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On the recovery and resolution of exponential relaxation rates from experimental data: Laplace transform inversions in weighted spaces

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Abstract. In three previous papers we have considered the problem of Laplace transform inversion when the unknown function is of bounded, strictly positive support. The improvement in resolution due to *a priori* knowledge of the support was quantified and methods for the choice of an optimum sampling of data were given.

In the present paper we discuss some undesirable edge effects encountered in practice with these methods and we indicate a way to refine such calculations by considering the problem of Laplace transform inversion in weighted L^2 spaces. A smoothly varying weight takes into account a partial knowledge of the *localisation* of the solution which can be estimated *a priori* from the knowledge of its first and second moments which are easily derived from the data before inversion. In such a way the reconstructed solution is forced to be small where it is likely to be small and the troublesome edge effects found in the previous methods are suppressed. The results show somewhat surprising improvements in typical inversions. The extensions of the method required for the analysis of sampled and truncated experimental data are also discussed and applied.

1. Introduction

In three previous papers (Bertero *et al* 1982, 1984a, b, hereafter referred to as I, II and III, respectively), the problem of Laplace transform inversion was considered assuming that the unknown function has a bounded, strictly positive support. By constructing the singular system of the finite Laplace transformation it was shown that *a priori* knowledge of this support allows an improvement beyond the general resolution limits derived by McWhirter and Pike (1978), in agreement with the results obtained by Ostrowski *et al* (1981) by means of numerical simulations. Furthermore the case of truncated, discrete data was considered and methods for obtaining optimum sets of data points were given.

In all these investigations the basic tool was the regularised solution obtained by means of a truncated singular function expansion. However the method has some unsatisfactory features. In practical situations the support of the unknown function is not known exactly although some estimations may be made from the experimental data since the derivatives of the Laplace transform $g(p)$ at the point $p=0$ are related to the moments of the unknown

function $f(t)$. The first and second moments provide information about the 'localisation' of $f(t)$ but not a precise estimation of its support.

A second and more serious difficulty originates from the behaviour of the functions at the edges of the support, say the interval $[1, \gamma]$. It is possible to prove that if we denote the singular functions associated with the singular values α_k, ordered in a decreasing sequence, by $u_k(t)$, $k=0, 1, 2, \ldots$, then $|u_k(1)| = \sqrt{\gamma}|u_k(\gamma)| \to \infty$ when $k \to +\infty$. Therefore the singular functions used in the inversion procedure are large precisely in those regions where the unknown function is presumably small. This fact gives rise to spurious and troublesome edge effects (cf the Gibbs phenomenon) which will be illustrated in the following by means of numerical simulations.

A way to overcome these difficulties is to look for solutions of the Laplace transform inversion in a weighted L^2 space. In such a way we are not forced to a rigid choice of the support, we can use the information contained in the knowledge of the lower moments of the unknown function and we can force the solution to be small in those regions where it is presumed to be small.

Let us introduce a positive 'profile' function $P(t)$ whose integral is equal to one. In fact we assume that $P(t)$ is one of a family of profile functions (uniform distributions, gamma distributions, normal or log–normal distributions, etc) parametrised in such a way that the first and second moments of $P(t)$ can be adapted to the experimental values of the corresponding moments of $f(t)$. Since it is always possible to put the first moment of $f(t)$ equal to one by means of a scaling of the variables, we assume that the first moment of $P(t)$ is also one. Furthermore we will denote the second central moment of $P(t)$ by Q:

$$Q = \int_0^{+\infty} (t-1)^2 P(t)\, \mathrm{d}t. \tag{1.1}$$

Then we consider the following problem: *given* $g(p)$, $0 < p < +\infty$, *find a function* f *satisfying the condition*

$$\int_0^{+\infty} \frac{f^2(t)}{P^2(t)}\, \mathrm{d}t < +\infty \tag{1.2}$$

and such that

$$g(p) = \int_0^{+\infty} \exp(-pt) f(t)\, \mathrm{d}t. \tag{1.3}$$

This problem is equivalent to the problem considered in I when the function $P(t)$ is proportional to the characteristic function of an interval $[a, b]$. The lower and upper bounds of the interval are related to Q by $a = 1 - \sqrt{3Q}$ and $b = 1 + \sqrt{3Q}$, and $P(t) = (12Q)^{-1/2}$ for $a \leqslant t \leqslant b$ (the procedure is meaningless when $Q > \frac{1}{3}$ since $a < 0$).

In § 2 we give a general outline of the problem of Laplace transform inversion in a weighted L^2 space in the cases of both continuous and discrete data. We consider regularised solutions given by truncated singular function expansions and we show how they are modulated by the profile function $P(t)$. As in I–III, this choice is justified by the fact that the singular values of the problem fall to zero very rapidly so that only a few components of $f(t)$ contribute to the data. Furthermore we give the explicit dependence of the singular system on the first moment of $P(t)$ when this is not equal to one.

In § 3 we consider the special case where $P(t)$ is a gamma distribution, in which case $Q < 1$. By means of numerical simulations we investigate the relation between the value of Q of the profile function and the value of the second central moment of $f(t)$. Finally, in § 4 we discuss the applications of the method to the analysis of experimental data.

2. Laplace transform inversion in weighted spaces

2.1. The case of continuous data

If $f(t)$ satisfies condition (1.2) and if we put

$$f(t)=P(t)\psi(t) \tag{2.1}$$

then $\psi \in L^2(0, +\infty)$ and the inversion of the Laplace transformation in the weighted L^2 space (1.2) is equivalent to the inversion in $L^2(0, +\infty)$ of the operator

$$(L\psi)(p)=\int_0^{+\infty} \exp(-pt)P(t)\psi(t)\,\mathrm{d}t. \tag{2.2}$$

By means of elementary computations the following proposition can be proved: *the operator L is of the Hilbert–Schmidt class in $L^2(0, +\infty)$ if and only if*

$$\mathrm{Tr}(L^*L)=\int_0^{+\infty} \frac{P^2(t)}{t}\,\mathrm{d}t < +\infty. \tag{2.3}$$

Therefore in the following we will assume that this condition is satisfied.

If we introduce the singular system of the operator L, which we denote as $\{\alpha_k; \psi_k, v_k\}_{k=0}^{+\infty}$, then the range of the operator L can be easily characterised and the solution of problem (1.2), (1.3) can be given. Since these are standard results, we omit the details. We wish only to point out that from the well known uniqueness theorem for the Laplace transform it follows that the *operator L is invertable (injective) if the support of $P(t)$ is $[0, +\infty]$, while the operator L^* is always invertable.* If the support of $P(t)$ is a bounded interval, say $[a, b]$, then the injectivity of L can be trivially restored by restricting the operator to $L^2(a, b)$.

As usual the α_k can be ordered in a decreasing sequence and $\alpha_k \to 0$ $(k \to +\infty)$ since the operator L is compact. The ψ_k form an orthonormal basis in $L^2(0, +\infty)$ (or $L^2(a, b)$) and also the v_k form an orthonormal basis in $L^2(0, +\infty)$. We notice that the singular functions $\psi_k(t)$ have the representation

$$\psi_k(t)=P(t)\varphi_k(t) \tag{2.4}$$

where $\varphi_k(t)$ is a square integrable function given by

$$\varphi_k(t)=\frac{1}{\alpha_k}\int_0^{+\infty} \exp(-tp)v_k(p)\,\mathrm{d}p. \tag{2.5}$$

By means of the variational characterisation of α_0^2 it is easy to prove that *$\varphi_0(t)$ and $v_0(p)$ are positive decreasing functions.* We also notice that the singular functions $u_k(t)$ which are orthonormal with respect to the weighted scalar product induced by condition (1.2) are given by

$$u_k(t)=P^2(t)\varphi_k(t). \tag{2.6}$$

In particular, $u_0(t)$ is roughly proportional to $P^2(t)$.

In the presence of noise an approximate, regularised solution of problem (1.2), (1.3) is given by a truncated singular function expansion which, as follows from equations (2.1) and (2.4), takes the form

$$\tilde{f}(t)=P^2(t)\sum_{k=0}^{K} \frac{g_k}{\alpha_k}\varphi_k(t) \tag{2.7}$$

where

$$g_k = \int_0^{+\infty} g(p) v_k(p)\, \mathrm{d}p. \tag{2.8}$$

The number of terms in a practical application of equation (2.7) is determined by the signal-to-noise ratio (see I).

As a concluding remark we give the explicit dependence of the singular system on the first moment of the profile function. This point is of importance for the applications.

Let μ be the first moment of the profile function which we denote by $P_\mu(t)$. Denote also by $\{\alpha_k(\mu); \psi_k(\mu, t), v_k(\mu, p)\}_{k=0}^{+\infty}$ the corresponding singular system. We notice that the profile function $P(t) = \mu P_\mu(\mu t)$ has a first moment equal to one and we denote the corresponding singular system by $\{\alpha_k, \psi_k(t), v_k(p)\}_{k=0}^{+\infty}$. Then, by means of elementary changes of variables, it is easy to prove that the following relations hold:

$$\alpha_k(\mu) = (1/\mu)\alpha_k \qquad \psi_k(\mu, t) = (1/\sqrt{\mu})\psi_k(t/\mu) \qquad v_k(\mu, p) = \sqrt{\mu}\, v_k(\mu p); \tag{2.9}$$

the multiplicative constants in the singular functions are chosen in order to preserve normalisation. The first of these relations has no effect on relative resolution.

2.2. *The case of discrete data*

When the Laplace transform is given only on a finite set of points, say $p_1, p_2, \ldots, p_n$, the problem (1.2), (1.3) is replaced by the following: *find a function $f(t)$ satisfying condition* (1.2) *and such that*

$$g(p_n) = \int_0^{+\infty} \exp(-p_n t) f(t)\, \mathrm{d}t \qquad n = 1, \ldots, N. \tag{2.10}$$

It is obvious that the solution of this problem is not unique, but uniqueness can be imposed by looking for a solution of smallest norm.

We write f in the form (2.1) and we denote by L_N the operator transforming $\psi \in L^2(0, +\infty)$ into the data vector $\boldsymbol{g}$ whose components are $g(p_1), \ldots, g(p_n)$ and whose norm is defined by

$$\|\boldsymbol{g}\|_N^2 = \sum_{n=1}^{N} w_n g^2(p_n) \tag{2.11}$$

where the w_n are suitable positive weights (see III). We also denote by $\{\alpha_{N,k}; \psi_{N,k}, \boldsymbol{v}_{N,k}\}_{k=0}^{N-1}$ the singular system of L_N. The $\alpha_{N,k}$ are again ordered in a decreasing sequence and the $\psi_{N,k}$ form an orthonormal basis in the subspace of $L^2(0, +\infty)$ spanned by the functions

$$\chi_n(t) = P(t) \exp(-p_n t) \qquad n = 1, \ldots, N \tag{2.12}$$

while the $\boldsymbol{v}_{N,k}$ form an orthonormal basis (with respect to the scalar product induced by the norm (2.11)) in the space of the data vectors. Furthermore, by noticing that the adjoint L_N^*, transforming a vector $\boldsymbol{v} = \{v(p_1), \ldots, v(p_n)\}$ into a function, can be expressed by

$$(L_N^* \boldsymbol{v})(t) = P(t) \sum_{n=1}^{N} w_n \exp(-t p_n) v(p_n), \tag{2.13}$$

we obtain a representation similar to (2.4), (2.5) for $\psi_{N,k}(t)$, namely

$$\psi_{N,k}(t) = P(t) \varphi_{N,k}(t) \tag{2.14}$$

where

$$\varphi_{N,k}(t)=\frac{1}{\alpha_{N,k}}\sum_{n=1}^{N} w_n \exp(-tp_n)v_{N,k}(p_n). \tag{2.15}$$

Again it is possible to prove that $\varphi_{N,0}(t)$ is a positive decreasing function and also that the components $v_{N,0}(p_n)$ are positive and decreasing for increasing p_n. Furthermore the analogues of the singular functions (2.6) are

$$u_{N,k}(t)=P^2(t)\varphi_{N,k}(t) \tag{2.16}$$

and $u_{N,0}(t)$ is roughly proportional to $P^2(t)$.

In the presence of noise the approximate filtered (regularised) solution of problem (1.2), (2.9) has an expression similar to (2.7):

$$\tilde{f}_N(t)=P^2(t)\sum_{k=0}^{K}\frac{g_{N,k}}{\alpha_{N,k}}\varphi_{N,k}(t) \tag{2.17}$$

where now

$$g_{N,k}=\sum_{n=1}^{N} w_n g(p_n)v_{N,k}(p_n). \tag{2.18}$$

In II–III two distributions of data points were considered: a set of *equidistant points*

$$p_n=d(n-1) \qquad w_n=d \qquad n=1,\ldots,N \tag{2.19}$$

where d is the distance between adjacent points, and a set of points forming a *geometric progression*

$$p_n=c\Delta^{n-1} \qquad w_n=(\ln\Delta)p_n \qquad n=1,\ldots,N \tag{2.20}$$

where c is the position of the first point and Δ the ratio between adjacent points.

By means of the same methods used in III it is possible to investigate the behaviour of $\alpha_{N,k}$ and $u_{N,k}$ (with fixed k) when the number of points tends to infinity and the distance between adjacent points tends to zero. The result is that they converge respectively to the singular value α_k and to the singular function u_k (with the same value of the index) of the problem with continuous data:

(*a*) in the case of a uniform distribution when $d\to 0$ and $N\to\infty$ in such a way that $Nd\to\infty$, and

(*b*) in the case of points forming a geometric progression when $c\to 0$, $\Delta\to 1$ and $N\to+\infty$ in such a way that $c^{(\Delta\ln N)}\to\infty$.

Finally, when the first moment of the profile function is not one, relations analogous to (2.9) hold true.

To compute a singular system in a practical case we need to choose a suitable profile function. In the next section we illustrate the method with a choice of $P(t)$ which leads to simple analytic calculations of the matrix operators required.

3. An example: the gamma distribution

We assume now that the profile function $P(t)$ is a gamma distribution

$$P(t)=\frac{\beta^\beta}{\Gamma(\beta)}t^{\beta-1}\exp(-\beta t) \tag{3.1}$$

whose first moment is unity and whose second central moment is given by $Q=1/\beta$. Condition (2.3) is satisfied when $\beta>1$, i.e. $Q<1$, and therefore the method cannot be applied to the reconstruction of very broad distributions.

The singular system of the operator (2.2), (3.1) can be computed using, for instance, the method used in I. However these rather time-consuming computations are not necessary for the following reasons: firstly, the case interesting in practice is the case of discrete data; secondly, as shown in III, by means of an optimum choice of few data points it is possible to obtain excellent approximations of the singular values and singular functions of the continuous case.

We comment now on some rough estimates of the first singular value α_0 and of the first singular function $u_0(t)$ in order to investigate their dependence on β, which will be determined from the experimental second moment of $f(t)$ as described in detail in § 4.

Since, as is confirmed by numerical computations to be presented shortly, the singular values fall to zero very rapidly, especially when β is large, a good approximation of α_0 is given by the inequality $\alpha_0 \leqslant [\mathrm{Tr}(L^*L)]^{1/2}$ and from equations (2.3), (3.1) we obtain

$$\alpha_0 \leqslant \frac{\beta}{\Gamma(\beta)} \frac{\Gamma^{1/2}(2\beta-2)}{2^{\beta-\frac{1}{2}}} \sim \frac{1}{2}\left(\frac{\beta}{\pi}\right)^{1/4} \qquad \beta \to \infty. \tag{3.2}$$

In particular, in the cases $\beta=2, 4, 8, 16$ we obtain the following upper bounds: $\alpha_0 \leqslant 0.707$, 0.645, 0.692, 0.795 (notice that $\mathrm{Tr}(L^*L)$ has a minimum as a function of β since it tends to infinity both for $\beta \to 1$ and for $\beta \to +\infty$). When β grows, namely when the profile function $P(t)$ becomes very narrow, α_0 grows while the other singular values decrease and, therefore, for a given signal-to-noise ratio there exists a value of β, say β_0, such that for $\beta \geqslant \beta_0$ it is possible to extract only one component of $f(t)$ from the data. In such a case the only information which can be extracted from the data is the second central moment Q and it is impossible to discriminate between two distributions having the same value of Q.

It follows from equation (2.6) that $u_0(t)$ is the product of $P^2(t)$ and a slowly decreasing function. If we neglect this factor and we normalise u_0 in such a way that its integral is equal to one, then the first moment and the second relative central moment of u_0 are given approximately by

$$\mu_0 \simeq 1-\frac{1}{2\beta} \qquad Q_0=\frac{\sigma_0^2}{\mu_0^2} \simeq \frac{1}{2\beta-1} \tag{3.3}$$

and therefore $\mu_0 \simeq 1$ and $Q_0 \simeq 1/2\beta$ when β is large.

In the case of discrete data, the singular system of the operator L_N can be computed by the same methods used in III as follows. The singular values $\alpha_{N,k}$ are the square roots of the eigenvalues of the symmetric, positive definite matrix (related to $L_N L_N^*$)

$$\bar{t}_{nm} = \sqrt{w_n w_m}\, S(p_n+p_m) \tag{3.4}$$

where

$$S(p) = \int_0^{+\infty} \exp(-pt) P^2(t)\, \mathrm{d}t = \beta \frac{\Gamma(2\beta-1)}{\Gamma^2(\beta)} \left(\frac{\beta}{p+2\beta}\right)^{2\beta-1}. \tag{3.5}$$

Furthermore the singular vectors $v_{N,k}$ are related to the eigenvectors $\bar{v}_{N,k}$ of the matrix (3.4) by the relation

$$\sqrt{w_n}\, v_{N,k}(p_n) = \bar{v}_{N,k}(p_n). \tag{3.6}$$

Finally, the singular functions $u_{N,k}(t)$ may be computed using equations (2.16) and (2.15).

3.1. Uniform sampling

When the data points and the weights are given by equation (2.19) we have verified, by means of many computations, that $N=32$ is an adequate number of data points for values of β ranging from 2 up to 16 (see also II). We have computed only the singular values greater than 10^{-3} and the distance between adjacent points has been chosen in order to minimise the ratio between the largest and the smallest computed singular value (condition number)—see II and III. As in our previous computations, we have found only one minimum; the results are reported in table 1.

We notice that $\alpha_{N,0}$ is greater than the estimate of α_0 given at the beginning of this section. This fact can be understood by noticing that $\mathrm{Tr}(L_N^* L_N) > \mathrm{Tr}(L^* L)$, as can be easily verified at least when the product Nd is sufficiently large. As in the case of α_0, $\alpha_{N,0}$ has a minimum between 2 and 4 as a function of β while the other singular values are decreasing functions of β.

In figure 1 we give the first six singular functions in the case $\beta=4$ ($N=32$, $d=0.65$) and in figure 2 the first four singular functions in the case $\beta=16$ ($N=32$, $d=0.3$). A remarkable feature, similar to that of the singular functions computed in III, is that $u_{N,k}(t)$ has exactly k zeros (the same property certainly holds true for $u_k(t)$). Furthermore it is also evident that $u_{N,0}(t)$ is roughly proportional to $P^2(t)$ and that the approximation is better in the case $\beta=16$ than in the case $\beta=4$.

3.2. Geometric sampling

Using geometrically sampled data, equation (2.20), we have tried to obtain reasonable approximations for the largest singular values using a number of data points equal to the number of required singular values. The motivation is that in our previous works (II and III) geometrical sampling was proved to be more efficient than linear sampling.

As an example we have investigated mainly the case $\beta=4$ and we have considered the first four singular values, i.e. the singular values greater than 10^{-2}. We have taken four data points and, for fixed Δ, equation (2.20), we have minimised the condition number with respect to c, the position of the first point.

For each value of Δ we have found only one minimum of the condition number $\alpha_{4,0}/\alpha_{4,3}$ and for $\Delta=2$, 3, 4, 5 the minimising values of c are respectively $c=1.4$, 0.4, 0.19, 0.12 with the corresponding condition numbers $\alpha_{4,0}/\alpha_{4,3}=76.7$, 50.0, 47.9, 53.5. Therefore the 'almost' best choice is $\Delta=4$, $c=0.19$ even though the minimum value of the condition number does not depend strongly on the dilation factor Δ, at least when Δ is in the range 3–5.

Table 1. Singular values in the case of 32 linearly spaced points for $\beta=2$, 4, 8, 16. (Next to each value of β is indicated the approximate value of d corresponding to the minimum of α_0/α_6 for $\beta=2$, of α_0/α_5 for $\beta=4$, and of α_0/α_3 for $\beta=8$, 16.)

	$\beta=2$ ($d=1.2$)	$\beta=4$ ($d=0.65$)	$\beta=8$ ($d=0.4$)	$\beta=16$ ($d=0.3$)
α_0	0.894	0.796	0.810	0.894
α_1	0.262	0.149	0.104	0.799×10^{-1}
α_2	0.997×10^{-1}	0.384×10^{-1}	0.186×10^{-1}	0.100×10^{-1}
α_3	0.403×10^{-1}	0.116×10^{-1}	0.398×10^{-2}	0.150×10^{-2}
α_4	0.153×10^{-1}	0.373×10^{-2}	—	—
α_5	0.529×10^{-2}	0.116×10^{-2}	—	—
α_6	0.170×10^{-2}	—	—	—

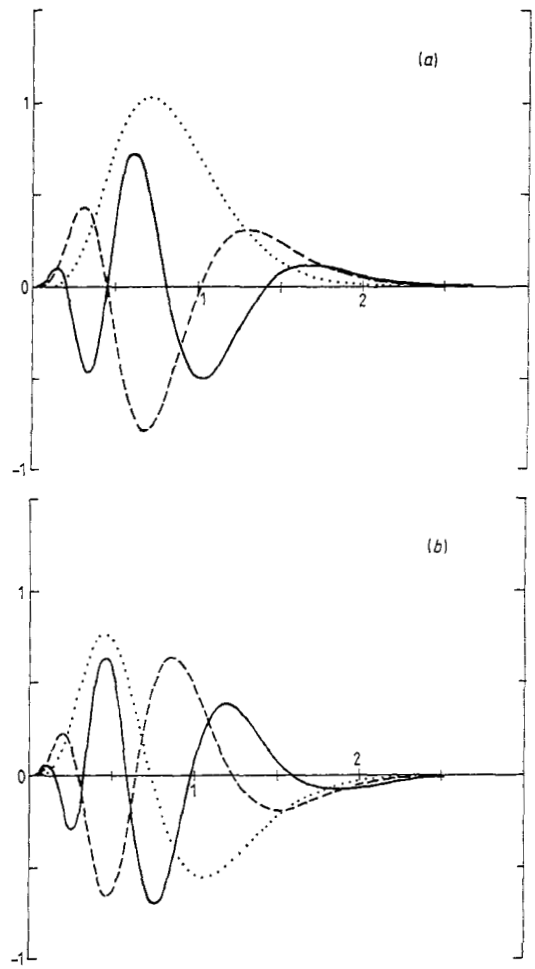

Figure 1. Singular functions in the case $\beta=4$ ($N=32$, $d=0.65$): (*a*) u_0 (dotted curve), u_2 (broken curve), u_4 (full curve); (*b*) u_1 (dotted curve), u_3 (broken curve), u_5 (full curve).

The singular values corresponding to $\Delta=4$, $c=0.19$ are

$$\begin{aligned} &\alpha_{4,0}=0.591 && \alpha_{4,1}=0.121 \\ &\alpha_{4,2}=0.233\times 10^{-1} && \alpha_{4,3}=0.123\times 10^{-1}. \end{aligned} \tag{3.7}$$

If we compare these values with those of the second column of table 1, we see that, except for the last one, they are smaller than the corresponding values of table 1. As a consequence the condition number is smaller in the geometric case (47.9) than in the linear case with 32 optimally placed points (68.7). This result proves that geometrical sampling is also more efficient than linear sampling in the case of Laplace transform inversion in weighted spaces.

The singular functions are quite similar to those of the linear case and therefore we do not illustrate them here. The variations in the positions of the zeros and of the maxima and minima with respect to the linear case (figure 1) amount only to a few per cent.

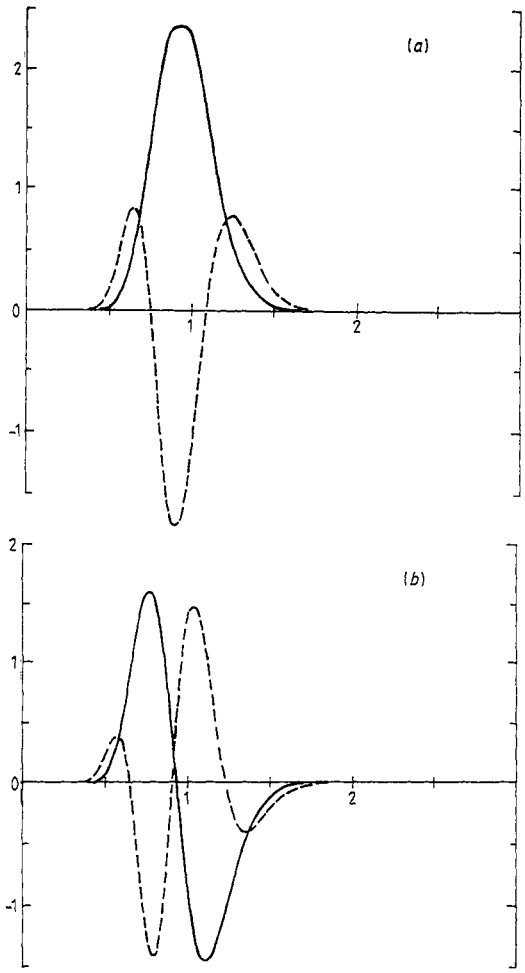

Figure 2. Singular functions in the case $\beta=16$ ($N=32$, $d=0.3$): (*a*) u_0 (full curve), u_2 (broken curve): (*b*) u_1 (full curve), u_3 (broken curve).

4. Applications

In most experiments in the field of photon correlation spectroscopy, of fluorescent decay, of sedimentation equilibrium, as well as in other areas of relaxation kinetics, the output of the experiment is the Laplace transform of an unknown distribution function $f(t)$. Some preliminary information about $f(t)$ can be obtained, without inversion of the Laplace transform, by means of the so called *cumulants method.* If we denote the first moment of $f(t)$ by $\bar{\mu}$ and the central moments of $f(t)$ by μ_n ($n=2, 3, 4, \ldots$) then by expanding the exponential in the Laplace integral around $\bar{\mu}$ we get

$$g(p)=\exp(-\bar{\mu}p)\left(1+\sum_{n=2}^{+\infty}\mu_n\frac{p^n}{n!}\right). \tag{4.1}$$

Then, by a polynomial fitting of the function $\ln g(p)$ (Köppel 1972, Pusey 1974, Ostrowski and Sornette 1983) it is possible to extract the first few moments of $f(t)$ from the data. In particular, we assume here that it is possible to obtain $\bar{\mu}$ and μ_2 and therefore the parameter

$$Q_{\exp} = \mu_2/(\bar{\mu})^2. \tag{4.2}$$

As already remarked, by means of a scaling of the variables it is always possible to put $\bar{\mu} = 1$ without changing the value of $Q_{\exp}$. We also assume that $Q_{\exp} < 1$.

The first question for the application of the method outlined in the previous section is the following: *given $Q_{\exp}$, what value of β $(= 1/Q)$ should be used for the profile function?*

Two choices are suggested rather naturally by qualitative considerations. The first one is to take $Q = Q_{\exp}$, i.e. $\beta = Q_{\exp}^{-1}$, since this choice assumes that $f(t)$ is small outside a region having the correct spread. The second choice is suggested by the remark made in § 2: $u_0(t)$, the first term in the truncated singular function expansion, is roughly proportional to $P^2(t)$ and if we consider this term as a first approximation to the unknown function then it is obvious to require $Q_0 = Q_{\exp}$ or, therefore, recalling equation (3.3), $\beta \simeq \frac{1}{2} Q_{\exp}^{-1}$.

In collaboration with N Ostrowski, K Lan and G de Villiers we have investigated both possibilities by means of numerical simulations. A separate analysis of the inversion of experimental data in the determination of polydisperity of suspended particles by photon correlation techniques is published elsewhere jointly with these authors (Bertero *et al* 1985). The main conclusions are as follows.

We have considered as test functions linear combinations of gamma distributions

$$f(t) = \sum_{m=1}^{M} \frac{c_m}{t_m} P(\beta_m; t/t_m) \tag{4.3}$$

where $P(\beta; t)$ is just the gamma distribution (3.1). The coefficients c_m and the first moments t_m satisfy the conditions

$$\sum_{m=1}^{M} c_m = 1 \qquad \sum_{m=1}^{M} c_m t_m = 1. \tag{4.4}$$

Furthermore the simulated value of $Q_{\exp}$ is given by

$$Q_{\exp} = \sum_{m=1}^{M} c_m \left((t_m - 1)^2 + \frac{t_m^2}{\beta_m} \right). \tag{4.5}$$

The Laplace transform of (4.3) is easily computed and is given by

$$g(p) = \sum_{m=1}^{M} \frac{c_m}{[1 + (t_m/\beta_m)p]^{\beta_m}}. \tag{4.6}$$

It can also be corrupted with additive noise, even if this point is not essential since in the method using truncated expansions error propagation can be controlled and estimated theoretically.

In our numerical simulations singular systems corresponding to various values of β were precomputed and stored so that, for a given data set, the truncated solution (2.17) can be computed very quickly using various values of β.

As a first example we consider a case where there is only one term in equation (4.2) with the following values of the parameters: $c_1 = 1$, $t_1 = 1$, $\beta_1 = 4$. We have used two values of β, namely $\beta = 2$ and $\beta = 4$. In figure 3(*a*) we give the reconstructions obtained using five terms in the case $\beta = 2$ and four terms in the case $\beta = 4$.

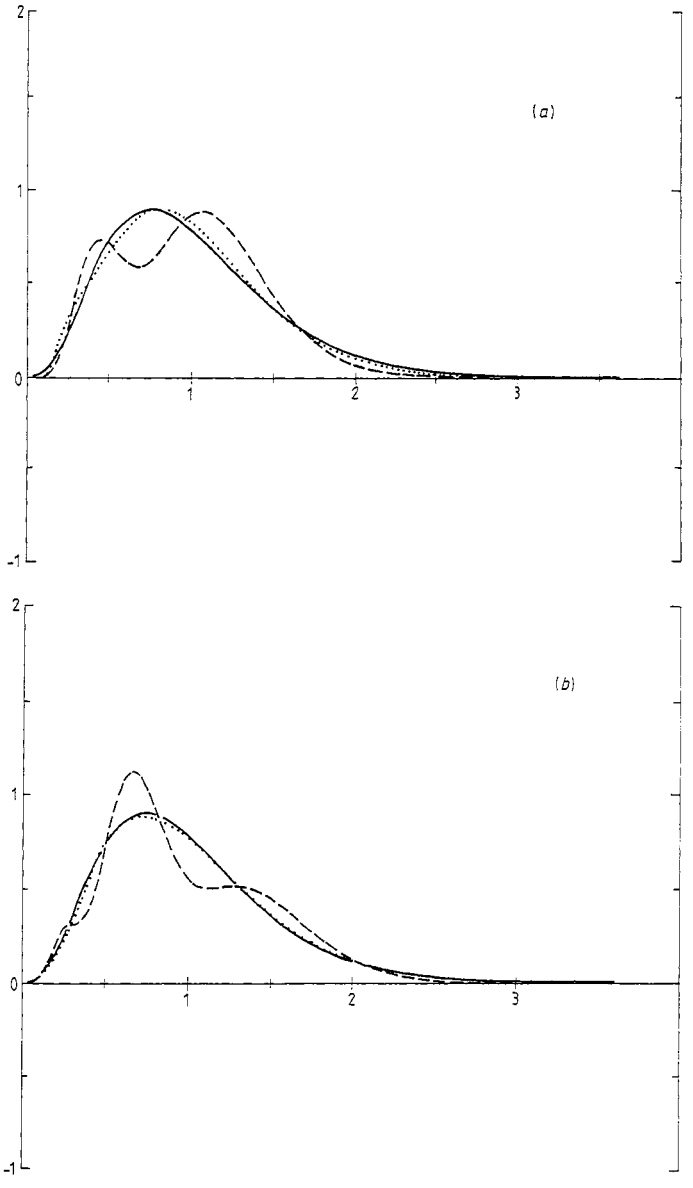

Figure 3. Reconstruction of a gamma distribution with $\beta_1 = 4$ (full curves) using singular functions with $\beta = 4$ (broken curves) and with $\beta = 2$ (dotted curves): (*a*) using singular values greater than 10^{-2} and (*b*) using singular values greater than 10^{-3}.

This is the maximum number of terms which can be used if we require that the condition number of the inversion procedure is less than 10^2. Furthermore in figure 3(*b*) we give the reconstructions corresponding to seven terms in the case $\beta = 2$ and six terms in the case $\beta = 4$ (condition number less than 10^3). We have used the singular systems described in § 3 corresponding to 32 linearly spaced and 'optimally' placed points.

It is evident that the choice $\beta=2$ gives a better result than the other and therefore, in this case, it seems convenient to adapt the value of β to the experimental data in such a way that $Q_{\text{exp}} \simeq Q_0$. This result has been confirmed by many other numerical simulations using

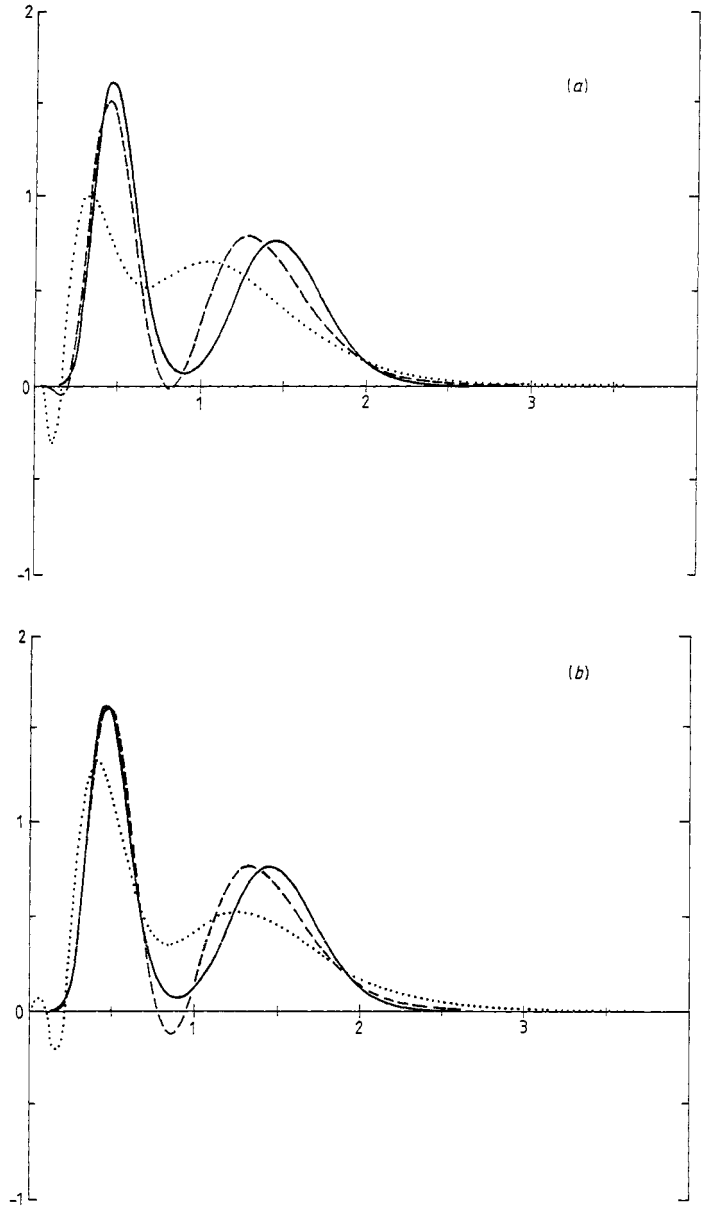

Figure 4. Reconstruction of a linear combination of two gamma distributions, equation (4.3), with $c_1=c_2=0.5$, $t_1=0.5$, $t_2=1.5$, $\beta_1=16$, $\beta_2=32$ (full curves) using singular functions with $\beta=4$ (broken curves) and with $\beta=2$ (dotted curves): (*a*) corresponding to singular values greater than 10^{-2} and (*b*) corresponding to singular values greater than 10^{-3}.

various functions with only one maximum and therefore the previous choice seems to be best when the unknown function has only one peak.

Unfortunately, the situation is somewhat different when $f(t)$ is known to have more than one peak. We again give as an example the reconstruction of a function in the class (4.3) which is a linear combination of two gamma distributions. The choice of the parameters is as follows: $c_1 = c_2 = 0.5$, $t_1 = 0.5$, $t_2 = 1.5$, $\beta_1 = 16$, $\beta_2 = 32$ ($Q_{\exp} = 0.293$). In figure 4 we give the reconstructions obtained using both $\beta = 2$ and $\beta = 4$ (the number of terms is the same as in figure 3) and in this case the choice $\beta = 4$ (namely $Q = 0.25$) seems to be more efficient than the other (corresponding to $Q_0 \simeq 0.33$). Therefore, if it is known that the unknown distribution has more than one peak, the higher value of β should be used.

We have also checked the capability of the method in discriminating point masses (delta functions) and therefore we have considered a test 'function' of the type

$$f(t) = \sum_{m=1}^{M} c_m \delta(t - t_m) \tag{4.7}$$

where the parameters again satisfy the conditions (4.4). In such a case

$$Q_{\exp} = \sum_{m=1}^{M} c_m (t_m - 1)^2 \tag{4.8}$$

and the Laplace transform is simply a linear combination of exponentials.

In order to show the improvement which can be obtained by means of the present method, in figures 5 and 6 we compare the results obtained by means of the singular system corresponding to $\beta = 1/Q_{\exp}$ with the results obtained by means of the singular

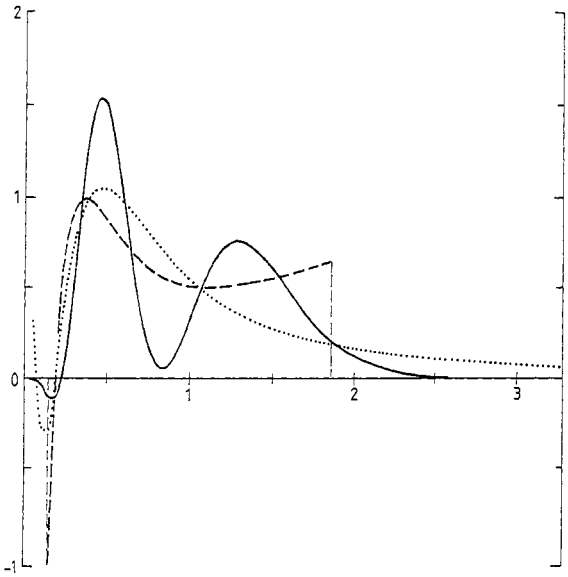

Figure 5. Reconstruction of two delta functions, equation (4.7), with $c_1 = c_2 = 0.5$, $t_1 = 0.5$, $t_2 = 1.5$ using the present method (full curve) with $\beta = 4$, the method with compact support (broken curve) and the eigenfunction method without constraint on the support (dotted curve). Here a signal-to-noise ratio of the order of 10^2 (see I–III) is assumed.

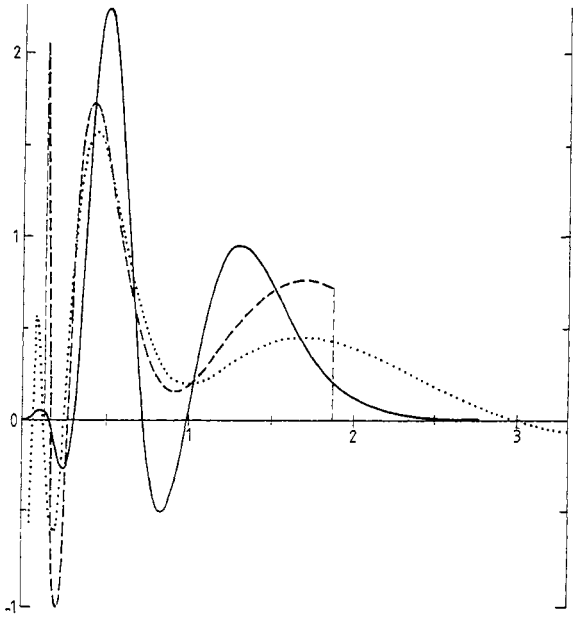

Figure 6. The same as in figure 5 but assuming a signal-to-noise ratio of the order of 10^3.

functions corresponding to a compact support (with $a=1-\sqrt{Q_{\exp}}$, $b=1+\sqrt{Q_{\exp}}$) and with the results obtained by means of the eigenfunction method of McWhirter and Pike (1978). The improvement obtained with the present method is impressive especially in the case of figure 5 where the required signal-to-noise ratio is of the order of 10^2.

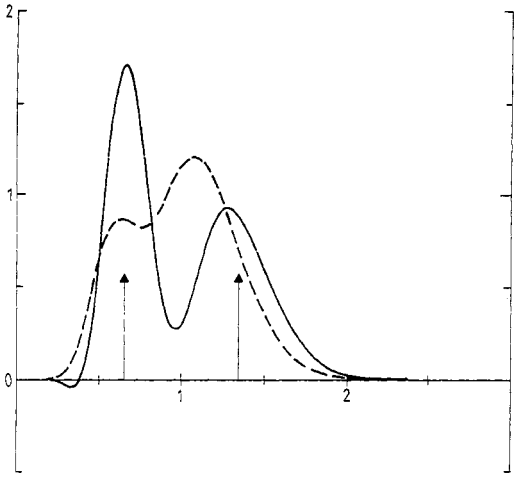

Figure 7. Reconstruction of two delta functions with $c_1=c_2=0.5$, $t_1=0.646$, $t_2=1.354$ ($t_2/t_1=2.1$), indicated by the arrows, using singular functions with $\beta=8$ in the case of a signal-to-noise ratio of the order of 10^2 (broken curve) and of the order of 10^3 (full curve).

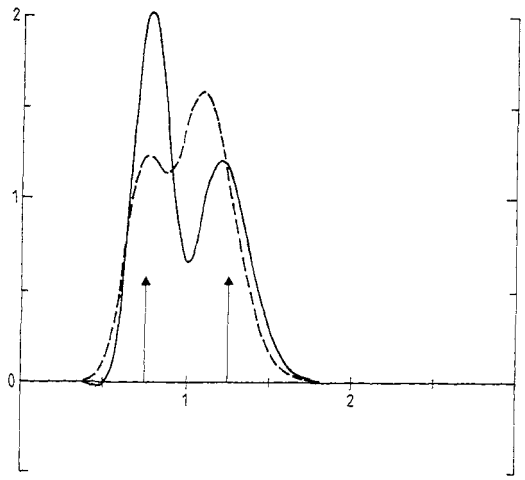

Figure 8. Reconstruction of two delta functions with $c_1 = c_2 = 0.5$, $t_1 = 0.75$, $t_2 = 1.25$ ($t_2/t_1 = 1.67$) using singular functions with $\beta = 16$ in the case of a signal-to-noise ratio of the order of 10^2 (broken curve) and of the order of 10^3 (full curve). The arrows indicate the positions of the delta functions.

Finally, in figures 7 and 8 we show that good resolution can be obtained even when Q_{exp} is small (0.125 in the case of figure 7 and 0.062 in the case of figure 8) provided one knows *a priori* that two components are present and β is chosen accordingly.

A remarkable feature of all the reconstructions obtained by the method of inversion in a weighted space is that the negative parts of the restored solution are not very important so that the constraint of positivity will not give a significant improvement in the quality of the solution.

Acknowledgment

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