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SOME COMMENTS TO DECONVOLUTION METHODS

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The problem of deconvolution is common to many branches of science, technology, medicine, etc. It always occurs when it is necessary to remove an instrumental distortion from a measured signal. The deconvolution belongs to the category of inverse problems which are often ill-posed, incorrect - the existence, unambiguity and stability of the solution are not *a priori* warranted. Connections among various deconvolution methods will be indicated, some practical recommendations will be given and examples from the deconvolution of X-ray diffraction profiles will be presented.

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1 Introduction

Many processes in nature and technology can be described as a transfer of an input $f(y)$ over some system S, which results in the output $h(x)$. If the system S is linear, the resultant output is the linear superposition

$$h(x) = \int_a^b f(y)g(x,y)dy\,, \tag{1}$$

where (a, b) is the interval, in which the functions f, g, h are defined.

If the properties of the system S are independent on the choice of the origin of the abscissa (time, position, ...), the function g is the same over all considered interval, i.e., g is a translational invariant and thus, the function of only the difference $(x - y)$. Eq. (1) is then changed into a convolution

$$h(x) = \int_a^b f(y)g(x-y)dy = \int_a^b f(x-y)g(y)dy\,. \tag{2}$$

The solution of the integral equation (1) and (2) for the unknown function f is called decomposition and deconvolution respectively. Equations (1) and (2) can be written in the operator form

$$Af = h\,, \tag{3}$$

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where unknown f has to be determined from the known A and h. This is so called the inverse problem, which is opposite to the direct problem – the estimation h from the known A and f. Inverse problems are often ill-posed, incorrect – the existence, unambiguity and stability of the solution are not *a priori* warranted. The stability means that the solution depends continuously on the data, which is very important for the treatment of really measured experimental data.

The system S is a measuring instrument in experimental sciences, for example an X-ray diffractometer. The function g is the instrumental function, which describes distortions (caused by geometrical and spectral factors) of a physical diffraction profile f (due to a small crystallite size and a microstrain) into really measured diffraction profile h. In optics, astronomy and image processing [1], the instrumental function g is called the point spread function. In radiation therapy, it is the elementary dose kernel [2] and in the theoretical physics, the function g has analogy in Green's function. In the communication theory or in the geophysics, the system S or the function g is considered as a filter of some input signal f, which should be restored from the output signal h.

The purpose of this contribution is to call attention to connections among methods of restoration developed in various branches and to facilitate the orientation in rapidly growing literature on these methods and among restoration procedures, which are contained in languages or programs, e.g. MATLAB, ORIGIN, etc.

2 Methods of restoration

Method of serial products [3] is the simplest method of deconvolution and cannot be suggested for a treatment of experimental data. It allows demonstrating why a large number of input data and a small ratio of widths of the function h and g lead to wrong results [4].

Method of the system of linear algebraic equations follows naturally from demands of practical computations. The integral in equation (1) is replaced by the sum and continuous functions are sampled in discrete points. Integral equation (1) is thus replaced by the system of linear algebraic equations

$$\sum_{i=0}^{n} w_i g_{ji} f_i = h_j + n_j \quad j = 0, 1, \ldots, n\,, \tag{4}$$

where $f_i = f(y_i)$, $h_j = h(x_j)$, $g_{ji} = g(x_j, y_i)$. Values $g_{ji} = g(x_j - y_i) = g_{j-i}$, appearing in the discretized form of the convolution (2), depend only on the difference of indices $j - i$. w_i denote weight factors, depending on the quadrature formula, which can be easily included in matrix elements of the system (4). The noise n_j is a very important factor. The system of linear algebraic equations (4) has usually the matrix form

$$\mathbf{h} = \mathbf{G}\mathbf{f} + \mathbf{n}\,. \tag{5}$$

Increased difficulties have appeared for a small ratio of widths of functions h and g and for input data with an increased fraction of noise $\mathbf{n}$. The higher dimension of the matrix $\mathbf{G}$ meant a stronger amplification of the noise in the process of matrix inversion. The decreasing step of variables x, y and the increasing number of equations in the system (5) leads to unfounded oscillations of the solution. A minimization of the second derivative of the solution was suggested

by Phillips [5] to suppress these oscillations. It may be expressed in matrix notation as the minimization of the quadratic form $(\mathbf{f}^T\mathbf{C}^T\mathbf{C}\mathbf{f})$, where

$$\mathbf{C} = \begin{pmatrix} 1 & & & & \\ -2 & 1 & & & \\ 1 & -2 & & & \\ & & 1 & \ddots & 1 \\ & & & & -2 \\ & & & & 1 \end{pmatrix} . \tag{6}$$

The solution is then obtained by the method of Lagrange multipliers

$$\mathbf{f} = (\mathbf{G}^T\mathbf{G} + \gamma\mathbf{C}^T\mathbf{C})^{-1}\mathbf{G}^T\mathbf{h}\,, \tag{7}$$

where γ is the reciprocal value of the Lagrange multiplier and it may be estimated by an iteration process [6]. An application of this *constrained least squares method* to the deconvolution of X-ray diffraction profiles is given in [7]. The *least squares method* follows from (7) for $\gamma = 0$

$$\mathbf{f} = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{h}\,, \tag{8}$$

and if $\mathbf{G}$ is a square matrix and if $\mathbf{G}^{-1}$ exists, then $\mathbf{f} = \mathbf{G}^{-1}\mathbf{h}$, which is the *simple inversion*.

The inverse matrix $\mathbf{G}^{-1}$ need not exist, so that it is necessary to use the Moore-Penrose pseudo-inverse matrix or singular value decomposition (SVD) method. An iteration form of SVD – the *truncated SVD method* [1] – is very convenient, because the index of truncation has the role of a regularization parameter. This parameter is a crucial notion in the regularization method, which can be used also to the regularization of the system of linear equations [8]. More simple iteration or relaxation methods are often successful. They are closely connected to the next method.

Iterative method of integral equation is based on the transformation of the Fredholm integral equation of the first kind (1) to the equation of the second kind, which can be solved by the iterative process. The recurrent formula

$$f^{(k+1)}(x) = f^{(k)}(x) + h(x) - \int_a^b f^{(k)}(y)g(x-y)dy\,, \tag{9}$$

holds with the initial approximation $f^{(1)}(x) = h(x)$ in the case of deconvolution [9]. The deconvolution is thus calculated by means of convolution, but the iteration process need not to converge. There is an optimal number of iterations. The recurrent formula (9) has the discretized form

$$f_i^{(k+1)} = f_i^{(k)} + \left(h_i - \sum_{l=1}^{n} f_l^{(k)} g_{i-l} \right) \quad i = 1, 2, \ldots, n\,, \tag{10}$$

which is a description of the Jacobi iteration method of the system of linear equations $\mathbf{G}\mathbf{f} = \mathbf{h}$ if the difference index $(i-l)$ is substituted by the couple indices i, l. Jansson [10] suggested to multiply the parentheses in (10) by factors (κ/g_{ii}), where κ is the relaxation parameter

$$f_i^{(k+1)} = f_i^{(k)} + \frac{\kappa}{g_{ii}} \left[h_i - \sum_{l=1}^{n} g_{il} f_l^{(k)} \right] \quad i = 1, 2, \ldots, n\,. \tag{11}$$

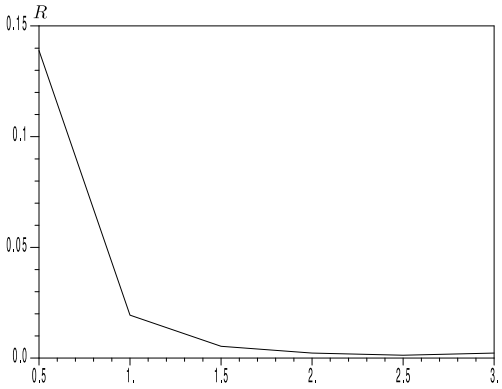

Fig. 1. The dependence of the residuum R on the relaxation factor κ' ($n = 9$).

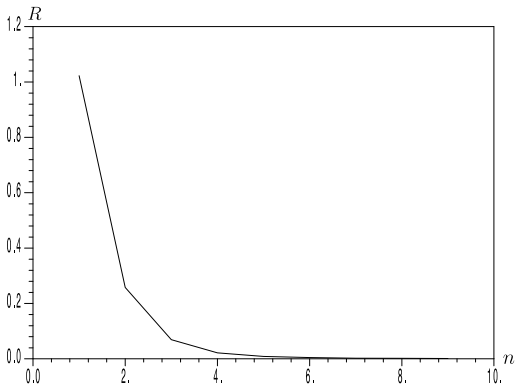

Fig. 2. The dependence of residuum R on the number of iterations n ($\kappa' = 2.5$).

This is the point-simultaneous overrelaxation method, which converges more rapidly than the system (10). Comparison of eqns. (10) and (11) indicates the Burger-van Cittert method in the discrete form to be a special case of the relaxation method with the choice $\kappa' = \kappa/g_{ii} = 1$, which is not optimal (Fig. 1). The optimum value of κ is connected with eigenvalues of the matrix $\mathbf{G}$ in eqn. (5) [11] or with the spectral radius of the corresponding Jacobi iteration matrix [12]. A suitable value of κ can also be obtained by the trial-and-error method [10], [13]. A small number of iterations is enough as a rule (Fig. 2).

The residuum R (in Fig. 1 and Fig. 2) is defined [14] by the equation

$$R = \frac{\sqrt{\sum_i \Delta_i^2}}{\sum_i h_i}\sqrt{n}\,, \tag{12}$$

where Δ_i is the difference between values h_i and $h_i^{(k)} = f^{(k)} * g$ (the asterisk indicated the convolution), n is the number of data.

Iterative ratio method proposed by Gold [15]

$$f_i^{(k+1)} = \frac{h_i}{[\mathbf{G}\mathbf{f}^{(k)}]_i} f_i^{(k)}\,, \tag{13}$$

gives often better results than original "difference" method of van Cittert [16]. Iterative ratio algorithm has also a continuous form [17]

$$f^{(k+1)}(x) = \left[\frac{h(x)}{f^{(k)}(x) * g(x)}\right]^{\mu} f^{(k)}(x)\,, \tag{14}$$

where exponent μ is an arbitrary number and it has a role of the relaxation parameter. It can be estimated by the trial-and-error method. Some care is necessary because of the possibility that $f_i^{(k)} = 0$. This can happen for some order of iteration k and some indices i as a consequence of noise. The following iterations are all zero for these indices i according to eqn. (13).

The relaxation parameter can constrain the iterations between prescribed limits, in addition to improvement of the convergence. Frieden [18] indicated general form of the variable relaxation parameter

$$\kappa(x) = C \left\{ 1 - 2[B(x) - A(x)]^{-1} | f^{(k)}(x) - \frac{1}{2}[A(x) + B(x)]| \right\} , \tag{15}$$

where C is a constant and $A(x)$ and $B(x)$ are limiting functions, *i.e.*, $A(x) \leq f(x) \leq B(x)$ for the continuous form of the van Cittert iterations

$$f^{(k+1)}(x) = f^{(k)}(x) + \kappa(x) \left[h(x) - f^{(k)}(x) * g(x) \right] . \tag{16}$$

Convergence of the van Cittert iterations exists if, and only if [19]

$$\left.\begin{array}{lll} |1 - G(\omega)| < 1 & \text{for} & G(\omega) \neq 0 \\ H(\omega)| = 0 & \text{for} & G(\omega) = 0 \end{array}\right\} , \tag{17}$$

where G and H are Fourier transforms of the functions g and h respectively. For details see [4] and references cited herein.

The iterative methods are very popular because of the possibility of terminating an iterative process when the noise is too strongly amplified and because of the possibility to introduce constraints on the solution. Therefore, new modifications of iterative methods have appeared, e.g. [14], [20], *etc*. A broader and more detailed review of the methods of restoration is given in [4].

3 Conclusion

All methods of restoration require a high quality of the input data. It means a high precision of the individual data and a high resolution of the instrument. More generally, the ratio of the widths of the functions h and g should be a higher as 2. Difficulties for a smaller value are illustrated in [21] by the *method of inverse filtering*.

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