Iterating Adjustment for Non-Linear Responses

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Background and Motivation

Within the adjustment-expert community it has been generally known that, in applications for which the linearity assumption is valid, there is no point in re-adjusting the just adjusted parameters by the simultaneously adjusted responses. Starting from a given parameter library *p* and a given set of measured responses *r*, and adjusting the former by the latter, we achieve an adjusted library p' and the corresponding set of adjusted responses r'. If we then *carefully* apply the adjustment prescriptions to these adjusted quantities, we realize that the re-adjusted library p'' is identical to p', as indeed is r'' to r'. A formal demonstration of the above was presented at the latest Symposium on Reactor Dosimetry [1].

Without loss of generality, we may assume that the input p and r data are uncorrelated. Then

$$p' = p - C_p S^{\dagger} C_d^{-1} d \ , \ \ r' = r + C_r C_d^{-1} d \quad , \qquad (1)$$

where S is the sensitivity matrix (of the responses with respect to the parameters); the components of the vector d are the so-called residuals, which are in fact the deviations of the calculated responses from their corresponding measured ones: $d = \bar{r}(p) - r$; the subscripted C's are the (given) uncertainty matrices respectively associated with p and r and

$$C_d = C_{\bar{r}} + C_r = S\,C_p S^{\dagger} + C_r \qquad (2)$$

obviously is the uncertainty matrix associated with d.

It is, however, self-evident that p' and r' are correlated. Their cross-covariance matrix in fact is

$$C_{p'r'} = C_p S^{\dagger} C_d^{-1} C_r \quad . \qquad (3)$$

An elementary, yet detailed, derivation of this equation, and indeed that of the entire conventional-adjustment *formulaire* is presented in Ref. 1. There it is demonstrated that using the prescriptions appropriate for the correlated input p' and r', the re-adjusted parameters and responses are identical to the respective input quantities, which proves our argument.

When responses are strictly linear in the parameters, then conventional adjustment is rigorously correct. However, except for such cases, the validity of the linearity assumption, and practically the effectiveness of the conventional adjustment procedure, depend on how close the representative parameter-space point of the adjusted library, p', is to the original-library point *p*. And this may only be *a posteriori* determined from the actual results of the particular application. To judge the effectiveness of the procedure, a common practice is to check to what extent $\bar{r}(p') \approx r'$.

And so, the question naturally arises of what one could do when the linearity assumption fails, namely when the results of a particular application are such that the recalculated responses $\bar{r}(p')$ are different from the adjusted responses r'. In such circumstances it would seem quite natural to re-adjust the just adjusted parameters by the simultaneously adjusted responses. A common argument to justify such a procedure, and to repeat it, i.e. to iterate the adjustment procedure, is that the process eventually converges.

This iterated solution, however, misses the point in that it is not, in fact, the solution of the original adjustment problem. Recall that conventional adjustment is supposed to find the library p' and the response set r' that, for uncorrelated p and r, minimize the quadratic form

$$Q(p',r') = (p'-p)^{\dagger} C_p^{-1} (p'-p) + (r'-r)^{\dagger} C_r^{-1} (r'-r) \ , \tag{4}$$

subject to the constraint

$$S(p'-p) + d = r' - r \ . \tag{5}$$

Well, the above "natural" iterated solution does not generally minimize the form of Eq. (4). In any event, we propose another iterative procedure of which the converged solution indeed minimizes this form.

A Basic Problem: to Reproduce One Response

We now propose to consider a very elementary adjustment problem, in order to elaborate on the salient points of the general problem. We will then discuss the inadequacy of the iterative solution that we have described. And finally we will examine a "new" procedure that we consider to be a proper one for solving the adjustment problem when the linearity assumption is unjustified.

Let us start from the very beginning. The problem we consider is that of adjusting a given parameter library p by just one measured response r, so that the adjusted library p' reproduce the given response.

The measured response determines a manifold in the parameter space, the locus of all points (libraries) p' that reproduce the response: $\bar{r}(p') = r$. The point p representing the given library is obviously not on the manifold (since it was implicitly implied that $\bar{r}(p) \neq r$). Now, the fundamental proposition of least-squares adjustment is that the optimal p' is the manifold point that minimizes $| p' - p |^2$. It is the manifold point nearest to the given p.

Now, if the (calculated) response $\bar{r}(p)$ is linear in the parameters, or if the optimal manifold point p' is close enough to p, we would be justified in approximating

$$\bar{r}(p') \approx \bar{r}(p) + (\partial \bar{r} / \partial p)\,(p'-p) \ , \tag{6}$$

where the second term on the right-hand side is the scalar product of the parameter-space gradient (evaluated at p), a row vector, by the column $p'-p$. Further, the calculated response at p', by definition, is r, so that Eq. (6) expresses a linear relation satisfied by the components of p'. Hence, letting p' vary under this constraint, there obtains a linear manifold that is the tangent hyper-plane to the manifold $\bar{r}(p') = r$, at its point nearest to p.

We denote the actual adjustments of the parameters by $x_n = p'_n - p_n$; and the sensitivity profile of our response by the row vector $s_n = \partial \bar{r} / \partial p_n$. Then Eq. (6) reduces to

$$sx + d = 0 \ . \tag{7}$$

The problem at hand is elementary: since x evidently is parallel to the vector $s^{\dagger}$, i.e. $x = \beta s^{\dagger}$, then obviously

$$sx + d = \beta ss^{\dagger} + d = 0 \quad \Rightarrow \quad \beta = -\frac{d}{ss^{\dagger}} \quad \Rightarrow \quad x = -\frac{d}{ss^{\dagger}} s^{\dagger} . \qquad (8)$$

A Numerical Example

We now illustrate the foregoing arguments by means of a manifestly non-linear example. Let us then consider a response that is a function of just two parameters, *a* and *b*:

$$\bar{r}(a,b) = ae^{-b} \quad . \qquad (9)$$

Let the given parameter "library" be (*a,b*) = (½,½), and the given measured value of the response $r = 1$. The curve determined by the given response is $b = \ell n\, a$. The curve point nearest to *p* is the point (1,0), since the normal to the curve at the latter point passes through the former. Indeed,

$$\frac{\partial \bar{r}}{\partial a} = e^{-b} \; , \; \frac{\partial \bar{r}}{\partial b} = -ae^{-b} \quad . \qquad (10)$$

Therefore the normal at (1,0) is the vector (1,–1), and this line is $b = 1 - a$, which obviously passes through (½,½).

Thus, any worthy adjustment procedure should take us from the library (½,½) to one as close as possible to (1,0). We also note that χ^2 = min x^2 = ½. Let us then see what happens if we apply the conventional procedure, i.e. the prescription of Eq. (8), to the problem at hand. After three iterations we find that $\bar{r}(p''') = 1.000652$, which practically reproduces r = 1, and the iteration process comes to its end. We therefore realize that p''' indeed lies on the curve determined by the given measured response, but it is away from the point nearest to the given p.

Thus the seemingly natural iteration procedure fails the criterion for acceptability. We will now consider another, more successful, scheme.

An Alternative Iteration Scheme

We now examine a different iteration procedure, and demonstrate that it does converge to the parameter point (1,0), as a deserving adjustment procedure should. The primary idea of the proposed procedure derives from the elementary observation that the normal to the curve determined by the measured response (b = ℓn a in our case), at the point p' nearest to the given-parameter point p, passes through the latter point. In other words, the desired p' is the foot of the perpendicular to the curve dropped from p. Thus, if s' is the sensitivity profile, the gradient, of the (calculated) response, evaluated at p', then $x = p' - p = \beta(s')^{\dagger}$. The problem, of course, is to find what the value of β is.

To find a relation of the given data that involves β, we expand the response about p':

$$\bar{r}(p) = \bar{r}(p') + \left.\frac{\partial \bar{r}}{\partial p}\right|_{p'} (p - p') + \varepsilon \quad , \qquad (14)$$

where ε represents the remainder in the Taylor expansion, which obviously does not vanish in our case of the non-linear response. We further recall that $\bar{r}(p) - \bar{r}(p') = \bar{r}(p) - r = d$. Thus the last equation may also be expressed as

$$s'x + d - \varepsilon = 0 \quad . \qquad (15)$$

And as we substitute $x = \beta(s')^{\dagger}$, we find that

$$\beta = \frac{\varepsilon - d}{s'(s')^{\dagger}} \quad . \tag{16}$$

This is fine, except that we know neither s' nor ε. Of course, if the linearity assumption holds, then s' can be replaced by s, the sensitivity profile evaluated at p, ε vanishes, and Eq. (16), as expected, reduces to Eq. (8).

In order to proceed, we first refer to the first conventional iteration. We will denote its result by p_0. We will henceforth reserve the notation p' for our target point (1,0). In any event, we start by approximating $s' \approx s(p_0) = s_0$. Using this approximation, we then refer to Eq. (14) to obtain a reasonable guess for ε, or rather for $\varepsilon - d$:

$$\varepsilon - d \approx r - \bar{r}(p_0) + s_0(p_0 - p) \quad . \tag{17}$$

And so our next guess for the adjusted parameters, by Eqs. (16) and (17), is now

$$p_1 = p + \frac{r - \bar{r}(p_0) + s_0(p_0 - p)}{s_0 s_0^{\dagger}} s_0^{\dagger} \quad . \tag{18}$$

To figure out the next "new" iteration, we refer to Eq. (18), in which we replace p_0 and s_0 by p_1 and s_1, so that:

$$p_2 = p + \frac{r - \bar{r}_1 + s_1(p_1 - p)}{s_1 s_1^{\dagger}} s_1^{\dagger} \quad . \tag{19}$$

Note that each iteration refers to the very given, original, parameters, using the preceding iteration just to improve the approximation of s' (by s_{n-1}) and of $\varepsilon - d$ (by means of p_{n-1}).

After three iterations we obtain $p_3^{\dagger}$ = (0.994056, –0.005577), which is close enough to the ideal (1,0), and that $\bar{r}(p_3) = 0.999615$, which indeed is practically r = 1, which means that we have reached our goal, and our proposed iteration scheme does work.

Prescriptions for the General Case

For the sake of clarity and completeness, we introduce a few definitions before spelling out the explicit general linearized least-squares prescriptions. Consider the following partitioned generalized vectors and matrices, namely the adjustment vector z, sensitivity matrix S_z, and the "grand" uncertainty matrix C:

$$z \equiv \begin{pmatrix} p' - p \\ r' - r \end{pmatrix}, \; S_z \equiv \begin{pmatrix} S & -1 \end{pmatrix}, \; C \equiv \begin{pmatrix} C_p & C_{pr} \\ C_{rp} & C_r \end{pmatrix} \quad , \tag{20}$$

where S is the conventional response-sensitivity matrix, and 1 the I×I unit matrix (I is the number of responses). Then the (apparently) "most" general (conventional) adjustment problem is to minimize $z^{\dagger}C^{-1}z$ subject to $S_z z + d = 0$. The solution of this conditional-minimum problem, also derived in Ref. 1, is

$$z = -CS_z^{\dagger}\left(S_z C S_z^{\dagger}\right)^{-1} d \quad . \tag{21}$$

This may be somewhat simplified, owing to the (trivial!) observation $S_z C S_z^{\dagger} = C_d$. And further, block multiplying the first two (partitioned) matrices on the right-hand side of Eq. (21), we may separately express the parameter and response adjustments:

$$p' = p + \left(C_{pr} - C_p S^{\dagger}\right) C_d^{-1} d \, , \; r' = r + \left(C_r - C_{rp} S^{\dagger}\right) C_d^{-1} d \quad . \tag{22}$$

Incidentally, the only difference between these prescriptions and the ones given in Eq. (1) is that here we also consider possible non-vanishing response-parameter cross covariances.

We therefore propose that if the conventional adjustment, for whatever reason, is deemed unsatisfactory, then adjustment should be iterated by the recursive prescription

$$p_{i+1} = p + \left(C_{pr} - C_p S_i^{\dagger}\right) C_{di}^{-1} \left[\bar{r}_i + S_i (p - p_i) - r\right] \quad , \tag{23}$$

where by C_{di} we mean that the sensitivity matrix which appears in the explicit expression of C_d is S_i, and where, as before, p_0 is the straightforward solution of conventional adjustment, i.e. p' of Eq. (22).

Recapitulation and Discussion

We have demonstrated that the proposed adjustment iteration scheme, at least in the case of the elementary exercise, indeed converges to the “library” of parameters that truly minimizes the quadratic form it is supposed to. On the other hand, the scheme that we (and others) had considered to be the naturally called for scheme, turned out to converge to a “library” that, though reproducing the measured response, does not minimize the required form.

We should now discuss the iteration scheme suggested by F.G. Perey [2]. He states that “solving a non-linear least-squares problem we must always linearize the model … [and this] involves an expansion, and the best expansion to make is about the solution.” His idea might have been similar to ours. In any event, in terms of our elementary problem it was easy to explain why this expansion point indeed was the best choice. However, in modifying Eq. (22) Perey’s statement, taken literally, seems to imply just replacing the sensitivity profile at the given p by the profile evaluated at the current library point. But, by some stunning intuition, Perey also expanded $\bar{r}(p)$, appearing in *d*, about the current set of parameters into $\bar{r}(p_i) + s_i(p - p_i)$. In other words, our iteration scheme is identical to that of Perey. And we might add that our analysis provides insight and justification for Perey’s iteration scheme, and demonstrates why it is just right.

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References:

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