

ARU – towards automatic unfolding of detector effects

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Abstract

This article presents the ARU algorithm, a general non-interactive algorithm for the unfolding of detector effects (resolution effects, efficiency, non-linear response) from one-dimensional data distributions. ARU uses an unbinned maximum-likelihood fit with a weighted regularization term, based on the relative information in the solution with respect to a reference distribution. The optimal regularization weight is found by minimizing the mean squared error of the solution. The algorithm's performance is demonstrated in a study of a toy data sets. The analysis shows that the bias on average is smaller than the statistical uncertainties which are properly estimated by the fit.

1 Introduction

The unfolding of detector effects from a measured distribution is a standard problem in particle physics, but a difficult one: the unfolding problem itself is ill-posed [1, 2] and has no unique solution. Several unfolding algorithms [3–7] are known to particle physicists, each with different strengths and weaknesses. This article describes the Automatic Regularized Unfolding (ARU) algorithm, strongly influenced by the works of Blobel [4] and Schmelling [6]. ARU is a regularized fit: a flexible parametrization with many free parameters is fitted to the data and softly constrained by a regularization term. The regularization term allows to reduce the freedom of the fit in a smooth way so that over-fitting is avoided.

ARU is a general non-parametric algorithm for unfolding one-dimensional data distributions that requires no user interaction. The unfolded solution that ARU chooses is optimal with respect to the principle of minimum mean squared error. The analysis of the data is completely unbinned with the advantage that no information is lost. The regularization adapts itself to the data distribution in order to minimize bias.

ARU's non-linear regularization term is a variant of the Kullback-Leibler divergence [8] between the solution and a reference distribution and measures the relative information in the solution with respect to the reference distribution. This choice is invariant to transformations and generalizes the principle of maximizing the entropy (minimizing the information) in the unfolded solution [2, 6]. The regularization introduces a bias as it pulls the solution to the reference. The bias is minimized by using a zero-order approximation of the solution as the reference distribution, obtained by correcting the original data distribution only for efficiency and calibration effects, but not for the critical resolution effects. This approach is invariant to coordinate transformations and self-consistent. If no resolution effects are present, the reference distribution becomes equal to the solution and the fit unbiased, despite the regularization.

In the following, we present the algorithm and close with a study of the performance of the algorithm on a larger number of toy Monte-Carlo data sets.

2 Basic concepts

ARU is a regularized fit. The unfolded solution is parametrized through a flexible and smooth function $b(x)$ which is forward-folded with the detector kernel $K(y, x)$ and fitted to the data under a soft constrain imposed by a regularization term. Many choices are possible for $b(x)$, but a parametrization with B-splines [9] is particularly suitable. A single B-spline is a unimodal, non-negative and piece-wise polynomial curve with finite support. It has non-zero derivatives up to a degree n and is defined on top

of a grid of m so-called knots x_i . The j -th B-spline is defined by the recursion

$$b_{j,0}(x) = \begin{cases} 1 & \text{if } x_j \leq x < x_{j+1} \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

$$b_{j,n}(x) = \frac{x - x_j}{x_{j+n} - x_j} b_{j,n-1}(x) + \frac{x_{j+n+1} - x}{x_{j+n+1} - x_{j+1}} b_{j+1,n-1}(x), \quad j = 0, \dots, m + n - 2 \quad (2)$$

ARU uses B-splines with $n = 3$ and the index n will be omitted in the following. The solution $b(x)$, a general distribution function, is parametrized as

$$b(x) = \sum_j c_j b_j(x), \quad (3)$$

with coefficients c_j . None of the usual boundary conditions are enforced on the B-spline curve which therefore has $m + 2$ free parameters. The solution $b(x)$ is not normalized; the normalization is also determined from the data. The knots of $b(x)$ need to be narrow enough to pick up all features of the unfolded solution. Above this point, the number of knots and their positions become uncritical. It is not possible to have too many knots, but it will not change the result but increases the computing time of the regularized fit described below.

The solution $b(x)$ is then forward-folded with the detector kernel $K(y, x)$ which quantifies effects of non-linear calibration, efficiency, and limited resolution on the true quantity x

$$f(y) = \int K(y, x) b(x) dx = \sum_j c_j \int K(y, x) b_j(x) dx = \sum_j c_j f_j(y), \quad (4)$$

yielding folded basis functions $f_j(y)$ of the folded solution $f(y)$ in the space of the observations. The folded basis functions $f_j(y)$ are computed numerically by the algorithm. Thanks to the linearity of the parametrization, this expensive step needs to be performed only once per application.

The folded solution $f(y)$ is then fitted to the data with the extended maximum-likelihood method [2, 10], i.e., by minimizing the negative log-likelihood function $L_1(\mathbf{c})$

$$L_1(\mathbf{c}) = \sum_j c_j F_j - \sum_i \ln f(y_i), \quad (5)$$

under the constraint $c_j > 0$, whereas $F_j = \int dy f_j(y)$ is the total integral of $f_j(y)$ and the y_i denote the observations.

Without an additional constrain, the parameters c_j will have a huge variance and the solution $b(x)$ will be dominated by oscillations that mainly represent noise. In order to compensate for this the combination $L(\mathbf{c}) = L_1(\mathbf{c}) + w L_2(\mathbf{c})$ is minimized for a given w with the regularization term

$$L_2(\mathbf{c}) = \int b(x) \ln \frac{b(x)}{g(x)} dx - \sum_j c_j B_j \quad (6)$$

and $B_j = \int dx b_j(x)$. The regularization term L_2 is a variant of the Kullback-Leibler divergence ($b(x)$ and $g(x)$ are not normalized). If only L_2 is minimized, $b(x)$ approaches $g(x)$. This narrows down the solution space but also introduces a bias. The bias can be reduced by choosing $g(x)$ properly, which will be discussed in the next section.

Minimizing $L(\mathbf{c})$ appears to be difficult since L_1 and L_2 are non-linear functions of \mathbf{c} . However, one can show that the curvature of both terms is always positive and thus only a single global minimum exists. Standard non-linear minimization algorithms will always converge to it, independent of the starting point.

3 Choice of the reference distribution $g(x)$

Eq. (6) vanishes if $g(x)$ is equal to the true solution [2]. Since the true solution is unknown, $g(x)$ can be made only as close as possible to the correct solution. The simplest choice is $g_{(0)}(x)$, a uniform distribution with the correct normalization of the final result

$$g_{(0)}(x) = \frac{1}{x_{m-1} - x_0} \sum_i \epsilon^{-1}(y_i), \quad (7)$$

whereas $\epsilon(y)$ is the efficiency, y_i are the data points, and x_0 and x_{m-1} the first and last knot position. With this choice our regularization becomes equivalent to the maximum entropy approach [2, 6].

An iterative approach comes to mind. The unfolding is started with $g_{(0)}(x)$ to obtain a solution $b_{(0)}(x)$, which is then used as $g_{(1)}(x) := b_{(0)}(x)$ to obtain $b_{(1)}(x)$, and so forth. Unfortunately, this approach enhances artificial fluctuations and cannot be used. Instead, we propose to unfold once with $g_{(0)}(x)$ and then use the folded solution $f_{(0)}(y)$ as $g_{(1)}(x)$

$$g_{(1)}(x) = f_{(0)}(\bar{y}(x)) \frac{1}{\epsilon(\bar{y}(x))} \frac{\partial \bar{y}}{\partial x} \quad (8)$$

whereas $\epsilon(y)$ describes the efficiency and $\bar{y}(x)$ the (possibly non-linear) average response of the detector. By doing so, we get an approximation that includes all effects except the resolution.

4 Choice of regularization weight

The choice of the regularization weight w is the choice of the trade-off between bias and variance. We minimize the mean integrated squared error (MISE) of the folded solution $f(y)$ to get an optimal compromise

$$\text{MISE}(f(y)) = \int dy E[(f(y) - f_{\text{true}}(y))^2] = \int dy \{V[f(y)] + (f(y) - f_{\text{true}}(y))^2\}. \quad (9)$$

The variance $V[f(y)]$ can be derived from the covariance matrix $\mathbf{V}[\mathbf{c}]$ of the coefficient vector \mathbf{c}

$$V[f(y)] \simeq \sum_i \sum_j \frac{\partial f(y)}{\partial c_i} \frac{\partial f(y)}{\partial c_j} V[\mathbf{c}]_{ij} = \sum_i \sum_j f_i(y) f_j(y) V[\mathbf{c}]_{ij}. \quad (10)$$

The analytical calculation of $\mathbf{V}[\mathbf{c}]$ is shown in the next section.

What remains is to estimate the bias. Since $f_{\text{true}}(y)$ is unknown, we apply the plug-in principle¹ [11] and replace $f_{\text{true}}(y)$ by the empirical distribution $f_{\text{emp}}(y) = \sum_i \delta(y - y_i)$ of the observations y_i . The empirical distribution $f_{\text{emp}}(y)$ is a maximum likelihood estimate of $f_{\text{true}}(y)$ if no other information is available. With these insights we can transform Eq. (9) after some steps into

$$\text{MISE}(f(y)) = \sum_k \sum_l (V[\mathbf{c}]_{kl} + c_k c_l) \phi_{kl} - 2 \sum_i f(y_i) + \text{const}. \quad (11)$$

The last term does not depend on w and therefore is irrelevant for the minimization. The matrix $\phi_{kl} = \int dy f_k(y) f_l(y)$ is computed numerically once per application of the algorithm.

The minimization of Eq. (11) as a function of the regularization weight w is carried out numerically. The coefficients c_i and the covariance matrix $\mathbf{V}[\mathbf{c}]$ are re-calculated in each step by minimizing $L(\mathbf{c})$.

¹Physicists use the plug-in principle (unintentionally) whenever they approximate the Poisson uncertainty of a count n by \sqrt{n} . In this case the unknown mean λ is replaced by its empirical value n .

5 Uncertainty of the solution

The variance of $b(x)$ is computed from the covariance matrix $\mathbf{V}[\mathbf{c}]$ of the coefficients analogue to Eq. (10). The covariance matrix is a sum of two contributions, one arising from the statistical term L_1 and one from the regularization term L_2 since we estimate the reference distribution $g(x)$ also from the data

$$\mathbf{V}[\mathbf{c}] = \mathbf{V}_1[\mathbf{c}] + \mathbf{V}_2[\mathbf{c}], \quad (12)$$

but $\mathbf{V}_2[\mathbf{c}]$ is usually negligible. Its contribution is only expected to be significant in ranges with poor detector efficiency $\epsilon(y)$.

In order to derive $\mathbf{V}_1[\mathbf{c}]$, we follow Blobel's discussion [1, 4] which also gives useful insight into the effect of the regularization. It starts with a Taylor expansion of $L(\mathbf{c})$ around a point \mathbf{c}_0 close to the minimum

$$L(\mathbf{c}) \simeq L(\mathbf{c}_0) + \mathbf{c}^T (\mathbf{h}_1 + w\mathbf{h}_2) + \frac{1}{2}(\mathbf{c} - \mathbf{c}_0)^T \mathbf{H}_1 (\mathbf{c} - \mathbf{c}_0) + w\frac{1}{2}(\mathbf{c} - \mathbf{c}_0)^T \mathbf{H}_2 (\mathbf{c} - \mathbf{c}_0), \quad (13)$$

with gradients $\mathbf{h}_{1,2}$ and Hesse matrices $\mathbf{H}_{1,2}$ of $L_{1,2}(\mathbf{c})$ evaluated at \mathbf{c}_0 .

Eq. (13) can be simplified by dropping all constant terms, this does not change the position of the minimum. Since \mathbf{H}_1 and \mathbf{H}_2 are symmetric, we can simplify to

$$L(\mathbf{c}) = \mathbf{c}^T (\mathbf{h}_1 + w\mathbf{h}_2 - (\mathbf{H}_1 + w\mathbf{H}_2) \mathbf{c}_0) + \frac{1}{2}\mathbf{c}^T \mathbf{H}_1 \mathbf{c} + w\frac{1}{2}\mathbf{c}^T \mathbf{H}_2 \mathbf{c}. \quad (14)$$

We now change into another coordinate system with the transformation matrix \mathbf{M} in which Eq. (14) takes its simplest form

$$\mathbf{c}^T = \bar{\mathbf{c}}^T \mathbf{M}^T = \bar{\mathbf{c}}^T \mathbf{U}_1^T \mathbf{D}_2^{-1/2} \mathbf{U}_2^T. \quad (15)$$

The matrices \mathbf{U}_1 and \mathbf{U}_2 are rotations. The first rotation \mathbf{U}_2 is chosen such that \mathbf{H}_2 becomes the diagonal matrix \mathbf{D}_2 . The matrix $\mathbf{D}_2^{-1/2}$ is also diagonal and defined as

$$D_{2jj}^{-1/2} = 1 / \sqrt{D_{2jj}}. \quad (16)$$

This scaling transformation turns \mathbf{D}_2 into the unit matrix. The matrix $\mathbf{D}_2^{-1/2}$ always exists, because all diagonal elements of \mathbf{D}_2 are positive. The unit matrix is invariant to any further rotation. These transformations applied to \mathbf{H}_1 lead to a another symmetric and positive-definite matrix $\tilde{\mathbf{H}}_1$. The last rotation \mathbf{U}_1 is chosen such that $\tilde{\mathbf{H}}_1$ turns into the diagonal matrix \mathbf{S} , and so we get

$$L(\bar{\mathbf{c}}) = \bar{\mathbf{c}}^T \mathbf{M}^T (\mathbf{h}_1 + w\mathbf{h}_2 - (\mathbf{H}_1 + w\mathbf{H}_2) \mathbf{c}_0) + \frac{1}{2}\bar{\mathbf{c}}^T \mathbf{S} \bar{\mathbf{c}} + w\frac{1}{2}\bar{\mathbf{c}}^T \bar{\mathbf{c}}. \quad (17)$$

The minimum of $L(\bar{\mathbf{c}})$ can now be calculated by solving $\nabla L(\bar{\mathbf{c}}) = 0$. The solution $\bar{\mathbf{c}}$ is compactly expressed as a combination of the two solutions $\bar{\mathbf{c}}_1$ and $\bar{\mathbf{c}}_2$ of the unregularized problem ($w = 0$, $L \equiv L_1$) and the purely regularized problem ($w \rightarrow \infty$, $L \equiv L_2$), respectively:

$$\bar{\mathbf{c}}_1 = \mathbf{S}^{-1} \mathbf{M}^T (\mathbf{H}_1 \mathbf{c}_0 - \mathbf{h}_1) \quad (18)$$

$$\bar{\mathbf{c}}_2 = \mathbf{M}^T (\mathbf{H}_2 \mathbf{c}_0 - \mathbf{h}_2) \quad (19)$$

$$\bar{\mathbf{c}} = (\mathbf{S} + w\mathbf{1})^{-1} (\mathbf{S}\bar{\mathbf{c}}_1 + w\bar{\mathbf{c}}_2). \quad (20)$$

It turns out that the transformed solution $\bar{\mathbf{c}}$ is a component-wise linear interpolation of the two extreme cases, since \mathbf{S} is diagonal. The mixture for each \bar{c}_i depends on the relative size of the weight w and $S_{ii} = \sigma_i^{-2}$, the inverse of the variance of the corresponding coefficient \bar{c}_{1i} . The regularization weight w effectively dampens coefficients with a large variance ($S_{ii} \ll w$).

Eq. (15) and Eq. (20) show the relation between the coefficients \bar{c}_{1k} , for which the variance S_{kk}^{-1} is known, and the coefficients c_i . We can obtain after successive error propagation

$$V_1[\mathbf{c}]_{ij} = \sum_k \frac{\partial c_i}{\partial \bar{c}_k} \frac{\partial \bar{c}_k}{\partial \bar{c}_{1k}} \frac{\partial c_j}{\partial \bar{c}_k} \frac{\partial \bar{c}_k}{\partial \bar{c}_{1k}} S_{kk}^{-1} = \sum_k M_{ik} M_{jk} \frac{S_{kk}}{(S_{kk} + w)^2}. \quad (21)$$

The second contribution $V_2[\mathbf{c}]$ to the total variance is also obtained from a different kind of error propagation. It starts with the known variance $V[\mathbf{d}]$ of the coefficient vector \mathbf{d} of $g(x) = \sum_l d_l b_l(x)$ and uses Eq. (A.2) from the appendix. The change $\delta \mathbf{H}$ after a variation $\delta \mathbf{d}$ is conveniently zero. For $\delta \mathbf{h}$, we get

$$\delta h_k = \frac{\partial h_k}{\partial d_l} \delta d_l = - \int dx \frac{b_k(x) b_l(x)}{g(x)} \delta d_l, \quad (22)$$

and thus finally obtain

$$V_2[\mathbf{c}]_{ij} = \sum_k \sum_l \sum_m \sum_p H_{ik}^{-1} H_{jl}^{-1} \frac{\partial h_k}{\partial d_m} \frac{\partial h_l}{\partial d_p} V[\mathbf{d}]_{mp}. \quad (23)$$

6 Monte-Carlo study

The method is demonstrated with a simple toy Monte-Carlo. The true distribution $t(x)$ is given by the sum of two Gaussians $N(\mu, \sigma)$ in the range $x \in [0, 1]$

$$t(x) = 0.3N(0.3, 0.1) + 0.7N(0.7, 0.05), \quad (24)$$

which form a shallow peak next to a sharp peak. The true distribution $t(x)$ is smeared out with a Gaussian kernel $K(y, x) = N(x - y, 0.1)$. ARU is applied to this data using 20 evenly spaced knots in the interval $[0, 1]$. This number is enough to pick up all features of the unfolded solution and further increasing the number does not change the result. Figure 1 shows the unfolding applied to a sample of 1000 events. The method picks up the true features and does not introduce artificial ones. Some bias is visible and expected, but it is of the same order as the estimated statistical uncertainty.

In order to show ARU's average performance, 2000 data sets are generated and unfolded, half of them with 100 events and the other half with 10000 events each. The results are shown in Fig. 2. The estimated uncertainty agrees well with the observed standard deviation. The average bias is comparable to the statistical uncertainty of the solution.

7 Conclusions and outlook

We presented ARU, an automatic algorithm to unfold detector effects from one-dimensional distributions. ARU tries to improve existing algorithms in several ways. It is a completely unbinned approach with a regularization term that is a variant of the Kullback-Leibler divergence between the solution and a reference distribution. The reference distribution is a smooth approximation to the final solution, obtained by correcting the data only for calibration and efficiency effects. We argue that this choice reduces the bias with respect to a maximum entropy regularization which we generalized with our approach. Our algorithm is based only on statistical information and therefore invariant to transformations of the data. The optimal regularization weight is found by minimizing the mean integrated squared error of the solution. An application of the algorithm to a large sample of toy data sets demonstrates the correct estimation of the statistical uncertainty and a regularization bias that is of the order of the statistical uncertainty.

The source code of ARU can be downloaded from Hepforge [12]. Future work will focus on the generalization of the algorithm to multi-dimensional distributions.

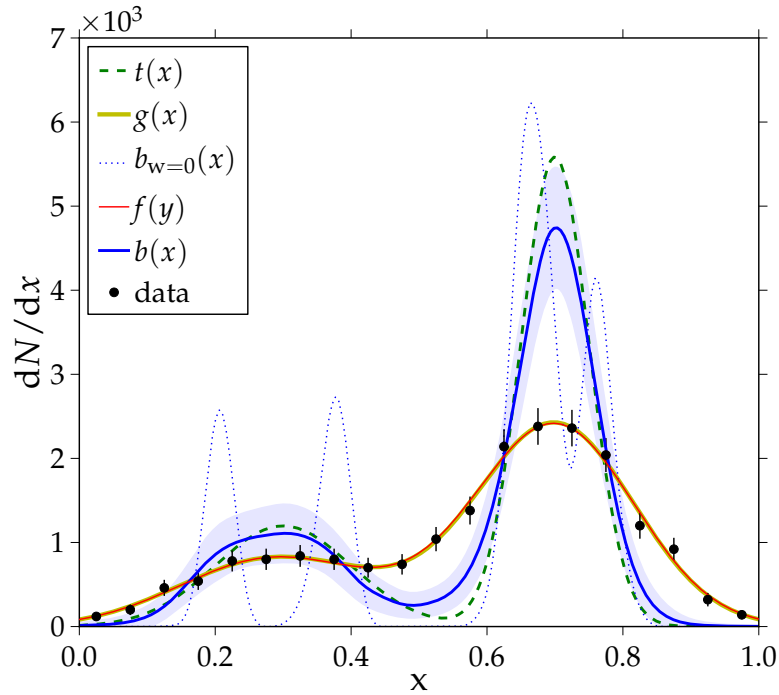


Figure 1: Unfolding of a toy data set of 1000 events. $t(x)$ is the true distribution, the points show a histogram of the smeared data. In this case, the folded solution $f(y)$ is on top of the reference distribution $g(x)$ used for regularization. The regularized solution $b(x)$ shows no undesired oscillations, in contrast to the solution $b_{w=0}(x)$, which is obtained if no regularization is applied.

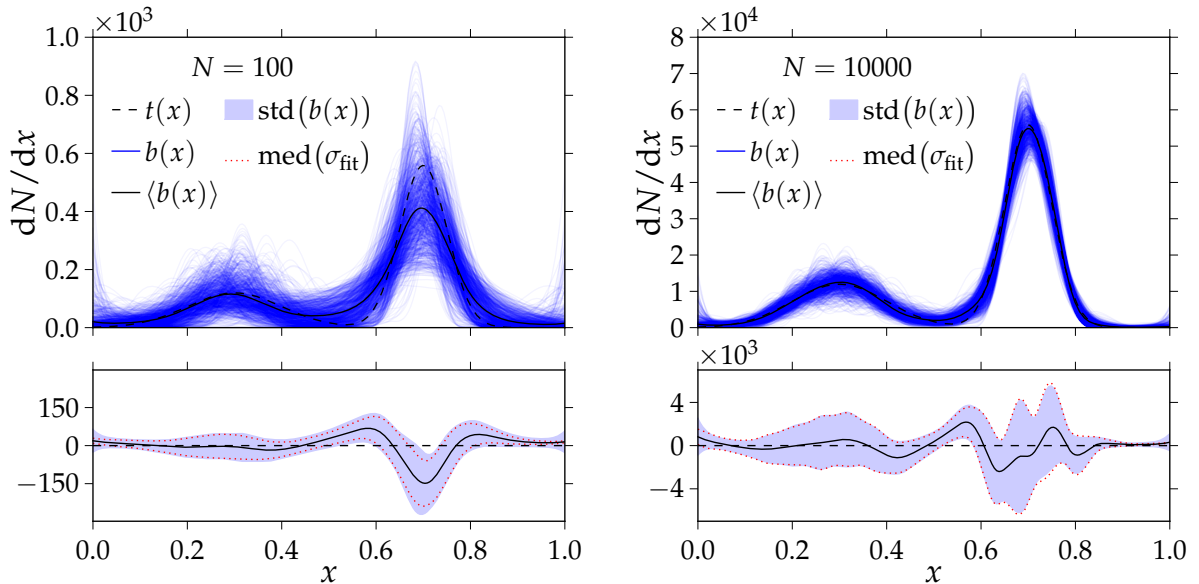


Figure 2: Monte-Carlo study of the unfolding method applied 1000 times to random toy data sets of 100 events (left) and 10000 events (right) each. The top plots show the true distribution $t(x)$ and the unfolded solutions $b(x)$ plotted transparently on top of each other. The bottom plots show the bias $\langle b(x) - t(x) \rangle$ of the unfolding, the standard deviation $\text{std}(b(x))$ of the unfolded set, and the median $\text{med}(\sigma_{\text{fit}})$ of the estimated uncertainty of the solution.

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Appendix

A Propagation of model uncertainties into a maximum-likelihood estimate

We will derive a formula that allows to propagate small changes in the likelihood function, for example due to systematic variations in the explanatory model, into its maximum likelihood estimate.

Let $L(c)$ be a general log-likelihood function. We expand it in a Taylor series up to second order with gradient \mathbf{h} and Hesse matrix \mathbf{H} around a point \mathbf{c}_0 . If \mathbf{c}_0 is close to the minimum of $L(c)$, the Taylor series will be a good approximation for $L(c)$ and the position of the minimum \mathbf{c} can be analytically calculated as

$$\mathbf{c} = \mathbf{c}_0 - \mathbf{H}^{-1}\mathbf{h}. \quad (\text{A.1})$$

We now regard a slightly changed $\tilde{L} = L + \delta L$ with according changes in gradient $\tilde{\mathbf{h}} = \mathbf{h} + \delta\mathbf{h}$ and Hesse matrix $\tilde{\mathbf{H}} = \mathbf{H} + \delta\mathbf{H}$. If \mathbf{c} is the minimum of the undisturbed function $L(c)$, Eq. (A.1) can be used to calculate the corresponding shift in the solution generated by the disturbance:

$$\begin{aligned} \delta\mathbf{c} &= \tilde{\mathbf{c}} - \mathbf{c} = -\tilde{\mathbf{H}}^{-1}\tilde{\mathbf{h}} \\ &= -(\mathbf{H} + \delta\mathbf{H})^{-1}(\mathbf{h} + \delta\mathbf{h}) \\ &= -(\mathbf{H}^{-1} - \mathbf{H}^{-1}\delta\mathbf{H}\mathbf{H}^{-1} + O(\delta\mathbf{H}^2))\delta\mathbf{h} \\ &= \mathbf{H}^{-1}(\mathbf{H}^{-1}\delta\mathbf{H} - \mathbf{1})\delta\mathbf{h} + O(\delta\mathbf{H}^2\delta\mathbf{h}), \end{aligned} \quad (\text{A.2})$$

where the Taylor expansion of $\tilde{\mathbf{H}}^{-1}$ was used and the fact that \mathbf{h} vanishes at \mathbf{c} . The last term $O(\delta\mathbf{H}^2\delta\mathbf{h})$ is of higher order and can be neglected for small disturbances in $L(c)$. The truncated formula is a powerful tool which allows to propagate systematic uncertainties of the explanatory model into the result without resorting to Monte-Carlo techniques in many cases. An example application is shown in Section 5.