СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E10-95-270

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REVERSIBLE MATHEMATICS — THE GLOBALLY ROBUST LEAST SQUARES

1995

1 Introduction

The standard linear model of data processing, i.e. the direct problem (folding, convolution etc.) looks 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 very elements of this mixed matrix–vector form, i.e. A, t, f and/or n, do not compose any algebraic group–this fundamental mathematical feature has been missed in the whole previously performed analysis. The immediate consequences are twofold: first, it is impossible to compute the matrix A by unfolding (1) [1], i.e. the matrix A becomes nonunique, and, second, the above mixed form can incorporate only additive errors.

In trying to get the solution of the inverse problem (unfolding, deconvolution etc.) like

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

where A^{-} is the inverse matrix of A, one usually encounters the irresistible fundamental computational instability.

We have succeeded in solving (2) under arbitrary input errors without any additional regularization used explicitely [1]. Here we describe some additional regularization means considered as an alternative to the above robust unfolding.

2 Local Robustization via Discrete Holder Norms

The discrete Holder norms are defined as [2]:

$$\| x \|_p = (\sum_{i=1}^{n} | x_i |^p)^{1/p} \tag{3}$$

The standard LSQ objective functional, G, being a squared discrete Holder norm with $p = 2$, i.e. the so-called Euclidean norm, has a scalar metric form [3], [4] to be minimized as

$$G = (f - t)^2 = MIN! \tag{4}$$

From a simple geometrical picture one can easily see that this constraint requires a minimum distance between the measured data vector f and the regressor (true solution) vector t.

The fragile, i.e. nonrobust or error-dependent, nature of this objective functional can be easily demonstrated by variating the measurement error of a single point from the set f. As a net result, the inherent statistical estimate, i.e. the mean value, will change according to the single point error value and the position of the regressor t will be changed accordingly. All the existing procedures of eliminating statistically "bad" points use an unlawfull means, since the final data set f becomes quite different as compared to the initial data set f.

Later on there were proposed some robust statistics based on the Manhattan norm, i.e. the discrete Holder norm with $p = 1$ [5]. This norm and the relevant metric forms possess, however, another instability feature, which one can clearly demonstrate by considering a set of the measured data f with equal errors – the position of the relevant regressor t between ambivalent halves of the set f is quite arbitrary. The inherent statistical estimate, i.e. the median, is, however, stable against single point error variations and in this sense is locally robust.

Analogous properties exhibits the so-called Chebyshev norm, i.e. the discrete Holder norm with $p = \infty$.

To sum up, any scalar objective functional G in the form of some discrete Holder norm or its involution modification, which can be imagined as a point in the G-space, is either fragile (nonrobust) or semi-fragile (locally robust).

3 Local Robustization via PTT (Philips–Twomey–Tikhonov)–Regularization

Another direction of the LSQ local robustization is associated with the PTT–regularization [6]. Here the drastic improvement is done by means of the

transfer to the vector objective functional G, which improvement is, unfortunately, compensated by the pseudo-scalar form of that functional:

$$G = \| At - f \| + \alpha \| t \| = G_1 + \alpha G_2 \tag{5}$$

where α is the so-called regularization parameter.

The integral form of the second term proposed by Philips [7]:

$$G_2 = \int [t'']^2 dx \tag{6}$$

can be used only for small input error cases, since any error–stricken function t is fractal-like and, consequently, has no analytical derivatives. The artificial approximation means like. e.g. spline techniques [8], are in fact implicit low–pass filtering tricks eliminating the most physically significant component of the unfolding solution.

Our direct tests of all PTT–regularized processing codes show that they provide the stable unfolding only for data sets f with the input relative errors $e = n/f \leq 1\%$ [1].

4 Global Reversible Robustization

4.1 Global Robustization via Integral Holder Norms

The transfer to the Holder integral analogs of the above discrete norms [2]:

$$\| f \|_P = [\int_a^b | f(t) |^p dt]^{1/p} \tag{7}$$

significantly improves the robustness of the inverse problem solution even in a simple scalar form. This enhanced stability is achieved, however, due to the same deterioriating low-pass filtering effect.

4.2 The All-Matrix Linear Model in an Integer Number Basis

The more mathematically sound and safe robustization can be achieved by means of the reversible all-matrix linear model [1]:

$$AT = F + N \tag{8}$$

solved within an integer number basis. The tested unfolding algorithm uses the Hermite or Smith Normal Forms (HNF or SNF) to factorize the apparatus matrix A. This factorization whithin the integer number basis does not require any divisions to be made, which is quite essential for an integer ring. The subsequent computation of the inverse matrix A^- is performed within a real number basis. The unfolding process is stable for arbitrary errors in the input data set f, thus producing satisfactory results without any regularization used.

4.3 Global Optimization

All the standard LSQ procedures are subject to two main defects: first, these use local optimization codes and, second, the most popular weighed LSQ procedures introduce a wrong mathematical object in the form of the Holder norm with $p \leq 1$. The latter, in turn, produces a set of virtual local minima. In addition, the minimized objective functional, G, is usually assumed to posses some analytical features, e.g. to be twofold differentiable.

All these facts appeal to the effective global optimization procedures to be used instead of ineffective standard local optimization ones. The developed till now global optimization codes ensure, however, the global character of the detected minimum with some probability $Prob < 1.0$ [9].

Our studies show [10], [11] that the most effective global optimization algorithms must incorporate both integration and an asymptotic search for the global minimum. The integration step ensures a low-pass filtering of all fractile-like nonanalytical singularities of the objective functional under study, i.e. it transforms an initial error-stricken functional into an analytical (smooth, monotone, differentiable etc. - VII) one, while the asymptotic search step ensures a reliable detection of the position of the global minimum. Unfortunately, the first step performs the filtering of the most physically informative "high frequency" component of the processed spectra. As a net result, such algorithms can be recommended for processing nonspectral objects like nucleon structure functions [12].

4.4 Global Optimization of Vector Objective Functional

Even the standard matrix-vector linear model (1) allows to construct in the G-hyperspace multidimensional vector objective functionals with a high degree of inherent robustness. The PTT-regularized objective functional (5) can be considered as a two-dimensional G-vector. A three-dimensional G-vector looks like

$$G = G_1 + G_2 + G_3 = \| At - f \|_p + \| f - t \|_p + \| t \|_p \tag{9}$$

Instead of transforming this vector functional into a (completely mathematically nonmotivated - VII) PTT-regularized quasi-scalar functional we postulate that any minimized vector is composed of minimized projections. In other words, the vector minimization requirement:

$$G = G_1 + G_2 + G_3 = MIN! \tag{10}$$

is considered to be equivalent to the three independent scalar minimization requirements:

$$G_1 = MIN! \ \& \ G_2 = MIN! \ \& \ G_3 = MIN! \tag{11}$$

realized by means of the global minimization codes cited above (see e.g. [11]). All these operations can be performed within a real number basis and the obtained results can be checked by a comparison with those obtained within an integer number basis by means of the HNF or/and SNF factorizations.

5 Analysis and Comments

One can easily see that the standard matrix-vector linear model (1) can be used only for an additive lathological (error) model with a nonunique apparatus matrix A. Some advanced factorization techniques like the SVD in a real number basis and/or the HNF and SMF in an integer number basis allow the unfolding problem to be reliably solved for arbitrary input error levels.

The transfer to the mathematically rigorous reversible all-matrix linear model (8) enables to incorporate arbitrary (multiplicative, compound etc.) lathological models with a unique apparatus function A. The potential possibility of factorizing the remaining matrices T, F and N provides a set of powerful novel unfolding versions.

6 Conclusions

Thus, the novel reversible approach provides the globally robust LSQ techniques specified by the main following features:

1. The first semi-globally robust LSQ solution can be obtained by means of some advanced SVD–factorizations of the matrix A with additional iterated SV–truncations or/and variations for a scalar or vector objective functional G within a real number basis.
2. The second globally robust LSQ solution can be obtained by means of some integral global optimization of a scalar or vector G within a real number basis.
3. The third globally robust LSQ solution can be obtained by means of some HNF– or/and SNF– factorizations of the matrices A, T, F and N for a scalar or vector G within an integer number basis.

7 Acknowledgments

The author would like to thank late Profs. H.Legendre and C.F.Gauss for their invention of classical LSQ techniques. The author also acknowledges the generous support provided by Prof.A.I.Malakhov within the SPHERE collaboration.

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Received by Publishing Department
on June 26, 1995.