Letters to the Editor

Comments on 'New Approach for Correction of Distortions in Spectral Line Profiles in Auger Electron Spectroscopy'

In a recent work[1] a new approach for the correction of spectral lineshapes was proposed. The method is universal and it is by no means restricted to a particular spectroscopy. There is no doubt that it is one of the significant achievements in solving the deconvolution problem.

However, one point remains unclear. The authors apply the non-linear Levenberg–Marquardt (LM) method to find the coefficients of the spline approximation used in their approach and the paper contains a subsection about the technicalities of this computational algorithm. The main idea being that the experimental spectrum and the deconvolved curve can be expressed as a linear combination of some basis functions (eqns (7) and (8) of Ref. 1), it should be obvious that the LM method is superfluous. The appropriate coefficients can be obtained by solving a simple system of linear equations. For the particular case of self-deconvolution presented elsewhere[2] a non-linear method is compulsory, but for the general problem of deconvolution it is unnecessary. This is not a point of principle but as the deconvolution problem is a practical one, we feel that it has some importance.

The gist of the new approach is to use the knowledge about the broadening effect upon some particular functions. These functions are Schoenberg's splines of order k, $B_{i,k}(x)$ (defined in eqn (5) of Ref. 1). A function $B_{i,k}(x)$ after a convolution with the function $V(x)$ is transformed into a new one:

$$B^*_{i,k}(x) = \int B_{i,k}(x-\Delta)V(\Delta)\,\mathrm{d}\Delta$$

An integral transformation of a linear combination of functions produces of course a linear combination of integrals:

$$\int \sum c_i B_{i,k}(x-\Delta)V(\Delta)\,\mathrm{d}\Delta = \sum c_i B^*_{i,k}(x)$$

The coefficients used to approximate the experimental spectrum

$$S(x) = \int D(x-\Delta)V(\Delta)\,\mathrm{d}\Delta$$

with the modified basis functions $B^*_{i,k}$ are the ones needed to approximate the original line $D(x)$ with the functions $B_{i,k}(x)$. If

$$S(x) = \sum c_i B^*_{i,k}(x) \qquad (1)$$

then

$$D_c(x) = \sum c_i B_{i,k}(x).$$

Obviously the convolution of $D_c(x)$ with $V(x)$ gives $S(x)$.

To implement this idea one needs first to compute the modified functions $B^*_{i,k}$ and then to find the appropriate coefficients. If, as usual, the values of $S(x)$ are known only for N points x_j, $j = 1 \ldots N$, Eqn (1) can be rewritten as a linear system of equations for the coefficients c_i, $i = 1 \ldots N_s$, where N_s is the number of splines:

$$\sum A_{ij} c_i = s_j$$

A_{ij} being $B^*_{i,k}(x_j)$ and $s_j = S(x_j)$. As a rule this is an over-determined system that can be solved with the *linear* least squares method:

$$\mathbf{c} = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}(\mathbf{A}^{\mathrm{T}}\mathbf{s})$$

This substantial simplification has been implemented in a program which consistently produces very good results.

Some practical questions about the number of splines needed, their order and how their knots are chosen arise. Such problems have been discussed already in a paper[3] where this approach to the deconvolution of experimental data has been investigated.

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Response to the comments of S. Kovatchev and A. Losev on 'New Approach for Correction of Distortions in Spectral Line Profiles in Auger Electron Spectroscopy' by A. G. B. M. Sasse, H. Wormeester and A. van Silfhout

We agree with the comments and we have also recognized these linear properties which can be useful for several applications when a deconvolution operation is needed. We found the same satisfying results. Furthermore, it can be proven that in the deconvolution calculation, our $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ and Kovatchev and Losev's $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ is a Toeplitz matrix. This mathematical property reduces the number of numerical operations significantly.[1] This mathematical property survives even in a two dimensional approach and with boundary splines included.[2] Nevertheless, we have chosen to present our scheme in the most general way because we do not want to exclude non-linear cases in solving equations for the type $\mathbf{A}x = y$[1] (for example the self-deconvolution problem). Furthermore, this non-linear approach has some advantages in solving the deconvolution problem when the whole spectrum is not available for the deconvolution. This can induce boundary effects which can be suppressed by specifically weighting a particular part of the spectrum. Also, constraints on the spline functions can easily be implemented to control the shape of the solution.

In summary, we believe that the comments which put stress on the linear features of our approach should have been included in our paper.[3] It would have increased its significance and therefore we are pleased with this comment that supports our achievement in solving (non)-linear problems ($\mathbf{A}x = y$) and the deconvolution problem in particular.

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