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REVERSIBLE MATHEMATICS — THE SECOND UNFOLDING SOLUTION AND THE BASIC SOURCE OF UNFOLDING INSTABILITY

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1 Introduction

The solution of the computationally unstable inverse problem (unfolding, deconvolution etc.) is one of the most difficult due to the mathematically noncontrollable solution process – e.g. all the existing algorithms and codes including the most powerful SVD (Singular Value Decomposition) do not allow to calculate explicitly ranks of the involved matrices. In addition, all the existing textbooks and handbooks on computational mathematics either do not deal with this problem at all or expose it as a second-hand item [1], [2].

Under these conditions any systematic attempts to solve the unfolding problem are of some significance *per se*. One of such attempts is the first mass production processing of high energy physics data specified by low statistics ($\leq 10E4$ event/bin) [3].

All the data processing in the above workshop has been done by means of the unfolding algorihm (BUA) developed in 1984 by V.Blobel at CERN [4].

Here we analyze the principal mathematical characteristics of the unfolding phenomenology including the Blobel's unfolding algorithm and consider the role of the Riemann-Lebesgue theorem as a potential source of inherent instabilities.

The newly found second form of unfolding solution suggests the real source of the fundamental computational instability.

2 Unfolding Phenomenology

It is well known that all the integral, differential, integro-differential, nonlinear etc. analytical (continuous) equations, when solved by means of a computer, are reduced to the discrete System of Linear Algebraic Equations (SLAE) like

$$At = f + n \tag{1}$$

where A – a square (apparatus) matrix, t – a column vector of true solution, f – a column vector of erroneous input data and n – a column vector of input data errors. The form (1) corresponds to the formulation of direct problem (folding, convolution etc.).

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Thus, the only purpose of data processing seems to be the solution of the corresponding inverse problem (unfolding, deconvolution etc.):

$$t = A^{-}(f + n) \tag{2}$$

where A^{-} is the inverse matrix of A.

In reality, due to the unavoidable obstacle in the form of the fundamental computational instability, any mass production data processing boils down to an odd mixture of some smoothing and fitting of the input data sets, i.e. of the vector f. Any smoothing in fact is a low-pass filtering, i.e. an implicit elimination of the most physically informative "high-frequency" data component. In turn, any practical data processing (i.e. fitting) deals only with the vector f and not with the vector t. Such fitting techniques are principally nonrobust (fragile or error–dependent) due to local optimization effects inherent in all modern Least SQuares (LSQ) computer codes.

Moreover, the very standard SLAE form (1) allows only the additive statistical errors to be analyzed. Any nonadditive and/or nonstatistical errors (systematic, multiplicative, compound etc.) cannot be described by this SLAE form.

2.1 Regular Unfolding

Generally, the apparatus matrix A can be factorized as [5]:

$$A = A_s A_r A_a A_c \tag{3}$$

where A_s – the particle sorting factor matrix, A_r – the apparatus resolution factor matrix A_a – the apparatus acceptance factor matrix and A_c – the apparatus correction factor matrix.

With $A_s = A_a = A_c = I^{\%}$, where $I^{\%}$ is the diagonal scalar unity matrix, we have $A = A_r$, i.e. the apparatus is completely described by its resolution factor matrix and we deal with the case of regular unfolding.

Then this matrix can be in turn partitioned as

$$A = I^{\%} + R \tag{4}$$

where R – the resolution residual factor matrix with the zero main diagonal.

The regular unfolding solution will look like

$$At = A_r t = (I^{\%} + R)t = f_{reg} = t + r \tag{5}$$

where r – the resolution residual (error) column vector.

2.2 Irregular Unfolding

The different kinds of irregular unfolding correspond to different factor matrices in (3) being unequal to $I^{\%}$, i.e.
$A_s \neq I^{\%}$
$A_a \neq I^{\%}$
$A_c \neq I^{\%}$
and their combinations.

Then the non-resolution errors (statistical, systematic, compound etc.) can be evaluated from

$$s = f - f_{reg} \tag{6}$$

where s – the non-resolution error column vector. In fact we can construct a chain algorithm with each step corresponding to some individual error evaluation.

The relevant deterministic error theory – lathology – is described in an accompanying paper [6].

3 Additive Instability Source Hypothesis – Riemann–Lebesgue Theorem

Notwithstanding the fundamental character of the unfolding computational instability, till now there is no exact identification data concerning its source. One possible explanation can be, however, inferred from SVD factorization studies of the apparatus Toeplitz matrix A. The resulting diagonal SV-matrix $S^{\%}$ provides a specific SV-spectrum, which usually consists of two components, i.e. a normal one with large $SV's \approx 1.0$ (SVL) and that composed of decreasing SV's down to small values $SV \approx macheps \approx E-06$ (SVS). The SVS component can be considered as a signal-plus-noise mixture and the subsequent truncation and optimization procedures support this assumption. This, in turn, suggests the instability source to be inherent in the very structure of the linear model.

In fact, the only presently proposed hypothesis about the origin of this instability is based on the Riemann-Lebesgue theorem [8], [9] well-known in the theory of Fourier series coefficients [10], [11], i.e.

$$\int_{\alpha\to\infty} A(x,s)\sin(\alpha * s)ds \to 0 \tag{7}$$

This Limiting Virtual Zero (LVZ) is usually added to the left-hand-side (l.h.s.) of the SLAE (1) in a discrete form to yield a solution with the superimposed periodic instability

$$SEF(m) = A^{-}(f+n) \tag{8}$$

where SEF - the Signature-Envelope Function in the form of a signature like sinus wave superimposed upon the envelope of the vector f and m - the bin number.

The Riemann-Lebesgue theorem is not, however, the only version of the LVZ - any converging series tending to zero will serve as well, i.e. the number of potential candidates is infinite.

4 The Second Unfolding Solution

The basic reversibility axiom requires an term-by-term equivalence relation between the left hand side and the right hand side of any equation to be really valid. As a consequence, any identity transforms like transfers of terms from one side to another or differentiation of both sides satisfy this axiom by definition.

So let us differentiate relation (1):

$$A't + At' = (f+n)' \tag{9}$$

to get the second general form of the inverse problem solution

$$t = (A')^{-}[(f+n)' - At'] \tag{10}$$

where all r.h.s. terms contain derivatives. The behaviour of numerical derivatives of error-stricken functions has been systematically studied ealier [7]. Their patterns closely fit those observed in solving (2), i.e. the SEF (8).

5 Blobel's Unfolding Algorithm (BUA)

It is useful to analyze the set of initial hypothesis forming the ground of the BUA [4]:

1. "The measured distribution differs from the true distribution by statistical errors".

This statement overestimates the role of statistical errors and excludes from the analysis systematic and other errors of different origin, since the standard data processing means cannot deal with these latter by definition.

2. "These errors are additive".

Again the analysis is too restricted because the standard linear model (1) cannot consider any nonadditive errors at all.

3. "The reconstruction of the true distribution from the measured one is called unfolding and it is a statistical estimation problem".

From our point of view, the unfolding (or deconvolution - VII) is a purely algebraic problem, especially, if one considers other nonadditive and nonstatistical errors.

4. "Acceptable unfolding results can be obtained by regularization methods".

The existing regularization methods use mathematically improper (quasiscalar - VII) objective functionals and inadequate local minimization techniques.

5. "The true distribution can be represented by some smoothed pattern e.g. in a spline form".

Any smoothing procedure is equivalent to a low-pass filtering, which eliminates the most physically informative "high-frequency" component of the measured data samples. In fact, any measured data sample is purely fractal due to point-to-point (bin-to-bin) errors of various kinds.

Other BUA hypotheses concern mainly computational means, but are also logically and mathematically unsafe.

6 Reversible Unfolding

As has been stated above, we consider the problem of unfolding as a purely algebraic one. We can postulate that in the absence of errors the unfolding like (2) has to be stable. This postulate becomes, however, invalid, if we are aware of the consequences following from the simple fact that the very elements of the standard mixed matrix-vector linear model (1), i.e. A, t and f do not form an algebraic group. One of such consequences is the impossibility of any unfolding relative to the matrix A:

$$A = ft^{-} \tag{11}$$

where t^{-} is the inverse vector of t. The product of the column vector f and of the row vector t^{-} is a matrix of rank one, i.e. a scalar, to result in a nonunique matrix A due to the purely Diophantine character of the initial linear model (1). This feature was somehow missed in the existing literature on linear model.

Now by means of simple reversible physical or/and mathematical transforms we shift to an all-matrix analog of (1):

$$AT = F \tag{12}$$

with the relevant reversible unfolding solution like

$$T = A^{-}F \tag{13}$$

and the corresponding solution for the apparatus matrix A.

The elements of the reversible linear model (12) form a group and are unique. For example, here the SVD techniques can be applied to all matrices to produce very simple symmetric algebraic structures. In addition, the novel model allows any error (lathological – see [6]) model to be incorporated in the simplest possible manner. Moreover, this linear model provides some mathematical means to analyze systematic errors of different origin [6].

Finally, by shifting to an integer number basis and using the matrix factorizations via the normal Hermite and Smith forms (NHF and NSF) one can continuously control the ranks of the involved matrices, while solving the unfolding problem (13) in a stable way under arbitrary input data errors without any regularization used [5].

The use of the advanced global regularization [12] and/or global optimization [13], [14] is supposed to provide additional means of the unfolding robustization.

7 Conclusions

The newly developed approach based on reversible mathematics produces the following results:

1. An identity differentiation transform provides the second unfolding solution.

2. The explicit form of this unfolding solution contains only derivative forms of the known linear model terms, thus indicating the general source of the fundamental computational instability.

3. Such an interpretation of the instability source justifies the transfer to an integer number basis performed earlier due to different mathematical reasons.

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