both $\vec{\mu}$ and $\vec{\nu}$, and if it is nonsingular, then $\vec{\mu} = R^{-1}\vec{\nu}$. In this case one can take the estimators for $\vec{\mu}$ to be

$$\hat{\vec{\mu}} = R^{-1}\vec{n} . \qquad (6)$$

This follows (see, e.g., Ref. [5]) from the likelihoods above for which the maximum-likelihood estimators for the ν_i are $\hat{\nu}_i = n_i$.

The most important properties of the estimators that we investigate here are the bias (difference between estimator's expectation and parameter's true values),

$$b_i = E[\hat{\mu}_i] - \mu_i , \qquad (7)$$

and the covariance matrix $\mathrm{cov}[\hat{\mu}_i, \hat{\mu}_j]$, in particular its diagonal elements (the variances) $V[\hat{\mu}_i]$ (also written $\sigma_{\hat{\mu}_i}^2$). In the Poisson case with a square nonsingular response matrix, the maximum-likelihood estimators have zero bias and their covariance equals the minimum variance bound (see, e.g., Ref. [5]). Nevertheless the variances are extremely large and in this sense the unfolding problem is said to be ill-posed [9]. In unfolding one therefore attempts to reduce the variance through some form of regularisation, and this necessarily introduces some bias.

2.2 Solutions to the unfolding problem

To suppress the large variance of the maximum-likelihood estimator one chooses a $\hat{\vec{\mu}}$ that does not correspond to the maximum of the log-likelihood $\ln L_{\max}$, but rather one considers a region of $\vec{\mu}$-space where $\ln L(\vec{\mu})$ is within some threshold below $\ln L_{\max}$, and out of these the distribution is chosen that is smoothest by some measure. This can be achieved by maximising not $\ln L(\vec{\mu})$ but rather a linear combination of it and a regularisation function $S(\vec{\mu})$, which represents the smoothness of the histogram $\vec{\mu}$. That is, the estimators $\hat{\vec{\mu}}$ are determined by the maximum of

$$\varphi(\vec{\mu}) = \ln L(\vec{\mu}) + \tau S(\vec{\mu}) , \qquad (8)$$

where the regularisation parameter τ determines the balance between the two terms. Equivalently one can take the regularisation parameter to multiply $\ln L(\vec{\mu})$, as done, e.g., in Ref. [5].

The regularisation function $S(\vec{\mu})$ can be chosen in a number of ways (see, e.g., Refs. [5, 23]). Two of the algorithms studied here (TUnfold and SVD; see Sec. 3.1) use Tikhonov regularisation [21] based on the mean squared second derivative of the unfolded distribution. For discrete bins $\vec{\mu}$, the Tikhonov regularisation function can be expressed as (see, e.g., [5])

$$S(\vec{\mu}) = - \sum_{i=1}^{M-2} (-\mu_i + 2\mu_{i+1} - \mu_{i+2})^2. \qquad (9)$$

If the regularisation parameter τ is set to zero one obtains the maximum-likelihood estimators (the "unregularised solution", cf. Sec. 3.1.7), which have zero (or small) bias but very

large statistical variance. In the limit of large τ the resulting $\hat{\vec{\mu}}$ is the maximally smooth distribution corresponding to the maximum of $S(\vec{\mu})$. This is independent of the data and thus has zero statistical variance, but results in a large bias.

Other algorithms to construct regularised estimators do not involve maximisation of a function such as the $\varphi(\vec{\mu})$ in Eq. (8). For example, the Richardson-Lucy [14, 17] iterative method, e.g., as implemented by D'Agostini [7] (see Sec. 3.1.1), a trial solution is successively updated. The number of updates plays the role of the regularisation parameter, such that zero iterations gives the maximally smooth trial solution and for a large number the estimators tend towards those of maximum likelihood. In the method based on Gaussian Processes (GP) by Bozson et al. [4] (see Sec. 3.1.5) the regularisation is set through the kernel function of the GP. For essentially all unfolding methods the analyst must choose, explicitly or otherwise, some parameter that regulates the degree of smoothness imposed on the solution and thus determines the trade-off between bias and variance in the estimators $\hat{\vec{\mu}}$.

2.3 Determining the regularisation parameter

Regularised unfolding thus requires a choice of algorithm by, for example, selecting a regularisation function $S(\vec{\mu})$, as well as some prescription for setting the degree of regularisation, e.g., through the parameter τ for Eq. (8) or the number of iterations used in the Lucy-Richardson algorithm. The regularisation parameter determines the trade-off between bias and statistical variance in the estimators $\hat{\vec{\mu}}$ that result. A quantity that represents this trade-off is the mean squared error (sum of bias squared and variance) averaged over the bins,

$$\text{MSE} = \frac{1}{M} \sum_{i=1}^{M} \left(V[\hat{\mu}_i] + b_i^2 \right) \ . \tag{10}$$

Minimising the (bin-averaged) MSE as defined above is one of the criteria investigated here for setting the regularisation parameter.

Another criterion that can be employed to set the degree of regularisation is based on the coverage probability of confidence intervals constructed for each bin of the true histogram, as proposed in Ref. [11]. These can be taken as extending between plus and minus one standard deviation about the estimator, i.e., $[\hat{\mu}_i - \sigma_{\hat{\mu}_i}, \hat{\mu}_i + \sigma_{\hat{\mu}_i}]$. Such an interval will contain the true value μ_i with a specified coverage probability and we take the average of these,

$$P_{\text{cov}} = \frac{1}{M} \sum_{i=1}^{M} P(\hat{\mu}_i - \sigma_{\hat{\mu}_i} < \mu_i < \hat{\mu}_i + \sigma_{\hat{\mu}_i} | \vec{\mu}) \ , \tag{11}$$

as a criterion that can be used to choose the regularisation parameter. For the unregularised estimators ($\tau \to 0$), P_{cov} tends towards the nominal coverage for a confidence interval of plus-or-minus one standard deviation about the maximum-likelihood estimator (assuming it is Gaussian distributed), i.e., $P_{\text{nom}} = 68.3\%$. As the amount of regularisation is increased, the standard deviations $\sigma_{\hat{\mu}_i}$ decrease, and thus the coverage probability also decreases. The recipe used in this paper is to select the regularisation parameter (τ or the number of iterations) such that $P_{\text{cov}} = P_{\text{nom}} - \varepsilon$ with the threshold $\varepsilon = 0.01$.

3 The RooFitUnfold framework

The RooFitUnfold framework provides a unified software environment in which various unfolding algorithms used in HEP are implemented. The framework currently implements all of the algorithms available in the RooUnfold package [1], in addition to the Gaussian Process unfolding method. The unique proposition of the RooFitUnfold framework is that it generalises the description of input distributions for unfolding problems as RooFit [22] probability models, whereas RooUnfold and most standalone unfolding implementation only accept histograms as input distribution.

The use of binned probability models as input extends the functionality of unfolding procedures to problems where uncertainties other than statistical uncertainties are important and must be propagated to the unfolded distribution. Such uncertainties can be generically expressed in terms of nuisance parameters that affect the binned physics distribution that is intended to be unfolded. Common uncertainties in HEP that are captured in nuisance parameters include uncertainties from simulation statistics and systematic uncertainties originating from theory and detector modelling. In this paper we will not make use of RooFitUnfold's ability to propagate nuisance parameters, but will exploit its unified implementation for the evaluation of the bias and variance of unfolding methods, allowing a comparison of the unfolding algorithms on equal footing.

Presently, RooFitUnfold has no specific technical handling of empty bins and low-statistics bins at the framework level, but will warn the user of (potentially) problematic input ingredients if the response matrix is not invertible, or if this inversion results in numerical stability problems. The choice of binning is considered to be responsibility of the user.

Section 3.1 will provide a brief overview of the unfolding methods implemented, Section 3.2 explains the role of MC simulation in determining unfolding ingredients, and Section 3.3 details the exact procedure that are used for the estimation of bias and variance of these methods in RooFitUnfold, which will be used in the results presented in Section 4/.

3.1 Overview of unfolding methods

In this overview a brief description of each method is given, with references to the general unfolding methodology presented in Sec. 2 where appropriate. Further details on each algorithm can be found in the references cited.

3.1.1 Richardson-Lucy (Iterative Bayes)

The RooUnfoldBayes algorithm uses the iterative method described by D'Agostini in [7]. Starting from equal probabilities in all bins, the solution is updated using a rule based on Bayes' theorem. In other fields this algorithm is known as Richardson-Lucy deconvolution [17, 14] and is typical of truncated expectation maximisation algorithms [8]. The regularisation strength corresponds to the number of iterations performed, with the solution approaching the maximum-likelihood estimator as the number of iterations increases.

3.1.2 Singular Value Decomposition (SVD)

The routine RooUnfoldSvd provides an interface to the TSVDUnfold class implemented in ROOT by Tackmann [20], which uses the Tikhonov unfolding method [21] in the manner described by Höcker and Kartvelishvili [10]. The data are modelled as Gaussian distributed resulting in a log-likelihood given by a sum of squares as in Eq. (5). Singular Value Decomposition is used to express the detector response as a linear series of coefficients. The regularisation parameter, equivalent to τ in Eq. (8), can be related to the singular values of the response matrix.

3.1.3 TUnfold

RooUnfoldTUnfold provides an interface to the TUnfold method implemented by Schmitt [18]. TUnfold uses Tikhonov regularisation and the log-likelihood is taken to have the sum-of-squares form of Eq. (5). TUnfold can automatically determine an optimal regularisation parameter by scanning the 'L-curve' [13].

3.1.4 Iterative Dynamically Stabilized (IDS)

The iterative, dynamically stabilized (IDS) unfolding method [15], is an iterative unfolding method that has a regularisation method based on the statistical significance of the difference between observed and simulated data. RooUnfoldIds uses a reweighting procedure that aims to stabilise the unfolding procedure against feature of the data that are not present in the model.

3.1.5 Gaussian Process (GP)

The unfolding method of Bozson et al. [4], as implemented in RooUnfoldGP, constructs the estimator for the true histogram as the mode of a posterior probability obtained using Bayesian regression. For Gaussian-distributed data the estimator for the true histogram is equivalent to the mean function of a Gaussian Process (GP) conditioned on the maximum likelihood estimator. The kernel function of the GP introduces regularisation, which has a natural interpretation as the covariance of the underlying distribution. This approach allows for the regularisation to be varied along the distribution.

3.1.6 Bin-by-bin

The bin-by-bin method implemented in RooUnfoldBinByBin defines estimators of the form $\hat{\mu}_i = C_i n_i$, where the 'correction factors' are computed for each bin using a Monte Carlo simulation of the true events and the detector's response as $C_i = \mu_i^{\mathrm{MC}}/\nu_i^{\mathrm{MC}}$. Further details and drawbacks of this method are discussed in Ref. [5].

3.1.7 Matrix Inversion

For the case of equal bins in the true and measured histograms ($M = N$) and assuming a nonsingular response matrix R one can construct the unregularised estimators of Eq. (6). RooUnfoldInvert performs inversion of the response matrix with singular value decomposition (TDecompSVD). The estimators have larger variances than from any regularised method but zero conceptual bias. This solution can be useful, e.g., if there is relatively little migration of events between bins so that the response matrix is almost diagonal. Even if in the case of greater migration and thus larger statistical variances, the unregularised solution can be used together with the full covariance matrix of the estimators to carry out a meaningful statistical test of a hypothetical true distribution.

3.2 Determining unfolding ingredients with Monte Carlo simulation

Simulated data from Monte Carlo (MC) models are used in RooFitUnfold to determine the response matrix R defined in Eq. (3), which is needed for all of the unfolding methods except the bin-by-bin method of Sec. 3.1.6. In addition, MC data are used to obtain model predictions for the true histogram $\vec{\mu}$ and the expected data histogram $\vec{\nu}$.

In a full Monte Carlo simulation in HEP one generates events each characterised by a true value of the variable in question x_{true} according to a given physical theory such as the Standard Model. The response of the detector is then also simulated resulting in a measured value x_{meas}. Suitably normalised histograms of the x_{true} and x_{meas} values are used

to determine the model's predictions for the true and expected data histograms $\vec{\mu}$ and $\vec{\nu}$. It is often the case that the MC samples are sufficiently large that we may neglect statistical uncertainties in these quantities.

The MC simulated events are also used in RooFitUnfold to determine the response matrix R. In practice the simulated events are used first to find the transfer matrix N_{ij} defined as the number of events found with x_{meas} in bin i and x_{true} in bin j. The response matrix is then

$$R_{ij} = \frac{N_{ij}}{\sum_{k=1}^{N} N_{kj}} \ .\tag{12}$$

A sufficiently large sample of simulated data and appropriate choice of binning is important to ensure that the response matrix determined in this way is sufficiently smooth and not overly influenced by statistical fluctuations.

3.3   Bias, variance and coverage estimation procedures

The calculation of the bias and variance of the estimators is based on a given choice for the true distribution $\vec{\mu}$, and in general these quantities can depend on this choice. For a given $\vec{\mu}$ one computes the expected observed histogram $\vec{\nu} = R\vec{\mu}$, and a simulated data sample $\vec{n}$ is generated with the n_i independent and Poisson distributed having mean values ν_i. We refer to this as a "toy" MC data set, $\vec{n}_k$, where $k = 1, \ldots, K$. In the studies shown below we have used $K = 1000$. Each dataset $\vec{n}_k$ is unfolded with the chosen method to acquire the estimates $\hat{\vec{\mu}}_k$. The variance for bin i is then calculated as

$$\sigma_{\hat{\mu}_i}^2 = \frac{1}{K-1} \sum_{k}^{K} \left((\hat{\mu}_i)_k - \frac{1}{K} \sum_{k} (\hat{\mu}_i)_k \right)\tag{13}$$

Using the same datasets the bias for bin i is calculated as

$$b_i = \frac{1}{K} \sum_{k}^{K} (\hat{\mu}_i)_k - \mu_i \ .\tag{14}$$

Under the assumption that the $\hat{\mu}_i$ are Gaussian distributed, the coverage probability P_{cov} of the intervals $[\hat{\mu}_i - \sigma_{\hat{\mu}_i}, \hat{\mu}_i + \sigma_{\hat{\mu}_i}]$, defined in Eq (11), can be calculated in closed form [12] using σ_{μ_i} and b_i as

$$P_{\text{cov}} = \Phi\left(\frac{b_i}{\sigma_{\hat{\mu}_i}} + 1\right) - \Phi\left(\frac{b_i}{\sigma_{\hat{\mu}_i}} - 1\right),\tag{15}$$

where Φ is the Standard Gaussian cumulative distribution function.

4   Comparison of methods

In this section we present a comparison of the performance of the unfolding methods described in Section 3.1. While realistic physics models and detector response functions in HEP rely on elaborate MC simulation packages that simulate both the physics and detector response from first principles, we opt in this study for simple and analytically expressed physics functions and resolution models. These analytical models represent a more portable benchmark than the elaborate simulation models, while still introducing a realistic level of complexity. Sections 4.1 and Sections 4.2 present results on an example model that is representative of unfolding problems commonly encountered in HEP, and is evaluated in situations where the response matrix sampled from the same or a different model, respectively, as the expected data. Section 4.3 will further explore the onset of bias for scenarios in which model of the expected data and the response matrix disagree, using a distortable bimodal distribution that is smeared with a Gaussian resolution model.

4.1 Study on smeared exponential distribution - SM

We define as benchmark model an exponential decay distribution, smeared with a resolution function that is loosely inspired on a calorimeter response:

$$
\begin{aligned}
f(x|\alpha) &= f_{\text{physics}}(x_{\text{true}}|\alpha) * f_{\text{detector}}(x_{\text{true}}, x) \\
&= (\alpha \cdot \exp(-\alpha \cdot x_{\text{true}})) * \text{Gauss}\left(x - x_{\text{true}}, 7.5, 0.5 \cdot \sqrt{x_{\text{true}}} + 2.5\right),
\end{aligned}
$$

where the $*$ symbol represents the convolution operator. We define two models variants, labeled SM ('Standard Model') and BSM ('Beyond the Standard Model'), that correspond to an exponential distribution with a slope α of 0.035 and 0.05 respectively. The true and expected distributions $\vec{\mu}$ and $\vec{\nu}$ corresponding to this model are defined by 20 uniformly sized bins in the range $[100, 200]$. The true distributions and data for SM and BSM, populated with 10000 and 14000 events respectively, are shown in Fig. 1, along with the SM transfer matrix.
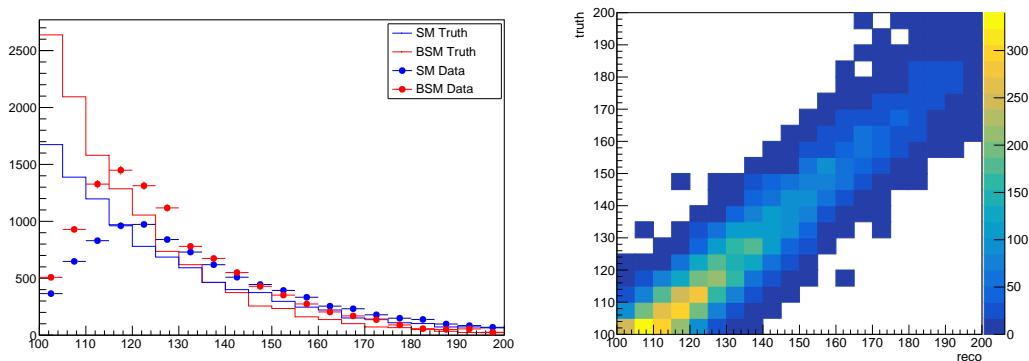
Figure 1: Left: The true distributions for the SM and BSM models and the corresponding smeared datasets. Right: the transfer matrix for the SM model, which is populated by the same events as the SM true distribution shown.

We first perform a standard unfolding benchmark using only the SM model: we compare for all methods the unfolded distributions of the SM data, obtained using the response matrix populated with data sampled from the same SM model, to the SM true distribution. In the top row of Fig. 2 the unfolded data is shown for every algorithm, along with the SM true distribution. Each panel also separately visualises the variance and bias of the unfolded distribution for each bin, calculated with the procedure described in Section 3.3 as well as corresponding coverage calculated with Eq. 15. In the visualisation of the bias for each bin, the statistical error $\sigma_{\hat{\mu}}$ is also shown to help guide the interpretation of observed fluctuations in the unfolded data. For each algorithm with a tuneable regularisation strength (Iterative Bayes, IDS, TSVD, TUnfold) two unfolding solutions are shown. These correspond to a regularisation strength that

1. unconditionally minimises the bin-averaged MSE , or

2. additionally requires the that the bin-averaged estimate of the coverage of the unfolded data reaches the target coverage of 68.3% within 1%.

The bottom row of Fig. 2 shows the average MSE and average coverage, i.e. the optimisation criteria used, as function of the regularisation strength parameter* Vertical lines indicate

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*NB: Although all plots are shown in the same format, the practical realisation and range of the regularisation strength parameter is different for each algorithm.

the chosen regularisation strengths that correspond to two solutions shown in the top pane. For the Gaussian Process and Bin-by-Bin algorithms, which have no tuneable regularisation parameter, as well as for the unregularised Matrix Inversion method only a single solution is shown.
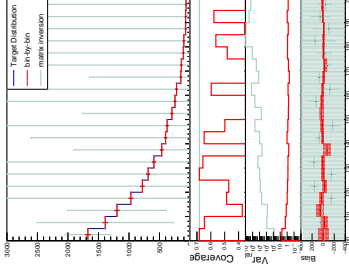
We observe that all tuneable methods (Iterative Bayes, IDS, TVSD, TUnfold) can reproduce the target distribution well, with an average bias consistent with zero in all bins. However, the solutions corresponding to the unconditionally minimised bin-averaged MSE substantially undercover for all four algorithms. Imposing the condition of correct bin-averaged coverage in the tuning largely rectifies this situation and results in a nearly uniformly correct bin-by-bin coverage, with only handful of bins undercovering by a few percent.

The Gaussian Process algorithm, which internally tunes its regularisation strength, performs well in regions far away from the lower observable boundary ($x > 120$) with uniformly good coverage and no significant bias. In the regime close to the boundary there is significant bias and undercoverage, which may be caused by boundary leakage effects related to the default choice of kernel function and might be mitigated with a different choice of kernel function. The unregularised Matrix Inversion method exhibits perfect coverage, but has a variance that is many orders of magnitude larger than that of any of the other algorithms, whereas the performance of the Bin-by-Bin method in terms of bias, variance and significant undercoverage is comparable to that of the tuneable methods.

4.2   Study on smeared exponential distribution - BSM

Next, we test the unfolding algorithms in a more challenging scenario that more closely reflect the reality of unfolding problems in HEP: the observed data, corresponding to an unknown distribution (the BSM model) has to be unfolded using a response matrix obtained for a known model (the SM distribution). The benchmark in this test is how well the SM-unfolded BSM distribution compares to the BSM true distribution. The use of the SM response matrix is a challenge for regularised methods in particular, since a too strong regularisation will bias the unfolded BSM distribution towards the SM distribution. Fig. 3 shows the results of this study, following precisely the same format as that of Fig. 2, and demonstrates that the four tuneable unfolding methods (Iterative Bayes, IDS, TVSD, TUnfold) can also reproduce the target distribution reasonably well in this more challenging benchmark. However, in a handful of bins the bias is notably increased w.r.t the first study. The observed coverage of these four methods is qualitatively similar to that of the first study: unconditional optimisation of the regularisation strength on the bin-averaged MSE leads to substantial undercoverage, which can again be largely and uniformly recovered through the imposition of a requirement on correct bin-averaged coverage in the regularisation tuning, albeit with a bit more variability in bin-by-bin coverage. For the Gaussian Process unfolding method the main difference with the SM benchmark result is the striking increase in variance for the low statistics bins in the region $x > 120$. A similarly striking increase in variance is also observed for the Matrix Inversion method, whereas the degradation of the performance of the Bin-by-Bin method is comparable to that of the tuneable algorithms.
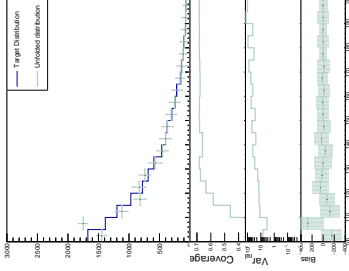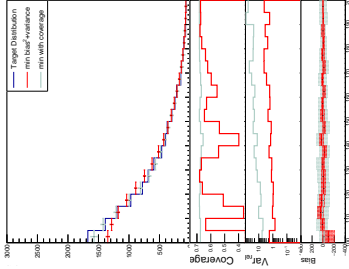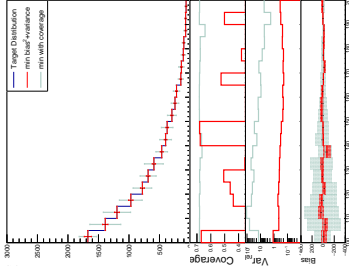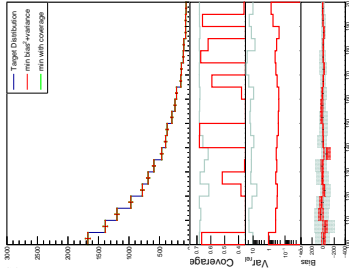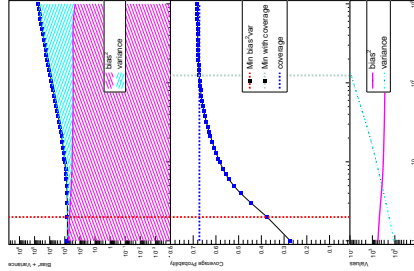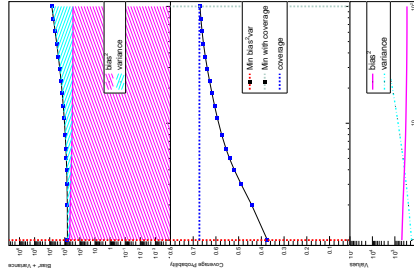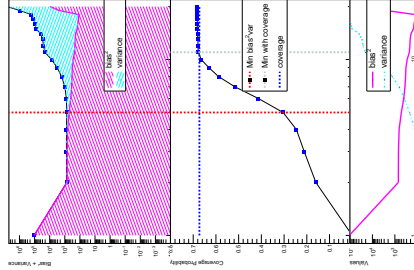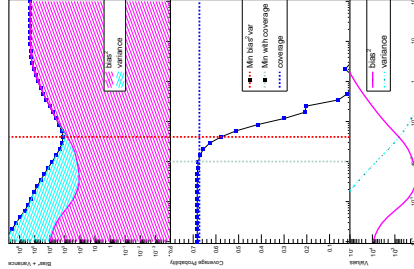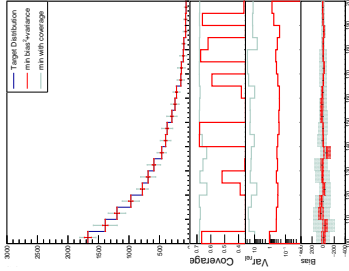
Figure 2: Comparison of the unfolding performance for the algorithms discussed in this paper. For each method, the top plot shows the unfolded SM data compared to the SM true distribution, where SM response matrix was used as input to the unfolding method. For the methods with a tuneable regularisation strength two unfolding solutions are shown: (1) with a regularisation strength corresponding to the unconditionally minimised MSE (red), and (2) with a conditionally minimised MSE with the requirement that the bin-averaged coverage reaches the target coverage within 1% (grey). The middle and lower panels of the top row plots display the bin-bin coverage, variance and bias estimates. For the bin-by-bin bias, the uncertainty of the toy-based estimate is shown with an error bar. Also overlaid on the bias plot is the statistical error of the unfolded data (i.e the RMS of the distribution of $\hat{\mu}$) to help guide the interpretation of observed fluctuations in the unfolded data. For the tuneable methods, the bin-averaged MSE and the bin-averaged coverage, which are used to tune regularisation strength, are shown as function of that strength in the bottom pane. The vertical lines in the bottom pane indicate the regularisation strength solutions chosen by the optimisation methods (1) and (2).
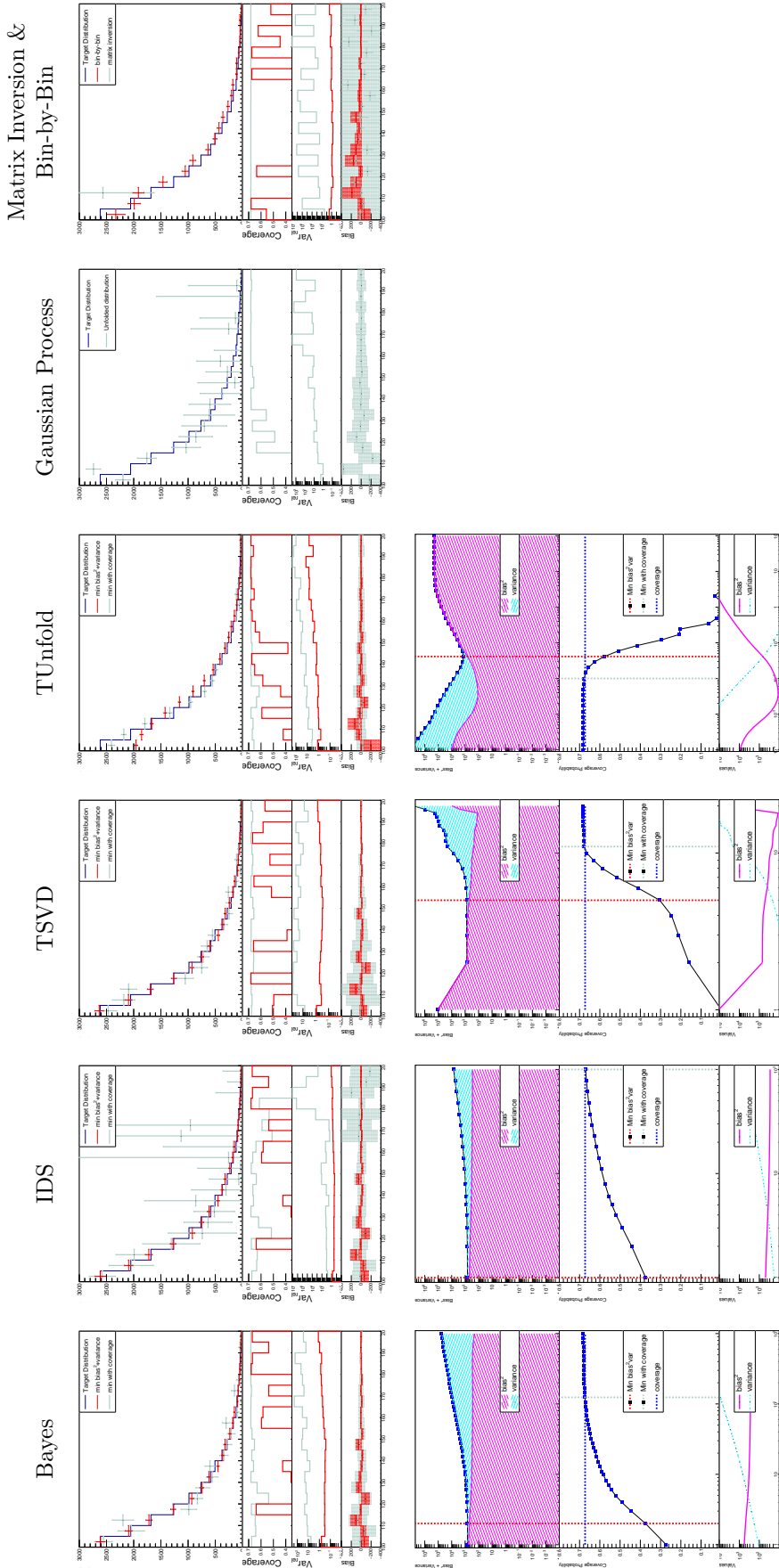
Figure 3: Comparison of the unfolding performance for the algorithms discussed in this paper. For each method, the top plot shows the unfolded BSM data compared to the BSM true distribution, where *SM* response matrix was used as input to the unfolding method. For the methods with a tuneable regularisation strength two unfolding solutions are shown: (1) with a regularisation strength corresponding to the unconditionally minimised MSE (red), and (2) with a conditionally minimised MSE with the requirement that the bin-averaged coverage reaches the target coverage within 1% (grey). In this result some of the unfolded data point fall outside the plot range, and are therefore not shown. The middle and lower panels of the top row plots display the bin-bin coverage, variance and bias estimates. For the bin-by-bin bias, the uncertainty of the toy-based estimate is shown with an error bar. Also overlaid on the bias plot is the statistical error of the unfolded data (i.e the RMS of the distribution of $\hat{\mu}$) to help guide the interpretation of observed fluctuations in the unfolded data. For the tuneable methods, the bin-averaged MSE and the bin-averaged coverage, which are used to tune the regularisation strength, are shown as function of that strength in the bottom pane. The vertical lines in the bottom pane indicate the regularisation strength solutions chosen by the optimisation methods (1) and (2).

4.3 Bimodal example

We use a bimodal distribution to further investigate unfolding biases in situations where the response matrix and the data are not sampled from the same model. The bimodal model for this study is the the sum of two Crystal Ball [16] functions, which is smeared by a simple Gaussian resolution model

$$
\begin{aligned}
f(x|\alpha) &= f_{\text{physics}}(x_{\text{true}}|\alpha) * f_{\text{detector}}(x_{\text{true}}, x) \\
&= (0.5 \cdot f_{CB}(x_{\text{true}}|\mu = 2.4, \sigma = 0.48, \alpha, n = 1) + \\
&\quad 0.5 \cdot f_{CB}(x_{\text{true}}|\mu = 5.6, \sigma = 0.48, \alpha, n = 1)) \\
&\quad * Gauss(x - x_{\text{true}}, 0, 0.4)
\end{aligned}
$$

where the Crystal Ball probability density function $f_{CB}(x|\mu, \sigma, \alpha, n)$ has a Gaussian core with mean μ and width σ, and a power law tail with power n below a threshold α that is expressed units of the Gaussian width σ. Thus, for $\alpha = \infty$ a Crystal Ball function is identical to a Gaussian distribution, whereas e.g. for $n = 1$ it follows a Gaussian distribution for $x > -1\sigma$ and a power law distribution $x \leq -1\sigma$. In the definition of the Crystal Ball function the normalisation factor for the power law tail is chosen such that the function is continuous and differentiable over the transition point. The true and expected data distributions $\vec{\mu}$ and $\vec{\nu}$ corresponding to this model are defined by 20 uniformly sized bins in the range $[-4, 4]$ and are populated with 10000 events. Fig. 4 shows the true distribution of the bimodal model for a range α values.
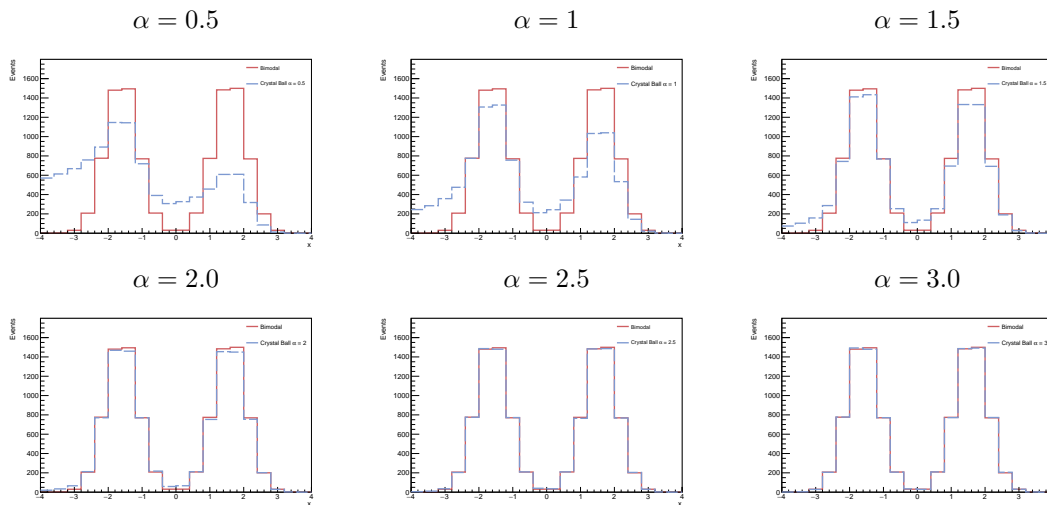

Figure 4: Visualization of the true distribution of the bimodal model for various values of the distortion parameter α.

Fig. 5 shows the bin-averaged unfolding bias of the tuneable algorithms (Iterative Bayes, IDS, SVD, TUnfold) for data sampled from the bimodal distribution with $\alpha = [0.5, 1, 1.5, 2, 2.5, 3]$ and unfolded with a response matrix with $\alpha = \infty$, with the regularisation strength always tuned to the unconditionally minimised MSE. Fig. 5 shows that the SVD, Iterative Bayes and IDS methods exhibit a strong unfolding bias that increases with the distortion for values of $\alpha < 2.5$. In contrast, the bin-averaged bias of TUnfold is almost independent on the model distortion, which may be explained by the fact that TUnfold regularises on smoothness, rather than the true distribution. As a result, TUnfold has the smallest bin-averaged bias for the strongest distortions ($\alpha = 0.5, 1, 1.5$), whereas SVD, Iterative Bayes and IDS have the (almost identical) best performance at low distortion ($\alpha = 2.5, 3$).
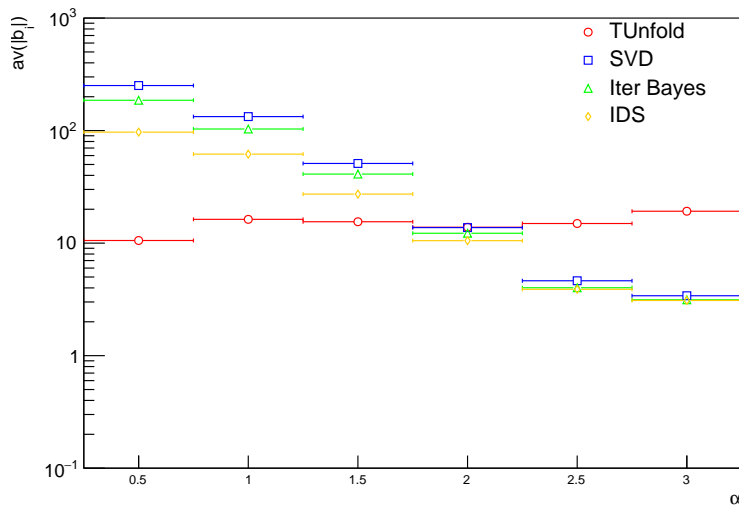
Figure 5: Comparison of the estimated bin-averaged bias of the tuneable unfolding algorithms when unfolding the distorted bimodal model with a response matrix obtained from the undistorted model. Results are shown for various distortion strengths, which increase in distortion with decreasing values of α (See Fig. 4). In this study, the regularisation strength for each algorithm has been unconditionally optimised on the MSE.

Fig. 6 shows the same comparison as Fig. 5, but with the average coverage condition imposed the regularisation optimisation. The dependence of average bias on the distortion is qualitatively the same for all methods, with TUnfold again being the least sensitive to distortions. In terms of absolute performance, TUnfold gives the smallest average bias for ($\alpha = 0.5, 1, 1.5, 2.0$) for medium to high distortion, where IDS outperforms for small distortions ($\alpha = 2.5, 3.0$).

Fig. 6 shows the performance of non-tuneable and non-regularised methods (Gaussian Process, Matrix Inversion, Bin-by-bin). The Gaussian Process and Matrix inversion methods demonstrate to be relative robust against distortion, with a minimal dependence of the average bias on the distortion parameter α, whereas the Bin-by-bin method shows a dependence that is comparable to that of the tuneable regularised methods. The robustness of the Gaussian Process method is a feature of its regularisation method, which relies only on smoothing, just like TUnfold. In terms of absolute performance, Matrix Inversion and Gaussian Process are on par with TUnfold for medium to large distortion scenarios ($\alpha = 0.5, 1, 1.5, 2$), while Gaussian Process unfolding is the clear winner for the low distortion $\alpha = 3$ scenario, likely due to the strongly Gaussian nature of the undistorted bimodal model.

5 Summary and conclusions

We have used the RooFitUnfold package, which provides a common framework to evaluate and use different unfolding algorithms, to evaluate the performance of seven unfolding algorithms used in HEP in terms of bias and coverage. The ability of RooFitUnfold to tune the regularisation strength of regularised unfolding methods with a common set of optimisation strategies has facilitated the comparative studies presented in the paper.

For the methods with a tuneable regularisation strength we observed that an optimisation of that strength solely on the smallest MSE does not automatically result in good coverage. For the studied example distributions we observed that the inclusion of a bin-averaged coverage criteria in the regularisation strength optimisation resulted in uniformly
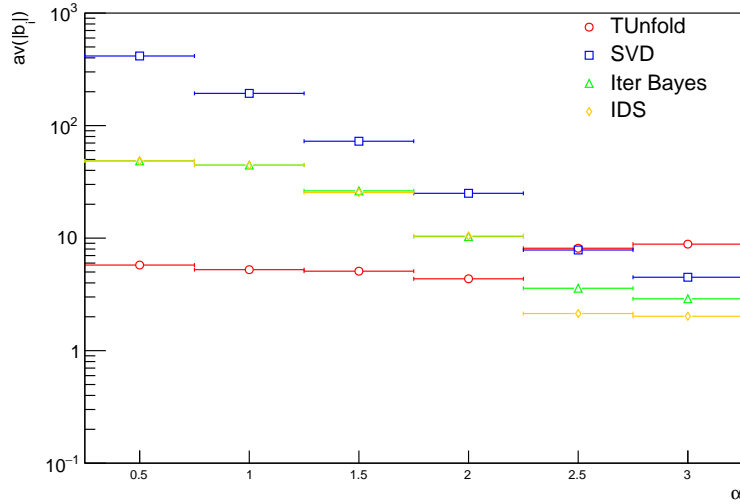
Figure 6: Comparison of the estimated bin-averaged bias of the tuneable unfolding algorithms when unfolding the distorted bimodal model with a response matrix obtained from the undistorted model. Results are shown for various distortion strengths, which increase in distortion with decreasing values of α (See Fig. 4). In this study, the regularisation strength for each algorithm has been optimised on the MSE with the condition that coverage is achieved with 1% of the target value

good coverage for all bins for the methods with a tuneable regularisation strength. While the unfolding bias always depends on the assumed true distribution, we observed for the bimodal example that this dependence was strongest for methods that regularise using the assumed true distribution.
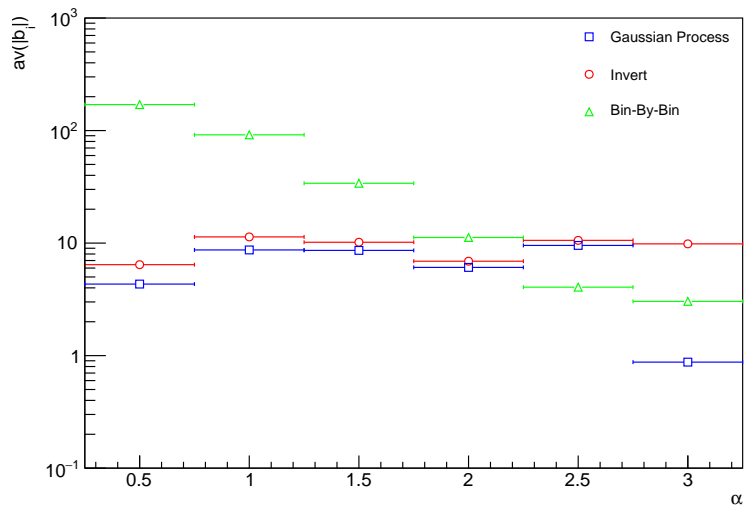
Acknowledgments

Figure 7: Comparison of the estimated bin-averaged bias of non-tuneable and non-regularised methods when unfolding the distorted bimodal model with a response matrix obtained from the undistorted model. Results are shown for various distortion strengths, which increase in distortion with decreasing values of α (See Fig. 4).

References

[1] T. Adye. Unfolding algorithms and tests using roounfold. PHYSTAT 2011, 2011.

[2] V. Blobel. Unfolding Methods in Particle Physics. In *PHYSTAT 2011*, pages 240–251, Geneva, 2011. CERN.

[3] V. Blobel. Unfolding. In O. Behnke, K. Kröninger, T. Schörner-Sadenius, and G. Schott, editors, *Data analysis in high energy physics: A practical guide to statistical methods*. Wiley-VCH, Weinheim, Germany, 2013.

[4] A. Bozson, G. Cowan, and F. Spanó. Unfolding with Gaussian Processes. 11 2018.

[5] G. Cowan. *Statistical Data Analysis*. Oxford University Pres, 1998.

[6] Cowan, G. A survey of unfolding methods for particle physics. *Conf. Proc. C*, 0203181:248–257, 2002.

[7] G. D'Agostini. A multidimensional unfolding method based on bayes theorem. 1995. Nucl. Instrum. Meth. A 362 (1995) 487.

[8] A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal Statistical Society, Series B*, 39(1):1–38, 1977.

[9] P. C. Hansen. The discrete picard condition of discrete ill-posed problems. *BIT*, 30(4):658–672, Nov. 1990.

[10] Hocker and Kartvelishvili. Svd-based unfolding: implementation and experience. PHYSTAT 2011, 2011.

[11] M. Kuusela and V. M. Panaretos. Statistical unfolding of elementary particle spectra: Empirical bayes estimation and bias-corrected uncertainty quantification. *Ann. Appl. Stat.*, 9(3):1671–1705, 09 2015.

[12] M. J. Kuusela. Uncertainty quantification in unfolding elementary particle spectra at the large hadron collider. pages 84–86, 2016.

[13] C. L. Lawson and R. J. Hanson. *Solving Least Squares Problems*. Society for Industrial and Applied Mathematics, 1995.

[14] L. B. Lucy. An iterative technique for the rectification of observed distributions. 79:745, Jun 1974.

[15] B. Malaescu. An iterative, dynamically stabilized method of data unfolding. arXiv:0907.3791.

[16] M. Oreglia. *A Study of the Reactions* $\psi' \to \gamma\gamma\psi$. Other thesis, 12 1980.

[17] W. H. Richardson. Bayesian-based iterative method of image restoration∗. *J. Opt. Soc. Am.*, 62(1):55–59, Jan 1972.

[18] S. Schmitt. TUnfold, an algorithm for correcting migration effects in high energy physics. *Journal of Instrumentation*, 7(10):T10003–T10003, oct 2012.

[19] F. Spanò. Unfolding in particle physics: a window on solving inverse problems. *EPJ Web of Conferences*, 55:03002, 2013.

[20] K. Tackmann. Svd approach to data unfolding. 1996. Nucl. Instrum. Meth. A 372 (1996) 469.

[21] A. N. Tikhonov and V. Y. Arsenin. *Solutions of Ill-posed problems.* W.H. Winston, 1977.

[22] W. Verkerke and D. P. Kirkby. The RooFit toolkit for data modeling. *eConf*, C0303241:MOLT007, 2003.

[23] G. Zech. Analysis of distorted measurements – parameter estimation and unfolding. 7 2016.