

Solution of inverse diffusion problems by operator-splitting methods

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Abstract

In this paper the inverse solution of the general (non-linear) diffusion problem or *backward heat conduction problem*. It is assumed that the direct solution can be satisfactorily modelled, for example by the finite difference method. The nature of the problem and typical approaches to its solution are briefly reviewed.

An operator-splitting method is introduced as a means of solving the inverse diffusion problem. An error analysis of the method is given, particularly for the application of the method to the simple diffusion equation. The method is applied to a range of test problems to illustrate the points of the analysis and to demonstrate the properties and performance of the method.

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1. Introduction

Many physical phenomena, such as fluid flow, heat conduction and semiconductor growth include a diffusion process. The action of the diffusion is a continuous process that has an increasing effect with time and typically manifests itself as a spreading and smoothing of the original distribution. Let the full effect of the diffusion process be written in operator notation as follows:

$$Kf = g, \tag{1}$$

where f is the original distribution, $K : X \rightarrow Y$ represents the operation of diffusion over the time interval and g the final distribution.

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Physical problems that include diffusion processes, such as those stated, can often be modelled by parabolic partial differential equation governing the concentration u , having the following general form

$$\frac{\partial u(x, t)}{\partial t} = D\nabla^2 u(x, t) + \text{first directional derivatives of } u. \quad (2)$$

The first term on the right-hand side of the equation is the diffusion term and the coefficient D (≥ 0) represents the rate of diffusion. Note that D need not be constant, it may for example be a function of position or time. The rate of diffusion may also vary with u as in material-dependent diffusion, resulting in a non-linear equation with $K = K(f)$. Often the first term is written $\nabla \cdot (D\nabla u)$ but by product differentiation the equation would again take the form (2). In the terminology of Eq. (1), $u(\mathbf{x}, 0) = f(\mathbf{x})$ and $u(\mathbf{x}, T) = g(\mathbf{x})$.

In general, typical diffusion problems, consisting of an initial distribution $u(\mathbf{x}, 0)$ and governed by an equation of the form (2), cannot be solved analytically. Numerical methods such as the finite difference method and the finite element method have been developed for their solution, simulating the relevant physical process through stepping forward in time t and re-computing the approximation to u at each time level (see [10,12], for example).

The inverse problem of solving the diffusion equation backwards in time—determining the initial distribution f from a final distribution g —is fundamental to much scientific enquiry. The classical example of inverse diffusion problems is the *backward heat conduction problem* in which the original temperature distribution in a material is to be determined from the distribution after an elapsed time. Such a problem is considered in Beck [1], although this book is more concerned with the *inverse heat conduction problem*, the estimation of the surface flux history of a heat conduction body. The author's interest in the inverse diffusion problems arise from their work in atomic mixing modelling [7,8,14] and the inverse problem of recovering the original material distribution [6].

In the forward numerical solution of parabolic partial differential equations like (2), it is generally found that the presence of the diffusion term (the first term on the right-hand side of (2)) improves the stability properties of the numerical method as it tends to damp away any of the numerical oscillations that may otherwise arise. However, in the backward numerical solution of the equations of the form (2), it is the diffusion term that causes the difficulty: simply employing the finite difference or finite element method with negative time steps is numerically unstable. The other terms on the right-hand side of (2) simply translate the solution and their effects are easily reversible.

Inverse diffusion problems are examples of *ill-posed* problems. Such problems—where the conditions placed on the governing equation are not classical and do not determine a unique solution—are also termed *Cauchy* problems. (see [4]). For diffusion problems, the smoothness that is inherent in the process results in a loss of resolution in the details of the original distribution. The inverse problem effectively suffers from insufficient information in g to determine a unique f . A further consideration is that in all practical applications the input to the inverse problem g will be measured data. It follows that some noise will be included in g . Since g should in theory be a smooth functions, the added noise in the measured g could easily place the measured g outside the set Y , the range of K , and there will be strictly no f such that $Kf = g$ (measured), $f \in X$.

The inversion method can only succeed if the original inverse problem—which will generally have no unique solution—is replaced by one that has a well-defined solution. The substitution of

a nearby problem for the original inverse problem is often termed (or is equivalent to) the *regularization* of the operator K . The inversion method must converge to the solution of the nearby problem. In Section 2 the general properties of the inverse problem and approaches to its solution are considered.

The purpose of this paper is to introduce an operator-splitting method for the iterative solution of inverse diffusion problems. The convergence of the resultant method is analysed, particularly in regard to observing Fourier solutions of the one-dimensional simple diffusion equation. The operator-splitting method is applicable to general non-linear diffusion problems. Results from the application of the method to Fourier components of the simple diffusion equation are given to illustrate the points of the analysis. The method is also applied to problems arising from selecting a general original f on the simple diffusion equation and it is applied to a typical non-linear diffusion equation to illustrate the usefulness of the method.

An Excel spreadsheet demonstration of the inversion method can be downloaded free from the www.scientific-computing.info web site.

2. Inverse solution methods

The purpose of this section is to discuss the nature of inverse problems and approaches to their numerical solution. There are a wide range of methods for solving inverse problems, two of which are particularly considered in this section: The Tikhonov method because of its importance and the fact that it helps to illustrate the general approach to inversion methods and the method of eigenfunction expansion, which will facilitate the understanding of the operator-splitting method that will be introduced in Section 4.

2.1. Nature of the diffusion problem

The nature of the diffusion problem and its inverse is illustrated in Fig. 1. The set X is the domain of K and Y is the range, where X and Y are subsets of normed linear spaces. The arrow labelled (a) shows the well-posedness of the forward operation; any $f \in X$ maps onto a unique $g \in Y$ (K is injective). The arrows labelled (b) illustrate the non-uniqueness of the inverse problem; $g \in Y$ (K is injective).

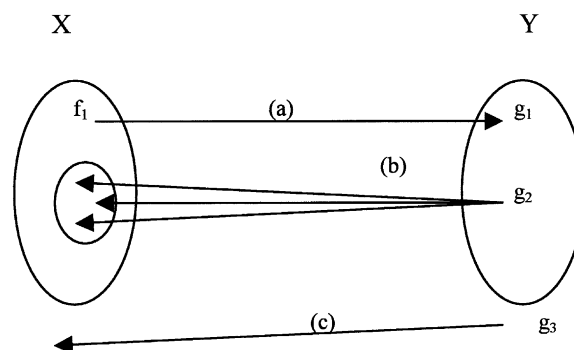


Fig. 1. Nature of the inverse problem.

there is a set of solutions $\{f: Kf = g\}$ (K is not surjective). The arrow labelled (c) represents the possibility discussed earlier, that a measured g^* may not be a member of Y since it contains noise. In this final case no $f \in X$ exists such that $Kf = g^*$.

It is illuminating to consider the analogies between the solution of inverse problems and the problem of solving the linear set of algebraic equations where the matrix is rank deficient (singular). For example consider the following equation:

$$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \mathbf{x} = \mathbf{b}. \quad (3)$$

For any given \mathbf{x}^* , matrix multiplication can be used to obtain the unique forward solution \mathbf{b}^* . For example $\mathbf{x}^* = [1, 2]^T \Rightarrow \mathbf{b}^* = [1, 1]^T$. However, when \mathbf{b} is known and \mathbf{x} is sought the fact that the matrix is singular means that there may be no solution and if there is a solution then it is not unique. The fact that the second component of \mathbf{x}^* does not effect the result of the forward operation is analogous to the loss of information that is a property of the forward operator that was discussed earlier. Furthermore, if the vector \mathbf{b}^* is perturbed, as it would be if it was affected by noise, then there may be no solution. For example if $\mathbf{b}^* = [1.01, 0.99]^T$ then a corresponding \mathbf{x}^* does not exist.

In developing a method for solving inverse problems, the aim is to reformulate the problem so that a unique solution is guaranteed (for the reformulated problem). To ensure existence of the solution, the data g could be smoothed to bring it into the range of K . Another approach is to widen the set of feasible solutions; $\{f: \|Kf - g\| < \varepsilon\}$, where $\varepsilon (>0)$ is a measure of the noise in g , and $\|\cdot\|$ is some suitable norm.

2.2. Tikhonov regularization

To ensure uniqueness, a typical approach is to seek an optimal solution in the space of feasible solutions. Examples of optimal solutions that are commonly used are minimum norm, minimum energy or maximum entropy. In the minimum norm example the inverse solution is defined as follows:

$$\min_{f \in X} \{\|f\|: \|Kf - g\| < \varepsilon\}. \quad (4)$$

The minimum norm method can be regarded as a constrained optimisation problem. Using Lagrange multipliers and dropping the constant ε allows us to substitute the problem (4) by the problem of minimizing the functional

$$\|f\|^2 + \mu \|Kf - g\|^2 \quad (5)$$

and taking the solution as $\mu \rightarrow \infty$. The second term in (5) enforces the constraint as a penalty function. Usually μ is fixed as a parameter (i.e., the limit is not taken) and the minimum found is taken as the inverse solution. Although some work is reported in the area, the selection of the value of μ is not straightforward in practice.

Reformulating the inverse problem in the form (5) is an example of Tikhonov regularization wherein a linear sum of the error functional $\|Kf - g\|^2$ and the smoothing functional ($\|f\|^2$ in (5)) is minimised in order to determine the inverse solution. A number of inversion methods are based

on the general approach of minimizing the combination of the error and smoothing functionals. A discussion of such methods is given in Chapter 18 of Press et al. [11].

The matrix equivalent of the regularization method (5) is the minimum norm solution of the rank deficient least squares problem (see Section 5.5 of [3]). Returning to the simple example (3), if $\mathbf{b} = [1, 1]^T$ then the solution \mathbf{x} is in the space $[1, \alpha]^T$, but the minimum norm solution is $[1, 0]^T$. The minimum norm solution of the matrix equation (3) illustrates a fundamental property of inversion methods: if a forward operator K is applied to a given function f to return a function g and an inversion method is applied to g , we should not expect the original function f to be returned.

2.3. Method of partial eigenfunction expansion

In order to develop the method of partial eigenfunction expansion, it must first be assumed that K is a linear operator. Let $\{\lambda_i, \varphi_i; i = 1, 2, \dots\}$ be the ordered set of eigenvalues and eigenfunctions of K . Hence given any g we may write

$$g(x) = \sum_{i=1}^{\infty} \alpha_i \varphi_i(x),$$

for any noise level ε (>0). Letting g be approximated by its first m eigenfunctions so that

$$g(x) = \sum_{i=1}^m \alpha_i \varphi_i(x) + \delta(x),$$

where $\|\delta\| < \varepsilon$. Now putting

$$f = \sum_{i=1}^m \frac{\alpha_i}{\lambda_i} \varphi_i,$$

ensures that f is a feasible solution of $\|Kf - g\| < \varepsilon$. The truncation of the eigenvalue expansion of g automatically tends the method towards the selection of a smooth solution.

2.4. Discussion

The inversion methods are developed through substituting the original $Kf = g$ by a nearby problem that has a unique solution. Accounting for noise in g using (4) widens the set of feasible solutions. Through seeking an optimal solution in this set or a solution that can be represented by a finite eigenvalue expansion, a deliberate bias has been included so that the resulting solution will have tend to have the desirable properties that have to be determined a priori.

In a mathematically determined (rather than a practical) test problem, we can begin with an original f , obtain the corresponding g using the forward operation. We can then test an inversion method through starting with g and trying to find an f^* such that $Kf^* = g$. However, the presence of an original f is also a priori information that biases the observer to expect an inverse solution similar to f . If the function g has been generated from an original function f then that f is not generally the solution of the nearby problem and we should not expect the numerical inverse solution to converge to it or necessarily regard the recovery of the original f as the aim of the inversion method. In practical situations the original f will often be unknown.

3. Properties of the simple diffusion equation

It is instructive to consider the properties of the simple diffusion equation

$$\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2}, \quad (6)$$

with $0 \leq t \leq T$ and $u(x, 0) = f(x)$ and $u(x, T) = g(x)$, to illuminate the nature of the diffusion operator K and its inverse. The equation is the one-dimensional form of the parabolic equation (2) with $D \equiv 1$ and the first derivative terms dropped. In the forward problem f is given and g is unknown: in the inverse problem g is given and f is unknown.

3.1. Fourier analysis

In the model problem (6), let $u(x, t)$ be expanded as a Fourier series. Let us consider one component of the Fourier series for f of angular frequency $N\pi$

$$f_N(x) = e^{iN\pi x}.$$

Substituting this into the model equation gives

$$g_N(x) = e^{-N^2\pi^2 T} e^{iN\pi x}$$

and hence that

$$g_N = k_N f_N,$$

where $k_N = e^{-N^2\pi^2 T}$.

3.2. First kind equation analogy

For the model equation, Eq. (1) can also be written in the form of a Fredholm integral equation of the first kind:

$$g(x) = \frac{1}{2\sqrt{\pi T}} \int_{-\infty}^{\infty} \exp\left\{-\frac{(x-y)^2}{4T}\right\} f(y) dy. \quad (7)$$

Discretising Eq. (7) using an integral equation method such as collocation results in a matrix-vector equation of the form

$$\underline{g} = K\underline{f}, \quad (8)$$

where $g_i = g(x_i)$, $f_i = f(x_i)$ and the x_i are the matching points.

The determination of g for the forward problem is simply the evaluation of an integral for each value of x . However, for the inverse problem, the solution f of (7) entails the solution of a Fredholm integral equation of the first kind. Such equations are notoriously difficult to solve, especially for integral operators with smooth kernels, such as the Gaussian kernel in (7). The matrix K in (8) will generally be severely ill-conditioned. An outline of the difficulties associated with methods for solving first kind equations is given in Miller [9].

3.3. Discussion

The Fourier analysis and the first kind Eq. (7) provide important information on some of the properties of the diffusion operator. For example the eigenvalues of the model problem (6) are

$$e^{(-N^2\pi^2T)},$$

for $N = 1, 2, \dots$. Hence the eigenvalues cluster and tend to zero as $N \rightarrow \infty$. It follows from the Fourier analysis that

$$f_N = e^{N^2\pi^2T} g_N$$

and so that the inverse problem effects a growth factor of

$$e^{N^2\pi^2T}$$

on the sinusoidal function g_N .

Eq. (7) demonstrates other interesting properties of the diffusion operator K . In particular, if f is a delta function then g is a Gaussian and if f is a step function then the discontinuity is smoothed in g to an error function. The general conclusion that can be drawn from this is that g is a C^∞ , continuously differentiable, function whereas f may belong to the space of C^0 or simply L_2 .

The danger of non-existence of a solution to the inverse problem can easily be demonstrated. For example for the model problem, if f is a delta function then g is a Gaussian function of greater and greater spread with T . If the result is observed at T then the precise form of the Gaussian distribution is given by (7). It might be thought that with g being a smooth function there should be no problem in returning a solution. However, if we attempt a time reversal of a greater value than T then there is no solution. Hence it is easily the case that an apparently benign function g can have no inverse.

4. Operator-splitting methods

In this section we turn to the main purpose of this paper: to describe and demonstrate the operator-splitting method form solving the inverse diffusion problem. The methods are derived through splitting the operator K . Just as the Tikhonov method (5) is analogous to the minimum norm solution of a rank deficient matrix, operator-splitting methods are similar to the Jacobi and related methods for the iterative solution of a linear system of equations. Operator-splitting methods are related to the *defect correction method* [13] and it is more commonly known as Landweber iteration, as considered in Chapter 6 of Engl et al. [2].

4.1. General derivation of the operator-splitting methods

In general, the method is initiated by determining that the solution belongs to a particular space of functions $Z \subseteq X$. Let the operator $B : Y \rightarrow Z$ be a mapping that forms an approximate inverse to the operator K . Applying the operator B to both sides of (1) gives

$$BKf = Bg. \tag{9}$$

Let us split the operator BK in (9), giving the following

$$\{I + (BK - I)\}f = Bg. \quad (10)$$

The $I : X \rightarrow Z$ in (10) is a generalised identity operator; $If^* \in Z$ is equivalent to the function $f^* \in X$ and I is surjective.

The following iterative solution method follows from operator-splitting:

$$If^{(0)} \leftarrow Bg, \quad (11)$$

$$If^{(n)} \leftarrow Bg + (I - BK)f^{(n-1)}. \quad (12)$$

The right-hand sides of the operation (12) can always be evaluated, provided the action of the operators B and K can be simulated. Since I is surjective its inverse exists and the solutions $f^{(0)}, f^{(1)}, \dots$ can be obtained from (11) and (12). It should be noted that the operator K could be non-linear (as could the operator B), in such cases the operators should exhibit their dependence on f .

In the method (11) and (12), a priori information about the nature of the solution is communicated to the successive approximations through the choice of the operator B and in particular its range Z . The selection of Z is crucial in determining the nature of the inverse solution, ensuring that the iteration (12) returns a physically acceptable solution in a pre-determined form. It is through the specification of Z that the *nearby problem* is determined in the operator-splitting method; the solution is not sought in its original space X but in the subspace Z . The technique can include that of *regularization by projection* (see [5] for example), in which Z is a space of finite-dimensional approximations.

4.2. Jacobi-like method

For most of the remainder of this paper, a particular example of the inversion method described in the previous section will be investigated. The approximate inverse operator B is taken to be the identity operator $Y \rightarrow Y$ (i.e., $Z = Y$). It will be demonstrated that this approximate inverse leads to an effective solution method.

In this case the method (11) and (12) simplifies to the following

$$\begin{aligned} If^{(0)} &\leftarrow g, \\ If^{(n)} &\leftarrow g + (I - BK)f^{(n-1)}. \end{aligned} \quad (13)$$

The successive solutions $If^{(n)}, n = 0, 1, 2, \dots$ all lie in the space Y , the same space as g . Recall from the discussion in Section 3.3 that the function g lies in a smoother space than the function f (ignoring the possibility of noise). Hence this method has the inbuilt property of returning a smooth solution.

In choosing the operator B to be the identity operator, the method exploits the property that the diffusion operator simply spreads the distribution and its effect is thus reasonably close to the identity operator. In operator terms, in the model problem of Section 3, choosing the identity operator for B is equivalent to approximating the Gaussian-like kernel of the diffusion operator by the Dirac delta

$$g(x) = \frac{1}{2\sqrt{\pi T}} \int_{-\infty}^{\infty} \exp \left\{ \frac{-(x-y)^2}{4T} \right\} f(y) dy \approx f(x) = \int_{-\infty}^{\infty} \delta(x-y) f(y) dy.$$

4.3. Comparison with Jacobi iteration

The operator splitting method with B as the identity operator is analogous to the Jacobi method for the solution of a linear system of equations. Reconsider the discrete form of the operator Eq. (1) and its discretisation as typified by the model problem in Section 3. We note that the diffusion problem can be written in the discrete form as a linear algebraic equation of the form

$$K\underline{f}^* = \underline{g}.$$

Let us split the matrix K into its diagonal and non-diagonal components so that

$$K = D + L + U,$$

where D is a diagonal matrix, L is lower triangular and U is upper triangular. Provided the diagonal elements are non-zero (as they must be for the Jacobi method) then by dividing each row of K by the diagonal element then we can rewrite the equation above with D as the identity matrix, without loss of generality. The Jacobi method then involves the iteration

$$D\underline{f}^{(n)} = \underline{g} - (L + U)\underline{f}^{(n-1)}.$$

Hence the application of the Jacobi method to the linear system of equations arising from the solution of the operator equation is equivalent to the operator-splitting method described in the previous subsection.

5. Analysis of the method for the model problem

In this section the properties of the operator-splitting method of the previous section are considered. In particular the convergence of the Jacobi-like method on the model problem is analysed.

5.1. Properties of the general method

Returning to the general operator-splitting method of Section 4.1, since the operator B of the previous section is an approximate inverse of K , then it is helpful to write

$$BK = I - R, \tag{14}$$

where $R : X \rightarrow Z$ can be regarded as the residual operator. It follows from (12) that

$$If^{(n)} = Rf^{(n-1)} + Bg \tag{15}$$

and that

$$If^{(n)} = (I^* + R + R^2 + \dots + R^{(n-1)})Bg, \tag{16}$$

where $I^* : Z \rightarrow Z$ is the identity operator. The series (16) is a Neumann series. The iterative method would always converge if $\|R\| < 1$, in which case (15) would be a contraction mapping and $Kf = g$ would have a unique solution.

If the function g has been obtained through applying the operator K to a function f then substituting Kf for g in (16) gives

$$If^{(n)} = (I^* + R + R^2 + \dots + R^{(n-1)})BKf$$

and hence that

$$\begin{aligned} If^{(n)} &= (I^* + R + R^2 + \dots + R^{(n-1)})(I - R)f \\ &= (I - R^n)f. \end{aligned}$$

It follows that the error $d^{(n)}$ in the approximation to f in the n th iterate is given by

$$Id^{(n)} = I(f - f^{(n)}) = R^n f \quad (17)$$

and the error $e^{(n)}$ in the corresponding approximation to g is

$$e^{(n)} = g - g^{(n)} = KI^{-1}R^n f. \quad (18)$$

5.2. Fourier analysis and the Jacobi-like method

Returning to the simple diffusion equation of Section 3, recall that the eigenvalues are $e^{-N^2\pi^2T}$ and hence they cluster and tend towards zero as $N \rightarrow \infty$. It follows that the corresponding $r_N = 1 - k_N$ lie in $[0, 1]$ and tend towards unity as $N \rightarrow \infty$. Thus, as a result of this, R is not a strict contraction mapping.

Let us now consider the domain of the diffusion equation to be $(x, t) \in [0, 1] \times [0, T]$ with $u(x, 0) = f(x)$, $u(x, T) = g(x)$ and $u(0, t) = u(1, t) = 0$. Given any particular eigenfunction $f_N = \sin(N\pi x)$, it follows from (18) that the error in iterate n is

$$d_N^{I(n)} = f_N - f_N^{(n)} = r_N^n f_N = (1 - e^{-N^2\pi^2T})^n \sin(N\pi x) \quad (19)$$

and

$$e_N^{I(n)} = g_N - g_N^{(n)} = k_N r_N^n f_N = e^{-N^2\pi^2T} (1 - e^{-N^2\pi^2T})^n \sin(N\pi x). \quad (20)$$

The eigenvalues of the model problem converge rapidly to zero. If λ is the eigenvalue corresponding to $N = 1$ then the complete set of eigenvalues form the sequence $\lambda, \lambda^4, \lambda^9, \lambda^{16}, \dots$ and these correspond to the eigenfunctions $\sin(\pi x), \sin(2\pi x), \sin(3\pi x), \sin(4\pi x), \dots$. Hence if the first eigenvalue is 0.9 then the simple diffusion equation (6) has eigenvalues 0.900000, 0.656100, 0.387420, 0.185302, 0.071790, 0.005726, 0.001179, 0.000197, 0.000026, ... to six decimal places. If the first eigenvalue is 0.5 then the eigenvalues are 0.500000, 0.062500, 0.001953, 0.000015, ... Since $r_N = 1 - k_N$ then the sequence $r_N, N = 1, 2, \dots$ converges quickly to N . It follows that the error term converges much more slowly to zero for the higher eigenfunctions. For example if the eigenvalues are 0.500000, 0.062500, 0.001953, 0.000015 then the r_N are 0.500000, 0.937300, 0.998047, 0.999985, ... In order to return a relative error of less than 1% the number of iterations required is 6, 71, 2355 and 30 7009 for the first four eigenfunctions. Test problems demonstrating

the convergence rates of the method on the eigenfunctions of the model problem are given in the next section.

5.3. Fourier analysis and the Jacobi-like method

The analysis of the previous section suggests that progress towards the inverse solution of the first eigenfunction of K is relatively rapid, with the rate of convergence declining as we pass through the eigenfunctions. The slower rate of convergence of the higher eigenfunctions is a positive property of the method: potentially, the iteration could be terminated before the higher eigenfunctions (ultimately the noise) affect the solution. For example the iteration could be terminated once iterate $f^{(n)}$ has the property that

$$\|Kf^{(n)} - g\| < \varepsilon,$$

where ε represents the uncertainty in g as a result of measurement or numerical error.

It is in this respect that the method is similar to the truncated eigenfunction expansion method described in Section 2.3. However, in this method the involvement of the higher eigenfunctions is naturally delayed in the method, rather than being deliberately removed.

6. Test problems and results

The Jacobi-like operator-splitting method described in the previous section is applied to a range of test problems in this section. To begin with, the method is used to solve the model diffusion problem (6) for Fourier components, then for a general function. However, the method is applicable to non-linear diffusion problems and results from the application of the method to such problems are also given.

As explained in the previous section, the operator-splitting methods require the numerical modelling of the forward operator K . For the test problems of this section the parabolic partial differential equations that represent the forward operator are discretised and solved using a finite difference method. An Excel spreadsheet with which the operator-splitting method can be directly tested is available through the *inverse problems* page of www.scientific-computing.info.

In the figures that follow the original function f is represented by the full line. The function g is the most damped dashed line. The other dashed lines follow the steady progress towards the inverse solution using the operator-splitting method. The number of iterations that each line represents can be worked out from the caption at the top of the figure.

6.1. Inverse solution of model equation for Fourier components

Fig. 2 shows the convergence of the inversion method on the first eigenfunction $\sin(\pi x)$ of the model diffusion equation (6) where the total diffusion is such that the amplitude is exactly halved (i.e., $\lambda = 0.5$). Recall that in the method that g is the first estimate of f .

Fig. 3 shows the results from the application of the method to $f(x) = (1/2)(\sin(\pi x) + \sin(\pi 3x))$. In this case g is not visibly distinguishable from g in Fig. 2 once the factor of 1/2 is taken into account. The results from the iteration show how the method initially pursues the solution of the first eigenfunction and then goes on to modify this with the third eigenfunction.

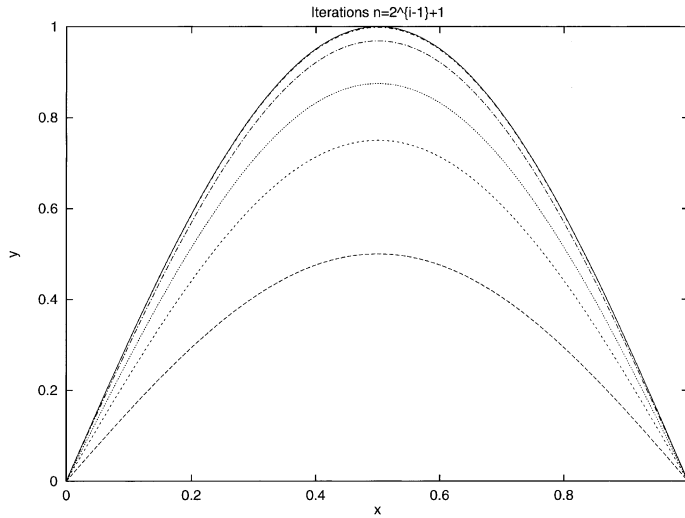


Fig. 2. Iterations for $f = \sin(\pi x)$, for the simple diffusion equation, $T = (\log 2)/\pi^2$.

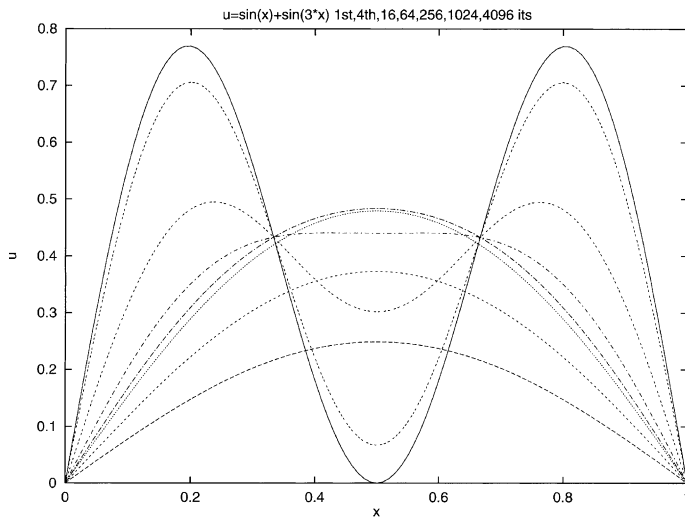


Fig. 3. Iterations for $f = 1/2(\sin(\pi x) + \sin(3\pi x))$, for the simple diffusion equation, $T = \log 2/\pi^2$.

6.2. Inverse solution of model equation for general functions

In Fig. 4 the method is applied to the inverse solution of the model problem with the original f being a \sin^2 function and the total diffusion being one-tenth that in the tests of Figs. 2 and 3. In this case, as in the case of functions that are not finite eigenfunction expansions, convergence to the original f is not observed.

In Fig. 5 the method is applied to a problem where the original f is a higher frequency \sin^2 function. The total diffusion in obtaining the $g(=f^{(0)})$ is just one-fortieth of the total diffusion

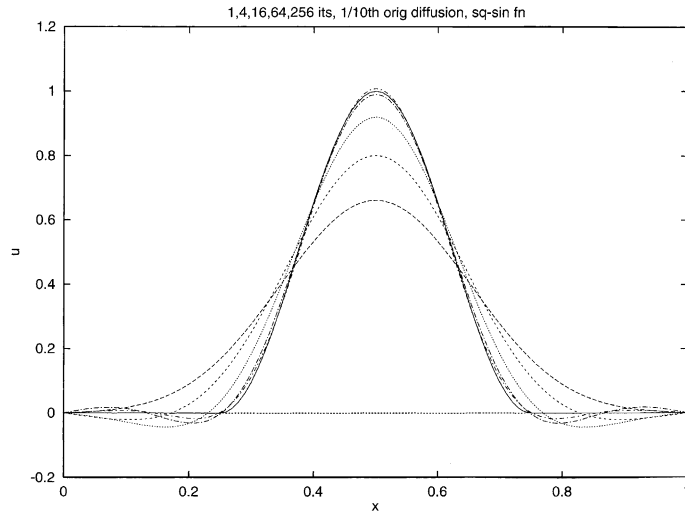


Fig. 4. Iterations for f , a \sin^2 function on $[0.25, 0.75]$, for the simple diffusion equation, $T = \log 2/(10\pi^2)$.

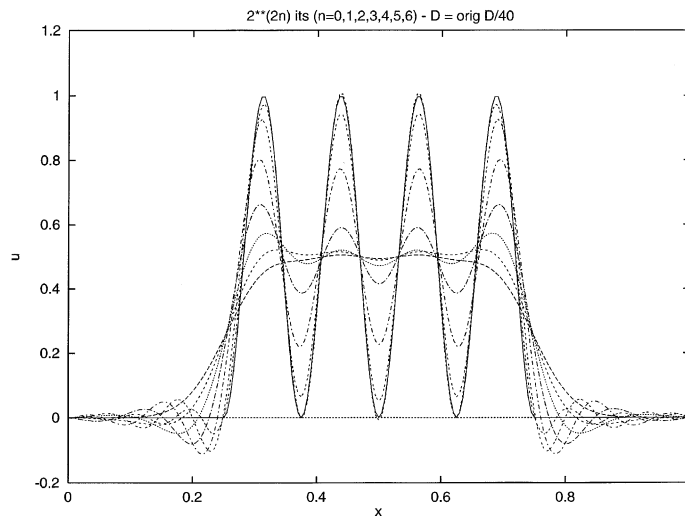


Fig. 5. Iterations for f , a \sin^2 function on $[0.25, 0.75]$, for the simple diffusion equation, $T = \log 2/(40\pi^2)$.

applied in Figs. 1–4. Even so, as has been observed earlier, higher frequencies decay much faster in the forward operation and most of the characteristics of f are apparently lost in g . However, the iterative solutions in the inversion method demonstrates that much of the quality of the original f can be recovered.

In Fig. 6 the inversion method is applied to a square wave. In this test problem the total diffusion is again one-tenth of that applied in Figs. 2 and 3. The figure shows that the original f is

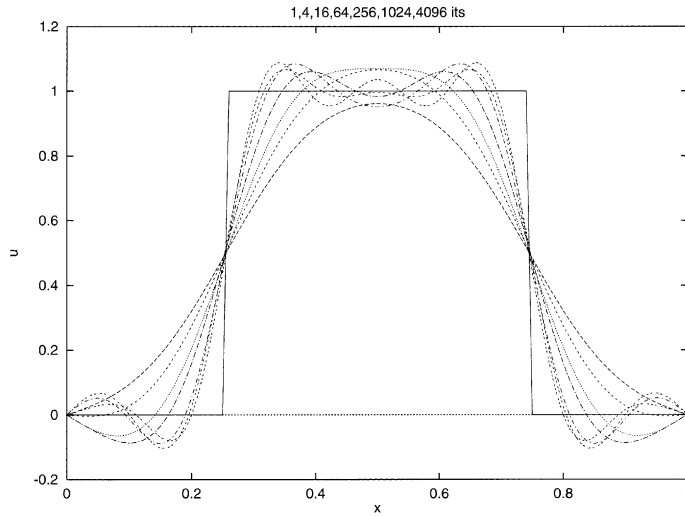


Fig. 6. Iterations for f , a square wave, for the simple diffusion equation, $T = \log 2/(10\pi^2)$.

discontinuous but g is a smooth function. As discussed earlier, the solution of the operator-splitting method mimics a truncated eigenfunction expansion and there is a similarity between the iterative solutions and those observed when fitting a square wave with a Fourier series.

6.3. Inverse solution of non-linear diffusion equation

In Figs. 7 and 8 the examples of Figs. 4 and 5 are repeated but this time with K a non-linear operator. In these cases $D = D(u) = 3/2 - u$. The same size and number of time steps are taken in

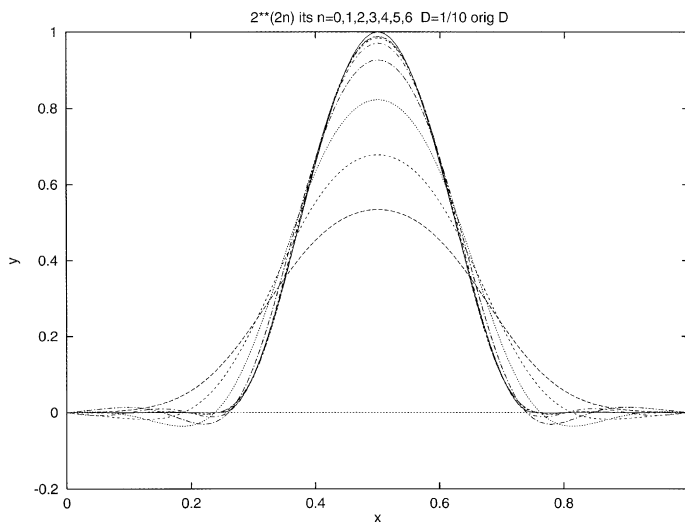


Fig. 7. Iterations for f , a \sin^2 function on $[0.25, 0.75]$, for the diffusion equation with $D = 3/2 - u$, $T = \log 2/(10\pi^2)$.

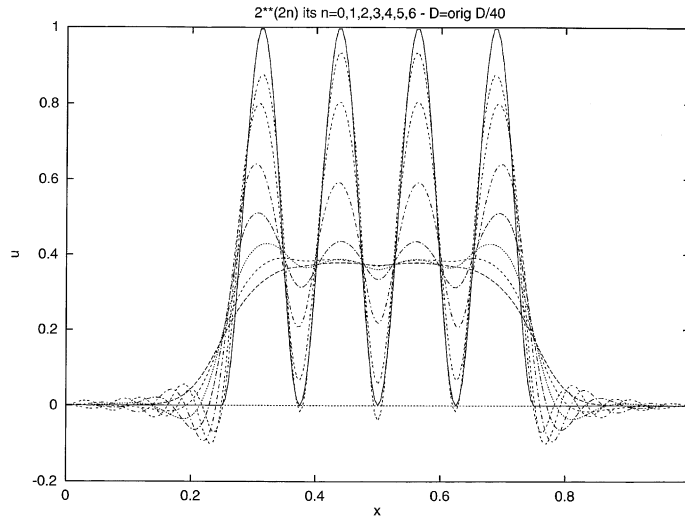


Fig. 8. Iterations for f , a \sin^2 function on $[0.25, 0.75]$, for the diffusion equation with $D = 3/2 - u$, $T = \log 2/(40\pi^2)$.

these examples as are taken in Figs. 4 and 5, respectively. Hence the total diffusion in the corresponding examples is approximately the same.

7. Concluding discussion

The general operator-splitting method of Section 5.1 provides a versatile means of solving inverse diffusion problems. It is for the method-developer to determine the approximate inverse operator B , and in doing so the nature of the inverse solution is determined.

A general error analysis of the operator-splitting method is given in Section 5.1. The error in the n th iterate is $R^n f$, but the fact that R is not necessarily a contraction simply reflects the ill-posedness of the original problem. In the case of the simple diffusion equation and provided f can be written as a finite sum of the first m Fourier components it is shown that

$$\|R\| = r_m = (1 - e^{-m^2\pi^2 T}) < 1$$

and hence that R is a contraction in this situation. Fig. 3 demonstrates the recovery of the original f when $m = 3$.

In practice g is measured data from a practical experiment and the forward operator used in the inversion method is a model and hence at a precise representation of the operator K . An extension of the analysis of this paper, examining the effect of an imprecise operator K , would also be of value.

The Jacobi-like operator-splitting method is a simple and remarkably effective method for solving inverse diffusion problems. In effect the method is similar to the method of partial eigenfunction expansion considered in Section 2.3, except for the important distinction that the former is applicable to non-linear as well as linear problems. In this paper results from a number of test problems have been used to demonstrate the effectiveness of the operator-splitting method

with $B = I$. The operator-splitting method has been successfully applied to practical problems by the authors [6].

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