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Linear regularizing algorithms for positive solutions of linear inverse problems

By M. BERTERO¹, P. BRIANZI², E. R. PIKE³, F.R.S., AND L. REBOLIA²

¹ *Dipartimento di Fisica dell'Università and Istituto Nazionale di Fisica Nucleare, I-16146 Genova, Italy*

² *Dipartimento di Matematica dell'Università, I-16132 Genova, Italy*

³ *Department of Physics, King's College London, University of London, Strand, London WC2R 2LS U.K.;*

Centre for Theoretical Studies, RSRE, Malvern, WR14 3PS, U.K.

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Linear-regularization methods provide a simple technique for determining stable approximate solutions of linear ill-posed problems such as Fredholm equations of the first kind, Cauchy problems for elliptic equations and backward solution of forward parabolic equations. In most of these problems the solution must be positive to satisfy physical plausibility. In this paper we consider ill-posed first-kind convolution equations and related problems such as numerical differentiation, Radon transform and Laplace-transform inversion. We investigate several linear regularization algorithms which provide positive approximate solutions for these problems at least in the absence of errors on the data. For noisy data the solution is not necessarily positive. Because the appearance of negative values can then only be an effect of the noise, the negative part of the solution should be negligible with a suitable choice of the regularization parameter. A price to pay for ensuring positivity is always, however, a reduction in resolution.

1. INTRODUCTION

In a series of recent papers a systematic application of the theory of singular systems has been made to a number of linear inverse problems in physics, for example, the finite Laplace transform inversion for recovering a distribution of diffusion constants in photon correlation spectroscopy (Bertero *et al.* 1985*b, c*), the Fraunhofer diffraction equation for recovering particle size distributions in light scattering (Bertero *et al.* 1985*a*) and the diffraction-limited imaging problem in scanning optical microscopy (Bertero *et al.* 1984 among others). The relation with information theory is discussed by Pike *et al.* (1984). Full account has been taken of the sampled and truncated nature of real experimental data and *a priori* knowledge of the location of the solution may be used to improve details in the reconstruction. The method is linear, non-iterative, fast in implementation and does not go beyond delivering the visible part of the object (solution). This is essentially the part of the object which is transmitted by the instrument under consideration (Pike *et al.* 1984) and it can be defined in a precise way as the orthogonal projection of the object onto the subspace spanned by the singular

functions corresponding to singular values greater than the inverse of the signal-to-noise ratio. The orthogonal complement of this subspace is the subspace of the invisible components of the object (for example high spatial frequencies not passed by a lens or attenuated by wave propagation). These are set to zero because they have no effect on the data measured.

It is often known that the object is positive. In such a case a commonly used argument is that to constrain the solution to be positive is thus adding *a priori* knowledge which must improve the inversion. A little thought on the singular function expansion of the solution will indicate the effect produced by an algorithm that uses the positivity constraint. In fact, the visible component of a positive function in general is not positive and the addition of invisible components does not modify the situation. For example, a positive δ -function has oscillating components at all frequencies and if those above a finite cutoff are removed, the visible projection is the well-known oscillating Airy function. Furthermore, the addition of invisible components is not sufficient to obtain a positive result: the addition of higher frequencies will have the effect of increasing the so-called side lobes. Therefore an algorithm producing a positive solution can introduce invisible components but it must necessarily perform some kind of windowing of both the visible and invisible components of the object. Such a windowing will be data-dependent. To our knowledge, no investigation of methods, such as maximum entropy, regularization plus positivity or Gerchberg-Papoulis plus positivity, has been done along the lines indicated above.

In this paper we investigate the possibility of obtaining positive solutions by means of a data-independent windowing of the visible components. This method, which is well known in signal processing where the objective is to reduce side-lobe strengths, has the advantage of being linear: the values of the visible components are weighted with a suitable window function to achieve the desired effects. Following this line we will consider and discuss several window functions having the property that, in the absence of noise, they give rise to a positive approximate solution if the object was positive. Any negative part in the reconstruction can therefore be attributed to the effect of noise and disregarded. A basic point is that, in this way, a positive solution is obtained at the cost of a concomitant loss of resolution when only visible components, in the sense specified above, are used. If this is tolerable, then these windows permit us to achieve positivity with a linear algorithm which thus retains the properties of speed and efficiency of inversion. We will show however that the above definition of invisible components must be modified to correspond with the *a priori* knowledge implied by the choice of window function.

The windowing method, as considered in this paper, is just a special case of the so-called regularization method for the solution of ill-posed first kind equations (Tikhonov & Arsenine 1977). For the convenience of the reader we recall here the definition of a regularizing algorithm. Assume that A is a linear continuous operator from the Hilbert space X into the Hilbert space Y and that the inverse of A , A^{-1} , exists but is not continuous (when A is not invertible one can consider the generalized inverse A^+ (Nashed 1976)). Then the problem: given $g \in Y$, find $f \in X$ such that

$$Af = g \tag{1.1}$$

is ill-posed. A linear regularization algorithm for the approximate solution of (1.1) (Tikhonov & Arsenine 1977; Groetsch 1984) is a one-parameter family $\{R_\alpha\}_{\alpha>0}$ of linear, continuous operators $R_\alpha: X \rightarrow Y$, such that

$$\lim_{\alpha \downarrow 0} \|R_\alpha A f - f\|_X = 0 \quad (1.2)$$

for any $f \in X$. The parameter α is called the regularization parameter. For a given value of α , $R_\alpha g$ is a stable approximate solution of (1.1) whenever g belongs to the range of the operator A . If we put

$$T_\alpha = R_\alpha A \quad (1.3)$$

then, as follows from (1.2), $T_\alpha: X \rightarrow X$ is a linear continuous approximation of the identity operator in X . In the case where T_α is an integral operator, the kernel of T_α is an 'impulse response function' describing the total effect of both the transmission by the instrument and the subsequent recovery procedure in terms of the algorithm R_α . If this function has the form of a central lobe flanked by decreasing side lobes, then the half-width of the central lobe may be used as a measure of the resolution achievable by means of R_α .

We give now the following definition: we say that a regularization algorithm $\{R_\alpha\}_{\alpha>0}$ has the positivity property if, for any $\alpha > 0$ and for any positive function f in the space X , the function $T_\alpha f$ is also positive. In other words the regularization algorithm provides a positive approximation of positive solutions for exact (noise-free) data.

If we apply such an algorithm to noisy data, we may get an approximate solution taking negative values. In the presence of noise, indeed, the data function g_ϵ can always be written in the following form

$$g_\epsilon = A f + h_\epsilon, \quad (1.4)$$

where f is the 'true' solution of the problem, assumed to exist and to be positive, and h_ϵ is a function, representing the effect of the noise, such that: $\|h_\epsilon\|_Y \leq \epsilon$. Then the approximate solution provided by the regularization algorithm is

$$R_\alpha g_\epsilon = T_\alpha f + R_\alpha h_\epsilon. \quad (1.5)$$

The first term of the RHS is positive but the second term can have negative values. These negative values, however, are an effect of the noise only and therefore one can expect that, by means of a suitable choice of the regularization parameter, they can be made negligible.

In §2 we investigate the problem of the inversion of convolution operators and we introduce several regularization algorithms having the positivity property. Among others we recall that defined by the triangular window, which is quite natural in the theory of the Fourier integral because it is related to Fourier-transform inversion in the sense of $(C, 1)$ -summability (Titchmarsh 1948). An interesting variational property of this window is proved in §3 where we indicate also an analogy between the windowing method and the Backus-Gilbert method (Backus & Gilbert 1968). In §4 we discuss a rather general recipe for the choice of the regularization parameter, which is usually called the discrepancy principle (Groetsch 1984), and we show that this method may justify the use of 'invisible'

components for an algorithm with the positivity property. In §5 two important problems are considered, numerical differentiation and Radon transform inversion. The use of the gaussian window is discussed and it is also shown that, for these problems, the usual Tikhonov regularizer (Groetsch 1984) has the positivity property. In §6 the windowing method introduced in §2 is extended to the inversion of Abel, Laplace and similar transforms, because for these problems the Mellin transform has a role similar to that of Fourier transform in the case of convolution equations. In §7 the inversion of convolution operators on the circle is considered and the relation between the triangular window and Fourier series summation by Cesàro means is discussed. Finally, in §8 we indicate possible applications of the results contained in this paper.

2. WINDOW FUNCTIONS FOR THE APPROXIMATE SOLUTION OF FIRST-KIND CONVOLUTION EQUATIONS

A very important example of a first-kind equation, such as (1.1), is provided by a convolution operator, i.e. an integral operator of the following form

$$(Af)(x) = \int_{-\infty}^{+\infty} K(x-y)f(y) dy, \quad (2.1)$$

where $K(x)$ is, for example, an integrable function. A problem of this type will be called a deconvolution problem. We will denote by $\hat{K}(\xi)$ the Fourier transform of $K(x)$.

We assume that X is $L^2(-\infty, +\infty)$, or a subspace of $L^2(-\infty, +\infty)$ defined by a suitable weighting function $\hat{p}(\xi)$ depending on the Fourier variable ξ

$$\|f\|_X^2 = (2\pi)^{-1} \int_{-\infty}^{+\infty} \hat{p}(\xi) |\hat{f}(\xi)|^2 d\xi, \quad (2.2)$$

and Y will always be $L^2(-\infty, +\infty)$. Under the previous assumptions A is a continuous operator whenever the function $|\hat{K}(\xi)|^2 \hat{p}(\xi)$ is bounded. The inverse operator A^{-1} exists if and only if the support of $\hat{K}(\xi)$ is $(-\infty, +\infty)$ and in such a case it is given by

$$(A^{-1}g)(x) = (2\pi)^{-1} \int_{-\infty}^{+\infty} [\hat{g}(\xi)/\hat{K}(\xi)] e^{ix\xi} d\xi. \quad (2.3)$$

Because the Fourier transform of the kernel tends to zero when ξ tends to infinity, A^{-1} is not continuous.

A broad class of linear regularizing algorithms for the approximate solution of equation (1.1), (2.1) can be obtained by introducing 'window' (or 'filter') functions depending on the variable ξ . We say that a one-parameter family of piecewise continuous functions $\{\hat{W}_\alpha(\xi)\}_{\alpha>0}$ is a family of window functions if the following conditions are satisfied (see, for instance, Tikhonov & Arsenine 1977, ch. 4)

- (i) $0 \leq \hat{W}_\alpha(\xi) \leq 1$, for any $\alpha > 0$ and any ξ ;
- (ii) $\lim_{\alpha \downarrow 0} \hat{W}_\alpha(\xi) = 1$, for any ξ ;
- (iii) for any $\alpha > 0$ there exists a constant c_α such that

$$|\hat{W}_\alpha(\xi)/\hat{K}(\xi)| \leq c_\alpha, \text{ for any } \xi.$$

Then, it is easy to show (Tikhonov & Arsenine 1977) that the family of linear operators, defined by

$$(R_\alpha g)(x) = (2\pi)^{-1} \int_{-\infty}^{+\infty} [\hat{W}_\alpha(\xi) \hat{g}(\xi) / \hat{K}(\xi)] e^{ix\xi} d\xi \quad (2.4)$$

provides a regularization algorithm for the approximate solution of problem (1.1), (2.1). The basic property (1.2), indeed, follows from the Parseval equality and the dominated convergence theorem.

We point out that the Tikhonov regularizer (Groetsch 1984) corresponds to the window function

$$\hat{W}_\alpha(\xi) = |\hat{K}(\xi)|^2 / [|\hat{K}(\xi)|^2 + \alpha \hat{p}(\xi)], \quad (2.5)$$

where $\hat{p}(\xi)$ is the weight function defining the norm of X , (2.2), and the method of truncated Fourier-transform inversion corresponds to the window function

$$\hat{W}_\alpha(\xi) = 1, \quad |\xi| < 1/\alpha; \quad \hat{W}_\alpha(\xi) = 0, \quad |\xi| > 1/\alpha. \quad (2.6)$$

When the regularization algorithm is defined by (2.4), the operator T_α , (1.3), is given by

$$(T_\alpha f)(x) = \int_{-\infty}^{+\infty} W_\alpha(x-y) f(y) dy, \quad (2.7)$$

where $W_\alpha(x)$ denotes the inverse Fourier transform of $\hat{W}_\alpha(\xi)$. It follows that *the regularization algorithm (2.4) has the positivity property if and only if $W_\alpha(x) \geq 0$ for any x* . We notice that the Tikhonov window (2.5) in general does not satisfy this condition. In §5, however, we discuss two important problems where the Tikhonov window has the positivity property.

2.1. Band-limited windows

Consider a family of window functions such that, for a given α , the support of $\hat{W}_\alpha(\xi)$ is interior to the interval $[-\Omega, \Omega]$ with

$$\Omega = 1/\alpha. \quad (2.8)$$

Using a standard terminology in electrical engineering and communication theory, we call the inverse Fourier transform of $\hat{W}_\alpha(\xi)$, i.e. $W_\alpha(x)$, a band-limited function with bandwidth Ω . An example is the window function (2.6), in which case $W_\alpha(x)$ is the well-known Dirichlet kernel

$$W_\alpha(x) = (\Omega/\pi) [\sin(\Omega x)]/(\Omega x) \quad (2.9)$$

and therefore the corresponding regularization algorithm does not have the positivity property.

A first very simple example of a band-limited window with the positivity property is provided by the triangular window

$$\hat{W}_\alpha(\xi) = 1 - \alpha|\xi|, \quad |\xi| < \Omega; \quad \hat{W}_\alpha(\xi) = 0, \quad |\xi| > \Omega. \quad (2.10)$$

$$\text{In which case} \quad W_\alpha(x) = (\Omega/2\pi) [\sin^2(\frac{1}{2}\Omega x)]/(\frac{1}{2}\Omega x)^2. \quad (2.11)$$

Notice that, for a given Ω (2.11) has a central peak with a width that is twice the width of the function (2.9) and smaller 'side-lobes'. This implies, for a fixed bandwidth, a loss in resolution by a factor of two. However, the 'optimum' choice

of Ω may not be the same in the two cases, as we will discuss in §4, and as a consequence the loss in resolution may be smaller than a factor of two.

Starting from the window function (2.10) one can build up other regularization algorithms with the positivity property as follows: take a set of n positive numbers a_k ($k = 1, \dots, n$), such that $a_1 + \dots + a_n = 1$, and put

$$\hat{W}_\alpha(\xi) = \sum_k a_k (1 - \alpha|\xi|)^k, \quad |\xi| < \Omega; \quad W_\alpha(\xi) = 0, \quad |\xi| > \Omega. \quad (2.12)$$

Then the conditions (i)–(iii) are satisfied and the corresponding function $W_\alpha(x)$ is a linear combination of the function (2.11) and of its autoconvolutions.

2.2. Gaussian and exponential windows

Another important family of window functions leading to regularization algorithms with the positivity property is

$$\hat{W}_\alpha(\xi) = \exp(-\tfrac{1}{2}\alpha\xi^2). \quad (2.13)$$

The corresponding functions $W_\alpha(x)$ are given by

$$W_\alpha(x) = (2\pi\alpha)^{-\frac{1}{2}} \exp(-x^2/2\alpha). \quad (2.14)$$

Obviously this window function cannot be used for any arbitrary deconvolution problem but only for those problems such that condition (iii) above is satisfied. In other words, the Fourier transform of the kernel must decay at infinity less rapidly than any gaussian. Applications of this window function will be discussed in §5.

Similar remarks apply also to the case of the exponential window

$$\hat{W}_\alpha(\xi) = \exp(-\alpha|\xi|) \quad (2.15)$$

in which case

$$W_\alpha(x) = (\alpha/\pi) (x^2 + \alpha^2)^{-1}. \quad (2.16)$$

It is interesting to notice that both the gaussian and the exponential windows do not exhibit ‘side lobes’.

3. WINDOW FUNCTIONS AND BACKUS-GILBERT AVERAGING KERNELS

The method of Backus and Gilbert (Backus & Gilbert 1968) applies to inverse problems with discrete data (Bertero *et al.* 1985c): find a square integrable function f such that

$$\int \phi_n(x) f(x) dx = g_n; \quad n = 1, \dots, N, \quad (3.1)$$

where the ϕ_n are given functions and the g_n are given numbers, the data of the problem. The method consists in looking for an ‘average’ of the unknown function $f(x)$ at any point x

$$\tilde{f}(x) = \int W(x, y) f(y) dy \quad (3.2)$$

(the analogy between this equation and (2.7) is obvious) the ‘averaging’ kernel $W(x, y)$ being expressed in terms of the functions ϕ_n as follows

$$W(x, y) = \sum_n a_n(x) \phi_n(y). \quad (3.3)$$

The functions $a_n(x)$ are determined from the normalization condition

$$\int W(x, y) dy = 1 \quad (3.4)$$

combined with an appropriate variational property of the following type

$$\int J(x, y) W^2(x, y) dy = \min. \quad (3.5)$$

An example of a particular weighting function $J(x, y)$ is, for instance (Backus & Gilbert 1968)

$$J(x, y) = (x - y)^2. \quad (3.6)$$

When the functions $a_n(x)$ have been determined by means of the equations (3.4) and (3.5), the 'average' solution $\hat{f}(x)$ is given by

$$\hat{f}(x) = \sum_n g_n a_n(x). \quad (3.7)$$

The previous procedure can be extended to deconvolution problems, such as those investigated in §2, in the following way. Assume that the Fourier transform of $f(x)$ is known on some band $[-\Omega, \Omega]$. This Fourier transform can be obtained from the Fourier transform of the real data function $g(x)$ as follows

$$\hat{f}(\xi) = \hat{g}(\xi)/\hat{K}(\xi), \quad |\xi| \leq \Omega. \quad (3.8)$$

Then it is quite natural to look for an 'average' solution of the following form

$$\hat{f}(x) = \int_{-\infty}^{+\infty} W(x - y) f(y) dy \quad (3.9)$$

with a band-limited 'averaging' kernel

$$W(x) = (2\pi)^{-1} \int_{-\Omega}^{+\Omega} \hat{W}(\xi) e^{-ix\xi} d\xi. \quad (3.10)$$

It is also natural to require that $W(x)$ is real and even. Then the conditions (3.4), (3.5) are replaced respectively by the following ones

$$\int_{-\infty}^{+\infty} W(x) dx = 1, \quad (3.11)$$

$$\int_{-\infty}^{+\infty} J(x) W^2(x) dx = \min. \quad (3.12)$$

In the case where $J(x)$ is given by (3.6), both $W(x)$ and $xW(x)$ are square integrable and therefore $W(x)$ is also integrable. It follows that the Fourier transform of $W(x)$, i.e. $\hat{W}(\xi)$, is absolutely continuous. Furthermore, thanks to the other assumptions on $W(x)$, $\hat{W}(\xi)$ is also real and even. It follows that $\hat{W}(\xi)$ is the solution of the following boundary value problem when $\xi \in [0, \Omega]$

$$\hat{W}''(\xi) = 0, \quad \hat{W}(0) = 1, \quad \hat{W}(\Omega) = 0 \quad (3.13)$$

and therefore

$$\hat{W}(\xi) = 1 - \xi/\Omega. \quad (3.14)$$

We conclude that the above extension of the Backus and Gilbert method is equivalent to the use of the triangular window and therefore has the positivity property.

The weight function

$$J(x) = x^4 \quad (3.15)$$

has also been used (Haario & Somersalo 1985). In such a case the function $\hat{W}(\xi)$ can be obtained by solving the following boundary-value problem

$$\hat{W}^{iv}(\xi) = 0; \quad \hat{W}(0) = 1, \quad \hat{W}'(0) = 0; \quad \hat{W}(\Omega) = 0, \quad \hat{W}'(\Omega) = 0 \quad (3.16)$$

whose solution is

$$\hat{W}(\xi) = 3(1 - \xi/\Omega)^2 - 2(1 - \xi/\Omega)^3. \quad (3.17)$$

The corresponding averaging kernel is given by

$$W(x) = (6\Omega/\pi) \{2[1 - \cos(\Omega x)]/(\Omega x)^4 - \sin(\Omega x)/(\Omega x)^3\}. \quad (3.18)$$

The averaging kernels (2.11) and (3.18) are plotted in figure 1 for the same value of Ω . The two kernels take the same value at $x = 0$ and have approximately the same width, i.e. they give the same resolution with the same value of the bandwidth. The averaging kernel corresponding to the weight function (3.15) does not have the positivity property, but the negative parts are quite small. Furthermore the 'side lobes' of this kernel are smaller than the 'side lobes' of the kernel (2.11). Therefore, even if the window (3.17) does not strictly satisfy the positivity property, it can have same advantages with respect to the triangular window. It is also interesting to notice that the kernel (3.18) is quite similar to the kernel corresponding to the so-called Hanning window (Kunt 1980)

$$\hat{W}(\xi) = \frac{1}{2}[1 + \cos(\pi\xi/\Omega)]. \quad (3.19)$$

In such a case the averaging kernel is

$$W(x) = \sin \frac{1}{4}[\Omega(x - \pi/\Omega)] \pi(x - \Omega/\pi) + \sin \frac{1}{2}(\Omega x) \pi x + \sin [\frac{1}{4}\Omega(x + \pi/\Omega)] \pi(x + \Omega/\pi). \quad (3.20)$$

A plot of the kernels (3.18) and (3.20) shows that they can hardly be distinguished in practice.

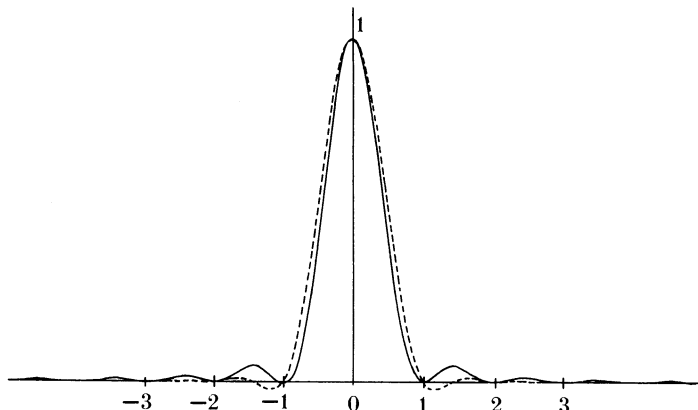


FIGURE 1. Comparison of the kernel (2.11) (full line) with the kernel (3.18) (dotted line) in the case $\Omega = 2\pi$.

4. THE DISCREPANCY PRINCIPLE

An important problem in regularization theory is the choice of the regularization parameter α . A rather general method is provided by the so-called discrepancy principle (see, for example, Groetsch 1984). For a given regularization algorithm and a given data function g_ϵ (1.4), one introduces the discrepancy function

$$\rho(\alpha) = \|\mathbf{A}\mathbf{R}_\alpha g_\epsilon - g_\epsilon\|_Y. \quad (4.1)$$

which is the norm of the difference between the real data and the computed data corresponding to the approximate solution $\mathbf{R}_\alpha g_\epsilon$. Then the discrepancy principle states that one must look for a value of α such that this norm is equal to the estimate ϵ of the norm of the error, i.e.

$$\rho(\alpha) = \epsilon. \quad (4.2)$$

In the case of a regularizing algorithm for the problem (1.1), (2.1), such as that of (2.4), the discrepancy function is given by

$$\rho^2(\alpha) = (2\pi)^{-1} \int_{-\infty}^{+\infty} \psi_\alpha(\xi) |\hat{g}_\epsilon(\xi)|^2 d\xi, \quad (4.3)$$

where

$$\psi_\alpha(\xi) = |\hat{W}_\alpha(\xi) - 1|^2. \quad (4.4)$$

An important property of $\rho(\alpha)$, which holds true for all the examples of window functions given in §§2 and 3, is that it is a continuous, increasing function of α , with $\rho(0) = 0$ and $\rho(+\infty) = \|g_\epsilon\|_Y$. Therefore, if the condition $\|g_\epsilon\|_Y > \epsilon$ is satisfied, there exists a unique solution of (4.2). If $\hat{\alpha} = \hat{\alpha}(\epsilon)$ is such a solution, then $\hat{\alpha} \rightarrow 0$ when $\epsilon \rightarrow 0$ as follows from the property $\rho(0) = 0$. It is also interesting to notice that, if we put

$$\nu(\alpha) = \|\mathbf{R}_\alpha g_\epsilon\|_X \quad (4.5)$$

then $\nu(\alpha)$ is a decreasing function of α for all the window functions introduced above. It follows that the approximate solution provided by the discrepancy principle is the solution of minimal norm among the regularized solutions compatible with the experimental data.

We prove now that the value of the bandwidth provided by the discrepancy principle in the case of the square window (2.6) is smaller than the value provided by the same criterion in the case of the triangular window (2.10). To this purpose we just notice that for the square window the function (4.4) is

$$\psi_{S,\alpha}(\xi) = 0, \quad |\xi| < \Omega; \quad \psi_{S,\alpha}(\xi) = 1, \quad |\xi| > \Omega, \quad (4.6)$$

whereas for the triangular window it is

$$\psi_{T,\alpha}(\xi) = (\alpha\xi)^2, \quad |\xi| < \Omega; \quad \psi_{T,\alpha}(\xi) = 1, \quad |\xi| > \Omega \quad (4.7)$$

and therefore, for any ξ , $\psi_{T,\alpha}(\xi) \geq \psi_{S,\alpha}(\xi)$. This implies the following inequality between the corresponding discrepancy functions

$$\rho_T(\alpha) \geq \rho_S(\alpha) \quad (4.8)$$

and as a consequence, $\hat{\alpha}_S \geq \hat{\alpha}_T$ or also $\Omega_S \leq \Omega_T$. As already remarked in the

Introduction, this result justifies the conclusion that the loss in resolution associated with the triangular window may be less than a factor of two. In fact, some Fourier components that are considered as invisible in the case of the square window can be added to the solution in the case of the triangular window. We also point out that similar conclusions can be obtained if the discrepancy principle is used for comparing the square window with the window (3.17) or with the Hanning window (3.19).

The previous result probably is not related to the particular criterion for the choice of the regularization parameter we have used. If we require, for instance, that the norm of the regularized solution takes a prescribed value, say E , and therefore we look for the value of α solving the equation $\nu(\alpha) = E$, $\nu(\alpha)$ being defined in (4.5), then we find again that the value of the bandwidth provided by this criterion in the case of the square window is smaller than the value provided in the case of the triangular or Hanning window.

We conclude this section with a few remarks about an important theoretical point: the convergence, when $\epsilon \rightarrow 0$, of the regularized solution $f_{\hat{\alpha}} = R_{\hat{\alpha}} g_{\epsilon}$ ($\hat{\alpha} = \hat{\alpha}(\epsilon)$ denotes the value of the regularization parameter given by (4.2)) to the true solution f of the problem as defined in (1.4). This result has been proved in the case of the Tikhonov regularizer (Groetsch 1984), which is given by (2.5) for deconvolution problems. A similar result has been proved in the case of truncated eigenfunction or singular function expansions and of several other regularizing algorithms (Vainikko 1982), provided that (3.2) is replaced by

$$\rho(\alpha) = \mu\epsilon, \quad (4.9)$$

where $\mu > 1$ is an arbitrary fixed number. No general result of this type seems to hold for the method of window functions described in §2. We give here a lemma which is an extension of results contained in Defrise (1986). This lemma will be used in the next section in connection with the problems of numerical derivation and Radon transform inversion.

LEMMA. *Let $\{R_{\alpha}\}_{\alpha>0}$ be a family of regularizing operators such that, for any α , $\|AR_{\alpha} - 1\| \leq 1$ and let $\hat{\alpha} = \hat{\alpha}(\epsilon)$ be the unique solution of (4.9). Then the following inequality holds true.*

$$\|f_{\hat{\alpha}} - f\|_X \leq (\mu - 1)^{-1} \|R_{\hat{\alpha}}\| \| (AR_{\hat{\alpha}} - 1) Af \|_Y + \|(T_{\hat{\alpha}} - 1)f\|_X, \quad (4.10)$$

where $f_{\hat{\alpha}} = R_{\hat{\alpha}} g_{\epsilon}$ and f is the true solution of the problem as defined by (1.4).

Proof. From the triangle inequality we get

$$\|f_{\hat{\alpha}} - f\|_X = \|R_{\hat{\alpha}}(g_{\epsilon} - Af) + R_{\hat{\alpha}}Af - f\|_X \leq \epsilon \|R_{\hat{\alpha}}\| + \|(T_{\hat{\alpha}} - 1)f\|_X. \quad (4.11)$$

Then, from (4.9), whose solution is $\hat{\alpha}$, using again the triangle inequality and the condition $\|AR_{\alpha} - 1\| \leq 1$, we obtain

$$\mu\epsilon = \|(AR_{\hat{\alpha}} - 1)g_{\epsilon}\|_Y = \|(AR_{\hat{\alpha}} - 1)(g_{\epsilon} - Af) + (AR_{\hat{\alpha}} - 1)Af\|_Y \leq \epsilon + \|(AR_{\hat{\alpha}} - 1)Af\|_Y. \quad (4.12)$$

It follows that

$$\epsilon \leq (\mu - 1)^{-1} \|(AR_{\hat{\alpha}} - 1)Af\|_Y \quad (4.13)$$

and by inserting this inequality in (4.11) we get (4.10). ■

A few remarks about this lemma may be made. First we notice that, for all the regularizing algorithms introduced in the previous sections, the condition $\|AR_\alpha - 1\| \leq 1$ is satisfied. Furthermore we know that for these algorithms the value $\hat{\alpha}$ of the regularization parameter provided by the discrepancy principle tends to zero when $\epsilon \rightarrow 0$. We conclude that we can apply the previous lemma and that if the following property holds true

$$\|R_\alpha\| \|(AR_\alpha - 1)Af\|_Y \rightarrow 0, \alpha \rightarrow 0, \quad (4.14)$$

then $\|f_{\hat{\alpha}} - f\|_X$ tends to zero when $\epsilon \rightarrow 0$, i.e. the regularized solution converges to the true solution.

5. NUMERICAL DIFFERENTIATION AND RADON TRANSFORM INVERSION

The computation of the derivative of a function, defined everywhere on $(-\infty, +\infty)$, can be formulated as the solution of a first-kind equation similar to those considered in the previous sections. Let X be a space of square integrable functions, the norm being defined as in (2.2) with

$$\hat{p}(\xi) = 1 + \xi^{-2}. \quad (5.1)$$

X is a space of square integrable functions having a square integrable primitive. Then consider the integral operator

$$(Af)(x) = \int_{-\infty}^x f(y) dy, \quad (5.2)$$

which is a continuous operator from X into $Y = L^2(-\infty, +\infty)$. The operator (5.2), indeed, can be viewed as a special case of operator (2.1) with

$$\hat{K}(\xi) = 1/(i\xi). \quad (5.3)$$

Then the computation of the derivative of a function $g \in Y$ is equivalent to the solution of the equation $Af = g$. This equation is obviously ill-posed and therefore regularization methods must be used for the approximate solution of this problem (Cullum 1971). We cannot summarize here the wide literature existing on the subject.

Our first remark consists in showing that, for the problem of numerical derivation as formulated above, the Tikhonov regularizer has the positivity property. From (2.5), (5.1) and (5.3) we get

$$\hat{W}_\alpha(\xi) = [1 + \alpha(1 + \xi^2)]^{-1} \quad (5.4)$$

and therefore the inverse Fourier transform of the Tikhonov window is positive because it is given by

$$W_\alpha(x) = (2\alpha\beta)^{-1} \exp(-\beta|x|), \quad (5.5)$$

where $\beta = (1 + 1/\alpha)^{\frac{1}{2}}$. As concerns the choice of the regularization parameter, one can obviously apply the general results that have been proved for the Tikhonov regularizer. In particular, the discrepancy principle (4.2) provides an approximate solution which converges to the exact solution when the error on the data tends to zero.

Another window which is often used in practical applications of this problem, such as the problem of edge detection (Torre 1986), is the gaussian window (2.13). As we have already remarked, this window has the positivity property. We will prove now that the discrepancy principle (4.9) with μ strictly greater than one, provides an approximate solution which also converges to the exact solution in the limit of zero error. For this purpose we will use the result derived from the lemma of §4. First of all notice that, in the present case

$$\begin{aligned}\|R_\alpha\|^2 &= \sup_{\xi} \{ \hat{\rho}(\xi) |\hat{W}_\alpha(\xi)/\hat{K}(\xi)|^2 \} \\ &= \sup_{\xi} \{ (1 + \xi^2) \exp(-2\alpha\xi^2) \} \leq 1/(2\alpha)\end{aligned}\quad (5.6)$$

and also

$$\begin{aligned}\|(AR_\alpha - 1)Af\|_Y^2 &= (2\pi)^{-1} \int_{-\infty}^{+\infty} |\hat{W}_\alpha(\xi) - 1|^2 |\hat{K}(\xi)|^2 |\hat{f}(\xi)|^2 d\xi \\ &= (2\pi)^{-1} \int_{-\infty}^{+\infty} |\exp(-\alpha\xi^2) - 1|^2 \xi^{-2} |\hat{f}(\xi)|^2 d\xi.\end{aligned}\quad (5.7)$$

It follows that

$$\|R_\alpha\|^2 \|(AR_\alpha - 1)Af\|_Y^2 \leq (2\pi)^{-1} \int_{-\infty}^{+\infty} \theta_\alpha(\xi) |\hat{f}(\xi)|^2 d\xi, \quad (5.8)$$

where

$$\theta_\alpha(\xi) = |\exp(-\alpha\xi^2) - 1|^2 / (\alpha\xi^2). \quad (5.9)$$

Because this function is bounded by 1, for any α and any ξ , and tends to zero for any ξ , when α tends to zero, from the dominated convergence theorem it follows that (4.14) is satisfied and the result stated above is proved.

The next problem we consider in this section is the inversion of the Radon transform, whose applications to several practical problems are well known (Herman 1979). Using standard notation, we define the Radon transform of a function $f(x, y)$ as follows

$$(\mathcal{R}f)(s, \theta) = \int_{-\infty}^{+\infty} f(s \cos \theta - u \sin \theta, s \sin \theta + u \cos \theta) du. \quad (5.10)$$

Then the back-projection operator $\mathcal{B} = \mathcal{R}^*$, acting on a function $h(s, \theta)$, is

$$(\mathcal{B}h)(x, y) = \int_0^\pi h(x \cos \theta + y \sin \theta, \theta) d\theta. \quad (5.11)$$

By using the back-projection operator the problem of the inversion of the Radon transform, i.e. of the solution of the first-kind equation $\mathcal{R}f = h$, can be reduced to the solution of the equation $Af = g$, where the operator A is defined by $A = \mathcal{B}\mathcal{R} = \mathcal{R}^*\mathcal{R}$ and $g = \mathcal{B}h$ are the back-projected data. The new equation is a convolution equation of the kind considered in §2, except for the fact that it is an equation for a function of two variables instead of one. As is well known the operator A is given by

$$(Af)(x, y) = \iint_{-\infty}^{+\infty} [(x-x')^2 + (y-y')^2]^{-\frac{1}{2}} f(x', y') dx' dy' \quad (5.12)$$

and by taking the Fourier transform one gets

$$(Af)\hat{f}(\xi, \eta) = 2\pi(\xi^2 + \eta^2)^{-\frac{1}{2}}\hat{f}(\xi, \eta). \quad (5.13)$$

To simplify the notation we will put $\mathbf{r} = \{x, y\}$ and $\boldsymbol{\zeta} = \{\xi, \eta\}$. Then we introduce a space of square integrable functions defined over R^2 , with a norm given by

$$\|f\|_X^2 = (2\pi)^{-2} \int_{R^2} (1 + |\boldsymbol{\zeta}|^{-2}) |\hat{f}(\boldsymbol{\zeta})|^2 d\boldsymbol{\zeta}. \quad (5.14)$$

It is easy to verify that the operator A is a bounded operator from X into $Y = L^2(R^2)$. We also notice that we can use all the formulae given in §2 if we replace $\hat{p}(\xi)$, $\hat{K}(\xi)$ respectively by

$$\hat{p}(\boldsymbol{\zeta}) = 1 + |\boldsymbol{\zeta}|^{-2}, \quad \hat{K}(\boldsymbol{\zeta}) = 2\pi |\boldsymbol{\zeta}|^{-1}. \quad (5.15)$$

As in the problem of numerical derivation, the Tikhonov regularizer has the positivity property when applied to the inversion of the convolution operator (5.12). From (2.5) and (5.15) we get

$$\hat{W}_\alpha(\boldsymbol{\zeta}) = (2\pi)^2 [(2\pi)^2 + \alpha(1 + |\boldsymbol{\zeta}|^2)]^{-1} \quad (5.16)$$

and the computation of the inverse Fourier transform, with a well-known integral representation of the modified Hankel functions, provides the following result

$$W_\alpha(|\mathbf{r}|) = (2/\pi\alpha) K_0(\beta|\mathbf{r}|). \quad (5.17)$$

Here $\beta = [1 + (2\pi)^2/\alpha]^{1/2}$ and K_0 denotes the modified Hankel function of order zero. Because $K_0(x) > 0$ for any x , the Tikhonov regularizer has the positivity property. Notice, however, that the function K_0 is not bounded in the neighbourhood of $x = 0$.

Finally, if we use a gaussian window to regularize the inversion of the operator (5.12), we can easily extend to this problem the computations performed in the case of the problem of numerical derivation in order to show that the choice of regularization parameter provided by the discrepancy principle (4.9), with μ strictly greater than one, provides an approximate solution which converges to the true solution of the problem when the error on the data tends to zero.

6. ABEL, LAPLACE AND SIMILAR TRANSFORMS INVERSION

In this section we investigate two important classes of first-kind integral equations which can be treated by using methods very similar to those developed in the previous sections for first-kind convolution equations. The corresponding integral operators indeed are, at least in one case, convolution operators commuting with the dilation group while the integral operators (2.1) commute with the translation group.

The first class of integral operators is defined as follows

$$(Af)(t) = \int_0^{+\infty} K(t/s)f(s)s^{-1}ds, \quad (6.1)$$

and the second class is the following one

$$(\hat{A}f)(t) = \int_0^{+\infty} K(ts)f(s) \, ds. \quad (6.2)$$

An important example of an equation of the first class is provided by the Abel equation which is obtained by taking

$$K(t) = (t-1)^{-\frac{1}{2}}, t > 1; \quad K(t) = 0, \quad 0 < t < 1 \quad (6.3)$$

and by identifying the unknown function with the function $f(s)s^{-\frac{1}{2}}$. As concerns the second class of integral operators, the most famous example is provided by the Laplace transform which is obtained by taking

$$K(t) = \exp(-t). \quad (6.4)$$

A common feature of the first kind equations associated with an operator of type (6.1) or (6.2) is that they can be treated by means of the Mellin transform. If we work in spaces of square integrable functions, then the appropriate definition of the Mellin transform of a function $f \in L^2(0, +\infty)$ is (we use here the same notation used in the previous sections for the Fourier transform)

$$\hat{f}(\xi) = \int_0^{+\infty} f(t) t^{-\frac{1}{2}+i\xi} \, dt. \quad (6.5)$$

As is well known (Titchmarsh 1948), if $f \in L^2(0, +\infty)$ then $\hat{f} \in L^2(-\infty, +\infty)$ and the following relation, which is just an extension of the Parseval equality, holds true

$$\int_0^{+\infty} |f(t)|^2 \, dt = (2\pi)^{-1} \int_{-\infty}^{+\infty} |\hat{f}(\xi)|^2 \, d\xi. \quad (6.6)$$

Analogously, the inversion formula of the Mellin transform of square integrable functions is given by

$$f(t) = (2\pi)^{-1} \int_{-\infty}^{+\infty} \hat{f}(\xi) \tau^{-(\frac{1}{2}+i\xi)} \, d\xi. \quad (6.7)$$

If we consider now the first-kind equation (1.1) with the operator A defined as in (6.1) and if we take the Mellin transform of both sides of this equation we get

$$\hat{g}(\xi) = \hat{K}(\xi)\hat{f}(\xi), \quad (6.8)$$

where $\hat{K}(\xi)$ is the Mellin transform of $K(t)$, as defined by (6.5). We see that the operator A is invertible if the support of $\hat{K}(\xi)$ is $(-\infty, +\infty)$. Furthermore, if the function $t^{-\frac{1}{2}}K(t)$ is integrable, then $\hat{K}(\xi)$ is continuous and tends to zero at infinity. As a consequence the operator A^{-1} is not continuous and the problem is ill-posed because the following equation holds true

$$(A^{-1}g)(t) = (2\pi)^{-1} \int_{-\infty}^{+\infty} [\hat{g}(\xi)/\hat{K}(\xi)] t^{-(\frac{1}{2}+i\xi)} \, d\xi. \quad (6.9)$$

Analogous considerations apply to the case of the integral operator (6.2). In such a case (6.8) is replaced by

$$\hat{g}(\xi) = \hat{K}(\xi)\hat{f}(-\xi) \quad (6.10)$$

and, if the kernel $K(t)$ satisfies the conditions stated above, the inversion formula (6.9) is replaced by

$$(A^{-1}g)(t) = (2\pi)^{-1} \int_{-\infty}^{+\infty} [\hat{g}(-\xi)/\hat{K}(-\xi)] t^{-(\frac{1}{2}+i\xi)} d\xi. \quad (6.11)$$

It is obvious now that (6.9) and (6.11) are completely analogous to (2.3). Therefore, as in §2, we can introduce regularizing algorithms defined in terms of families of window functions $\{\hat{W}_\alpha(\xi)\}_{\alpha>0}$ which depend now on the Mellin variable ξ . These functions of course must satisfy conditions (i)–(iii) of §2. Then the corresponding regularizing operators R_α are obtained by inserting the function $\hat{W}_\alpha(\xi)$ in (6.9) or (6.11). In both cases the operator T_α is given by

$$(T_\alpha f)(t) = \int_0^{+\infty} W_\alpha(t/s) f(s) s^{-1} ds, \quad (6.12)$$

where $W_\alpha(t)$ is the inverse Mellin transform of $\hat{W}_\alpha(\xi)$. It follows that the regularizing algorithm has the positivity property if $W_\alpha(t) \geq 0$ for any value of t .

We give now expressions for the functions $W_\alpha(t)$ corresponding to the window functions considered in §2. For the square window we have

$$W_\alpha(t) = (\Omega/\pi) t^{-\frac{1}{2}} \sin[\Omega \ln(t)]/[\pi \ln(t)], \quad (6.13)$$

and in the case of the triangular window we have

$$W_\alpha(t) = (\Omega/2\pi) t^{-\frac{1}{2}} \sin^2[(\frac{1}{2}\Omega) \ln(t)]/[(\frac{1}{2}\Omega) \ln(t)]^2. \quad (6.14)$$

Notice that (6.13) and (6.14) are obtained respectively from (2.9) and (2.11) just by putting $x = \ln(t)$ and multiplying by $t^{-\frac{1}{2}}$. In the same way the functions $W_\alpha(t)$ corresponding to the gaussian and exponential windows are obtained.

As follows from (6.12), the impulse response associated with a given window function, i.e. the response to the unit impulse $f(t) = \delta(t-a)$, is given by $a^{-1}W_\alpha(t/a)$. The typical behaviour of this function for the square and triangular window, as well as for all the other windows, is that the principal peak becomes broader and

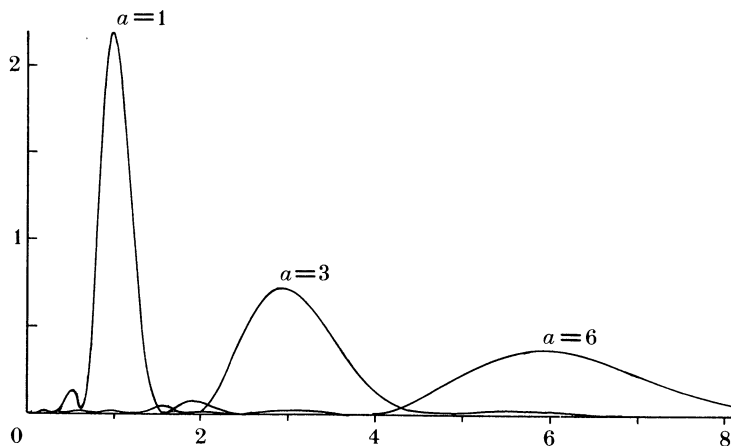


FIGURE 2. Plot of the function $a^{-1}W_\alpha(t/a)$, corresponding to the kernel (6.14) with $\Omega = 4\pi$, for various values of α .

lower as a increases. Furthermore, the ratio between the peak values corresponding to two different positions of the δ -function, say a_1 and a_2 , is approximately a_2/a_1 and it is independent of Ω which is related to the regularization parameter by (2.8). The function $a^{-1}W_\alpha(t/a)$, in the case of the kernel (6.14), is plotted in figure 2 for various values of a .

7. CONVOLUTION OPERATORS ON THE CIRCLE

Another important case where it is easy to introduce regularization algorithms with the positivity property is that of convolution operators on the circle, namely the case of integral operators having the following form

$$(Af)(x) = (2\pi)^{-1} \int_{-\pi}^{+\pi} K(x-y)f(y) dy, \quad (7.1)$$

where $K(x)$ is a periodic function with period 2π . Several classical ill-posed problems such as analytic or harmonic continuation on a disc and the determination of periodic solutions of the backward heat equation or of the Cauchy problem for the Laplace equation (Miller 1964) can be reduced to the inversion of an operator of the type (7.1).

The problem (1.1), in the case where the integral operator is defined by (7.1), can obviously be solved by means of Fourier series expansions. If we denote by f_n the Fourier coefficients of $f(x)$, by g_n the Fourier coefficients of $g(x)$ and by k_n the Fourier coefficients of $K(x)$, then the following relation holds true

$$g_n = k_n f_n \quad (7.2)$$

and therefore the operator A is invertible if and only if all the Fourier coefficients k_n are different from zero. In such a case the inverse operator is given by

$$(A^{-1}g)(x) = \sum_{n=-\infty}^{+\infty} (g_n/k_n) e^{inx}. \quad (7.3)$$

Because the Fourier coefficients k_n tends to zero when n tends to infinity, the operator A^{-1} is not continuous in $L^2(-\pi, \pi)$.

Regularization algorithms can be defined in terms of families of window coefficients $\{w_{\alpha,n}\}_{\alpha>0}$ satisfying conditions similar to conditions (i)–(iii) of §2 and precisely

- (i') $0 \leq w_{\alpha,n} \leq 1$, for any $\alpha > 0$ and any n ;
- (ii') $\lim_{\alpha \downarrow 0} w_{\alpha,n} = 1$, for any n ;
- (iii') for any $\alpha > 0$ there exists a constant c_α such that

$$|w_{\alpha,n}/k_n| \leq c_\alpha \text{ for any } n.$$

Then it is easy to show that the family of linear operators defined by

$$(R_\alpha g)(x) = \sum_{n=-\infty}^{+\infty} (w_{\alpha,n} g_n/k_n) e^{inx} \quad (7.4)$$

provides a regularization algorithm for the problem (1.1), (7.1). Furthermore the operator T_α , (1.3), is given by

$$(T_\alpha f)(x) = (2\pi)^{-1} \int_{-\pi}^{+\pi} W_\alpha(x-y) f(y) dy, \quad (7.5)$$

where

$$W_\alpha(x) = \sum_{n=-\infty}^{+\infty} w_{\alpha,n} e^{inx}. \quad (7.6)$$

Also in this case the regularizing algorithm (7.4) has the positivity property if and only if the function $W_\alpha(x)$ is positive.

The most simple regularizing algorithm is provided by the truncation of the Fourier series expansion of the solution. This corresponds to the use of the following square window

$$w_{\alpha,n} = 1, \quad |n| \leq N; \quad w_{\alpha,n} = 0, \quad |n| > N, \quad (7.7)$$

the relation between N and the regularization parameter being given by

$$N = [\alpha^{-1}]. \quad (7.8)$$

The function $W_\alpha(x)$ corresponding to the square window is the well-known Dirichlet kernel of the theory of Fourier series expansions

$$W_\alpha(x) = \sin[(N + \frac{1}{2})x] / \sin(\frac{1}{2}x) \quad (7.9)$$

and therefore this algorithm does not have the positivity property. On the other hand, if we consider the triangular window

$$w_{\alpha,n} = 1 - |n|/(N+1), \quad |n| \leq N; \quad w_{\alpha,n} = 0, \quad |n| > N \quad (7.10)$$

then the corresponding function $W_\alpha(x)$ is the Fejér kernel of the theory of Fourier series expansions

$$W_\alpha(x) = \sin^2[\frac{1}{2}(N+1)x] / [(N+1) \sin^2(\frac{1}{2}x)], \quad (7.11)$$

which has the positivity property. As is known this kernel is obtained when one considers Fourier series summation by Cesàro means.

Other window functions with the positivity property can be obtained by a procedure analogous to that defined by (2.12). It is interesting to point out that the gaussian window

$$w_{\alpha,n} = \exp(-\alpha n^2) \quad (7.12)$$

has again the positivity property because the corresponding function $W_\alpha(x)$ is just a periodic fundamental solution of the heat equation, the time variable being identified with the regularization parameter α . As is known the positivity of this solution follows from the maximum principle for the heat equation.

A very interesting problem is to investigate the possibility of introducing regularization algorithms with the positivity property for Toeplitz integral operators, i.e. integral operators having a structure similar to that of the operators (7.1)

$$(Af)(x) = \int_{-a}^{+a} K(x-y) f(y) dy, \quad (7.13)$$

where now $K(x)$ is *not* a periodic function (a is a fixed given number). A well-known example of such an operator is that investigated by Slepian and co-workers

(Slepian & Pollak 1961) which is obtained by taking $K(x) = \sin(Wx)/\pi x$ with W fixed.

Under very general conditions on the function $K(x)$, the operator (7.13) is compact in $L^2(-a, +a)$ and, when the function $K(x)$ is real and even, it is also self-adjoint. Then one can use eigenfunction expansions to solve the problem (1.1), (7.13) and introduce regularizing algorithms by means of a windowing of these eigenfunction expansions. We are not able to build up for this problem windowing methods with the positivity property. We have, however, strong numerical evidence, based on numerical computations performed for several kernels, that the use of the triangular or of the Hanning window produces a considerable reduction of the negative lobes which are present in the case of the square window. We give an example in figure 3. This corresponds to the integral operator (7.13) in the case $a = 1$ and $K(x) = 1/\cosh(bx)$ with $b = \frac{1}{4} \ln(2)$. This integral operator is related to the problem of finite Laplace transform inversion (Bertero *et al.* 1982) and its eigenfunctions are also eigenfunctions of a second-order self-adjoint differential operator (Bertero & Grünbaum 1985). In the figure we plot the kernel of the integral operator T_a obtained by taking 20 terms in the eigenfunction expansion and using a triangular window. In practice, we plot the response to several unit impulses $f(x) = \delta(x-c)$. Except for values of c very near to ± 1 the response function is essentially positive.

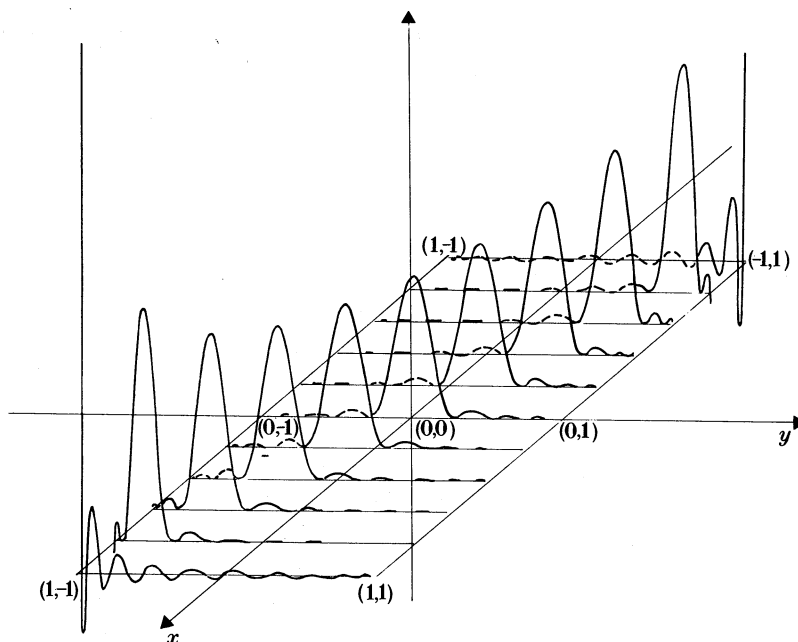


FIGURE 3. Plot of the impulse response obtained by means of a triangular windowing of the eigenfunction expansion corresponding to an operator of the type (7.13). The kernel is specified in the text.

8. CONCLUDING REMARKS

In this paper we have introduced several regularization methods, for deconvolution and similar problems, having the interesting property of producing positive approximate solutions in the absence of noise. As we have shown, however, positivity is always obtained at the cost of a loss in resolution. This feature implies that these methods are not convenient for those problems, such as finite Laplace transform inversion (Bertero *et al.* 1985*a*, 1982), where the number of degrees of freedom is quite small. In other words these methods are not convenient for severely ill-posed or ill-conditioned problems. On the other hand they can have interesting applications to those problems, such as the inversion of Fraunhofer diffraction data (Bertero *et al.* 1985*a*), where the number of degrees of freedom can be rather large and therefore a loss in resolution is not dramatic. Further work is in progress along these lines.

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