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Abstract

A method is presented in this paper for estimating solutions of ill–posed problems in the form of Fredholm integral equations of the first kind, given noisy data. In this paper we consider the method of constrained regularization for the numerical solution of Fredholm convolution equations of the first kind. In this method optimal amount of smoothing may be computed, based on the data and the assumed known noise variance.

AMS(MOS) Subject Classification: 65R20, 45A05, 65R30, 45B05, 45D05

Key Words Constrained regularization, Fourier extrapolation, convolution equation, cross-validation, filter function.

1. Introduction.

Inverse problems posed as Fredholm integral equations of the first kind are common, but their solution is among the more difficult tasks of numerical mathematics. A subset of these problems is the Fourier convolution type equations

$$g(x) = \int_{-\infty}^{\infty} k(x-y)f(y)dy \tag{1.1}$$

where $g(x)$ is given as data and $k(x)$ is a given analytic function. ¿From a computational point of view the most serious problem with (1.1) is that it is ill–posed, i.e., small variations in g can produce large variations in f, when g is given as experimental (noisy) data.

For many years ill–posed problems have been considered as mere mathematical anomalies. However it appeared in early sixties that this attitude was erroneous and that many ill–posed problems, generally inverse problems [10], arose from practical situations. Nowadays, a systematic study of these problems has undoubtedly proved of great relevance in many fields of applied physics [4, 5, 9].

The use of constraints in solving Fredholm integral equations of the first kind has been investigated by several authors [2, 3, 5, 8, 10, 11, 12, 13, 17, 19]. It has become apparent that the need for constrained information depends on the degree of ill–posedness of the problem as characterized by the decay rate of the kernel spectrum and also the smoothness of the solution. Thus for mildly ill–posed problems, optimal smoothing methods are often sufficient in themselves to give satisfactory numerical solutions, but the negative lobes are there [14, 15]; on the other hand, for severely ill–posed problems, the improvements introduced by positivity constraints have been clearly demonstrated in this paper.

2. Description of the Method

We estimate the solutions of (1.1) where we know in advance that f is nonnegative and hence our estimate $\underline{f}_N$ is constrained to be nonnegative.

Let $\underline{f}_N = (f(x_0), f(x_1), \dots f(x_{N-1}))^T$ and consider the p–th order regularization functional in T_N (trigonometric polynomials of degree at most N),

$$C(\underline{f}_N; \lambda) = \|\hat{K}\psi^H \underline{f}_N - \psi^H \underline{g}_N\|_2^2 + \lambda \underline{f}_N^H \psi \hat{J} \psi^H \underline{f}_N \qquad (2.1)$$

where

$$\hat{K} = \psi^H K \psi$$

and

$$\hat{J} = \mathrm{diag}[(i\tilde{\omega}_q)^{2p}] \qquad (2.2)$$

where ^ denotes the Fourier transform and

$$\tilde{\omega}_q = \begin{cases} \omega_q, & 0 \le q < \frac{1}{2}N \\ \omega_{N-q}, & \frac{1}{2}N \le q < N-1 \end{cases}$$

and $\omega_q = \frac{2\pi q}{T}$ where T is the period $= Nh$ and N is the number of data points. ψ represents the DFT (Discrete Fourier Transform) matrix in equation (2.1) and ψ^H is the Inverse DFT., i.e., $\psi\psi^H = \psi^H\psi = I$ and $\psi_{rs} = \frac{1}{\sqrt{N}} \exp\left(\frac{2\pi i}{N} rs\right), \quad r, s = 0, 1, 2, \dots, N-1.$

Let $\underline{f}_\lambda$ be the minimizer of (2.1) subject to $\underline{f}_N \ge \underline{0}$, with components $f_{\lambda,n}$. The indices $n_1, n_2, \dots, n_L$ for which $f_{\lambda,n} \ge 0$ are an important class for many physical applications, e.g., density functions, and are first determined. These constraints have been applied to problems in image restoration by Thompson

[12, 13] and with prior choice of smoothing. Let E be the $N \times L$ indicator matrix of indices $n_1, n_2, \ldots, n_L$, that is E has a unit element in m–th row and n–th column if $m = n_j,\ j = 1, 2, \ldots, L$ and zeros elsewhere. Let $N = 4$ and $L = 2$. Further let A be a 4×4 circulant matrix, $A = \begin{bmatrix} a_0 & a_1 & a_2 & a_3 \\ a_3 & a_0 & a_1 & a_2 \\ a_2 & a_3 & a_0 & a_1 \\ a_1 & a_2 & a_3 & a_0 \end{bmatrix}$ and $E = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$. Then $AE = \begin{bmatrix} a_0 & a_2 \\ a_3 & a_1 \\ a_2 & a_0 \\ a_1 & a_3 \end{bmatrix}$ and $E^H AE = \begin{bmatrix} a_0 & a_2 \\ a_2 & a_0 \end{bmatrix}$ which is circulant. In what follows we denote by I the set of indices $(n_1, n_2, \ldots, n_K)$ of inactive constraints.

The constrained minimizer of (2.1) is

$$\underline{f}_\lambda = E(E^H \psi \hat{K}^H \hat{K} \psi^H E + \lambda E^H \psi \hat{J} \psi^H E)^{-1} E^H \psi \hat{K}^H \psi^H \underline{g}_N. \qquad (2.3)$$

Defining $\underline{g}_\lambda = K \underline{f}_\lambda$, there exists an $N \times N$ influence matrix $A_L(\lambda)$ satisfying $\underline{g}_\lambda = A_L(\lambda) \underline{g}_N$. It can be shown that

$$A_L(\lambda) = \psi \hat{K} \psi^H E \left(\sum_K + \lambda \sum_J \right)^{-1} E^H \psi \hat{K}^H \psi^H \qquad (2.4)$$

where

$$\sum_K = E^H \psi \hat{K}^H \hat{K} \psi^H E$$

and

$$\sum_J = E^H \psi \hat{J} \psi^H E$$

with the property that

$$\text{Trace}(I - A_L(\lambda)) = N - L + \lambda \ \text{Trace}(B) \qquad (2.5)$$

where

$$B = \sum_J \left(\sum_K + \lambda \sum_J \right)^{-1}.$$

Wahba [17, 18, 19] argues that the optimal λ in the constrained setting may be found by minimizing

$$V(\lambda) = \frac{\|\hat{K}\psi^H \underline{f}_\lambda - \psi^H \underline{g}_N\|^2}{\left[\frac{1}{N}(N - L + \lambda \text{ Trace } (B)\right]^2}. \tag{2.6}$$

Clearly $\underline{f}_\lambda$ depends nonlinearly on E as well as on λ and so E must be recomputed whenever $\underline{f}_\lambda$ is computed. These iterations can be computationally expensive. Moreover $V(\lambda)$ in (2.6) need not be a continuous function of λ.

For given λ, Wahba [17, 18] uses a quadratic programming algorithm to minimize (2.1) subject to $\underline{f}_N \geq \underline{0}$. A unique minimum always exists (Butler [2]). Having found E and f_λ, she then computes B by solving the L linear system.

We observe that

$$\psi(\hat{K}^H \hat{K} + \lambda \hat{J})\psi^H \tag{2.7}$$

is a circulant matrix, so is $\sum_K + \lambda \sum_J$ (see the expressions of $\sum_K$ and $\sum_J$ on page 4) and consequently $E(\sum_K + \lambda \sum_J)^{-1} E^H$ is also circulant. Thus in equation (2.4) $A_L(\lambda)$ is clearly circulant.

In principle, we can use the L–dimensional DFT (Discrete Fourier Transform) to evaluate $A_L(\lambda)$, thus avoiding the necessity of solving the L–linear system in equation (2.7), which is computationally an expensive procedure.

Now consider

$$\hat{K}\psi^H E(\sum_K + \lambda \sum_J)^{-1} E^H \psi \hat{K}^H = \text{ diag } (\tilde{z}_{q;\lambda}) \tag{2.8}$$

where

$$\tilde{z}_{q;\lambda} = \begin{cases} z_{q;\lambda}, & q \in I \\ 0, & q \notin I \end{cases}$$

and

$$z_{q;\lambda} = \frac{|\hat{K}_{N,q}|^2}{|\hat{K}_{N,q}|^2 + N^2\lambda\tilde{\omega}_q^{2p}} \tag{2.9}$$

$\hat{K}_{N,q} = \sum_{n=0}^{N-1} K_n \exp(-i\omega_q x_n)$, $p = 2$ and λ the regularization parameter to be determined.

¿From equations (2.7) and (2.8), it follows that

$$A_L(\lambda) = \psi \text{ diag } (\tilde{z}_{q;\lambda})\psi^H$$

and so from equation (2.6) we have

$$V(\lambda) = \frac{\frac{1}{N}\left[\sum_{q\in I}(1 - z_{q;\lambda})^2|\hat{g}_q|^2 + \sum_{q\notin I}|\hat{g}_q|^2\right]}{\frac{1}{N}\left[N - L + \sum_{q\in I}(1 - z_{q;\lambda})^2\right]}. \tag{2.10}$$

We minimize $V(\lambda)$ in equation (2.10) by making a linear search in λ. The function is not always continuous because the index I changes with λ. At each step we minimize $C(\underline{f}_N; \lambda)$ in equation (2.1) subject to nonnegativity constraints using NAG quadratic programming subroutine E04LBF, which yields the index set I for any given λ. All calculations are done using double precision because the examples tested are severely ill–posed. When a minimizing value of λ is found, the corresponding $\underline{f}_\lambda$ is given by NAG subroutine E04LBF. We conclude that the indicator set I plays a key role in the algorithm. It affects the filter function $z_{q;\lambda}$ and ultimately affects the expression for $V(\lambda)$.

3. Optimal Convergence.

Here we shall discuss the optimal convergence of the case of convolution equation

$$\int_0^T k(x-y)f(y)dy = g(x) \tag{3.1}$$

in which the function k is periodic with period T, expanding k in a Fourier series

$$k(x-y) = \sum_{q=-\infty}^{\infty} \hat{k}_q \exp\left(\frac{2\pi i}{T}q(x-y)\right) \tag{3.2}$$

where $\hat{k}_q$ is the Fourier coefficient, i.e.,

$$\hat{k}_q = \int_0^T k(y)\exp\left(\frac{2\pi i}{T}qy\right)dy = \overline{\hat{k}}_{N-q}\,. \tag{3.3}$$

We shall assume that

$$|\hat{k}_q| \simeq q^{-\ell} \quad \ell > 1, \qquad [6]$$

and so the Fourier series is uniformly convergent.

4. Test Problems

Problem 1: This problem has been taken from Phillips [10] and Judith [8] and has a noisy data function g with a maximum absolute error of about 0.7%. The noise results purely from quadrature errors. The equation is

$$\int_{-30}^{30} K(x-y)f(y)dy = g(x) \tag{4.1}$$

where $K(x), g(x)$ and $f(x)$ are given in Table 1. The number of grid points $= N = 32$.

Problem 2. This problem has been taken from Turchin [14]. It is modified to take the wider kernel to make the problem severely ill–posed. We have

$$\int_{-3.2}^{3.1} K(x-y)f(y)dy = g(x) \tag{4.2}$$

where f is the sum of the two Gaussian functions

$$f(x) = 0.5\exp\left[-\frac{(x+0.4)^2}{0.18}\right] + \exp\left[\frac{(x-0.6)^2}{0.18}\right] \tag{4.3}$$

with essential support $-1.7 < x < 1.5$. By the essential support of $f(x)$, we mean that part of its domain for which $|f(x)| > \epsilon$ where $\epsilon \geq 0$ (is small) e.g. $\epsilon = 1\%$ of $\max|f(x)|$.

The kernel $K(x)$ is given by

$$K(x) = \begin{cases} (5/12)(-x+1.2) & , \quad 0 \leq x < 1.2 \\ (5/12)(x+1.2) & , \quad -1.2 \leq x < 0 \\ 0 & , \quad |x| \geq 1.2 \end{cases} .$$

Also the essential support of $g(x)$ is $-2.5 < x < 2.7$. The number of grid points $= N = 64$, $g(x)$ is given in Table 1 as as an experimental data.

5. Addition of Random Noise to the Data Function

In solving Problem 2, we have considered the data functions contaminated by varying amounts of random noise. To generate a sequence of random errors of the form $|\epsilon_n|$, $n = 0, 1, 2, \ldots, N-1$, we have used the NAG Algorithm G05DAA which returns pseudo–random real numbers taken from a normal distribution of prescribed mean A and standard deviation B.

To mimic experimental errors we have

$$A = 0 \text{ and } B = \left(\frac{x}{100}\right)\left(\max_{0\leq n\leq N-1} |g_n|\right) \tag{5.1}$$

where X denotes a chosen percentage, e.g., 0.7, 1.7 and 3.3. Thus the random error ϵ_n added to g_n, does not exceed $3X\%$ of the maximum value of $g(x)$.

6. Numerical Results

In this section we describe the application of the two methods discussed in sections 2 and 3, over the same test problems enlisted in section 4.

Problem 1.

Constrained Method. This method worked very well and the results are shown in Table 2 and Fig. (1).

Problem 2

Constrained Method. This is a severely ill–posed problem. For accurate data the method yielded perfect solution resolving the two peaks very clearly.

(i) With 0.7% noise level, the constrained method gave a very good result as shown in Table 2 and Fig. (2).

(ii) With 1.7% noise level, again the constrained method yielded a very good result as shown in Table 2 and Fig. (3).

(iii) With 3.3% noise level, the constrained method performed reasonably well and the result is shown in Table 2 and Fig. (4).

7. Concluding Remarks

1. The constrained regularization method worked very well for severely ill–posed problems, even with higher levels of noise. In fact, the constrained method can cope with noise level equal to about 10% in severely ill–posed problems and yielded exceedingly excellent results as shown in Table 2 and in Figs. 1-4.

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Table 1

x_n	g_n	k_n	f_n
−30.0	0.0100	0.1184	0.0000
−28.0	0.0110	0.1311	0.0000
−26.0	0.0100	0.1464	0.0000
−24.0	0.0170	0.1651	0.0000
−22.0	0.0305	0.1883	0.0006
−20.0	0.0405	0.2179	0.0000
−18.0	0.0585	0.2563	0.0000
−16.0	0.0869	0.3077	0.0000
−14.0	0.1309	0.3788	0.0000
−12.0	0.2018	0.4816	0.0000
−10.0	0.3235	0.6380	0.0000
−8.0	0.5469	0.8914	0.0000
−6.0	0.9621	1.3333	0.0019
−4.0	1.6301	2.1483	0.0345
−2.0	2.4047	3.5103	0.0965
0.0	2.9104	4.3600	0.1321
2.0	2.8912	3.0628	0.1096
4.0	2.4586	1.6329	0.0584
6.0	1.9049	0.8806	0.0349
8.0	1.4144	0.5095	0.0173
10.0	1.0282	0.3137	0.0107
12.0	0.7411	0.2021	0.0028
14.0	0.5409	0.1341	0.0005
16.0	0.4083	0.0906	0.0000
18.0	0.3214	0.0906	0.0000
20.0	0.2623	0.0413	0.0000
22.0	0.2201	0.0269	0.0000
24.0	0.1580	0.0089	0.9000
26.0	0.1886	0.0165	0.0000
28.0	0.1270	0.0031	0.0000
30.0	0.0780	0.0013	0.0000

Table 2

Constrained Regularization Method

Test Problem	N	Noise Level	λ	$\|f - f_\lambda\|_2$	Figures
Problem 1	32	0.7%	1.0×10^{-4}	1.793×10^{-2}	1
Problem 2	64	clean data	2.10×10^{-15}	6.81×10^{-3}	2
Problem 2	64	0.7%	1.614×10^{-9}	4.79×10^{-2}	2
Problem 2	64	1.7%	7.402×10^{-9}	7.511×10^{-2}	3
Problem 2	64	3.3%	1.296×10^{-8}	1.005×10^{-1}	4

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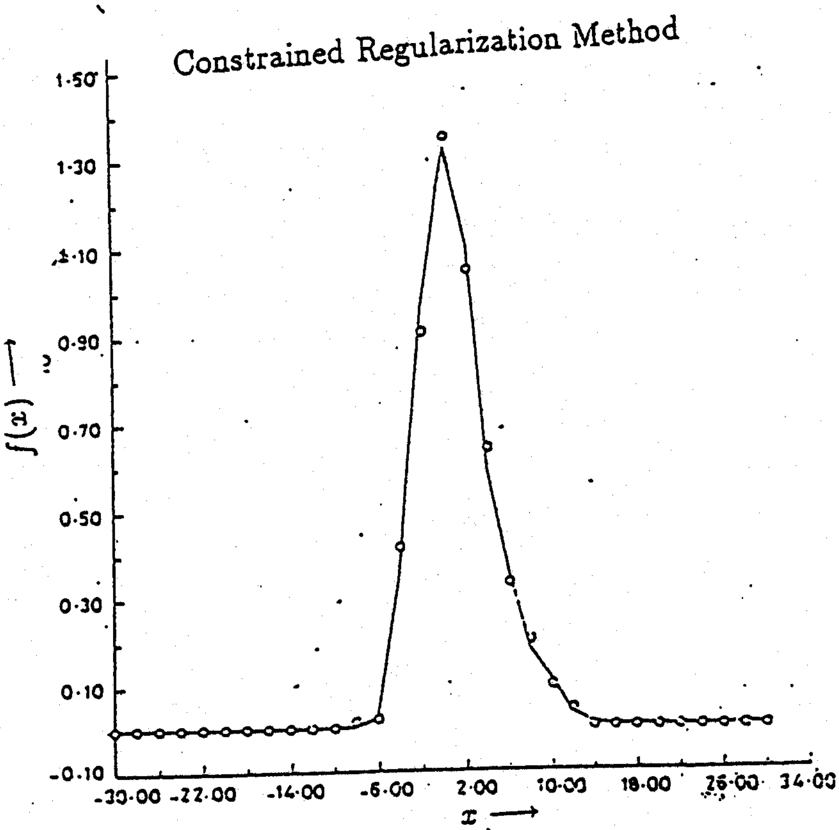

Fig (1) TRUE SOL.
SOL. FOR 0·7% ERROR

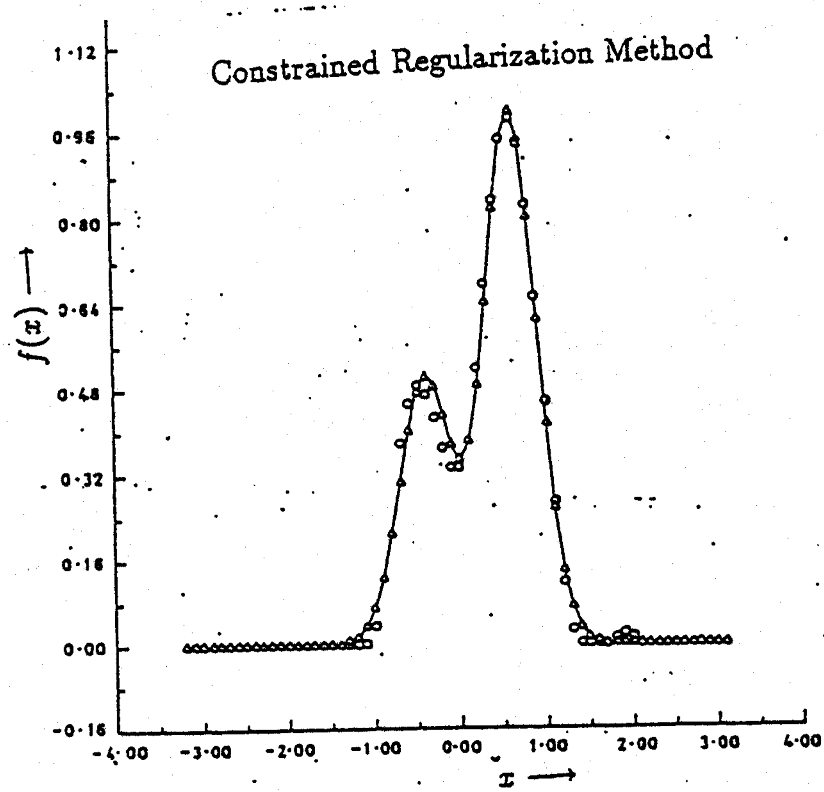

Fig (2) TRUE SOL.
NUM. SOL. CLEAN DATA
SOL. FOR 0·7% ERROR

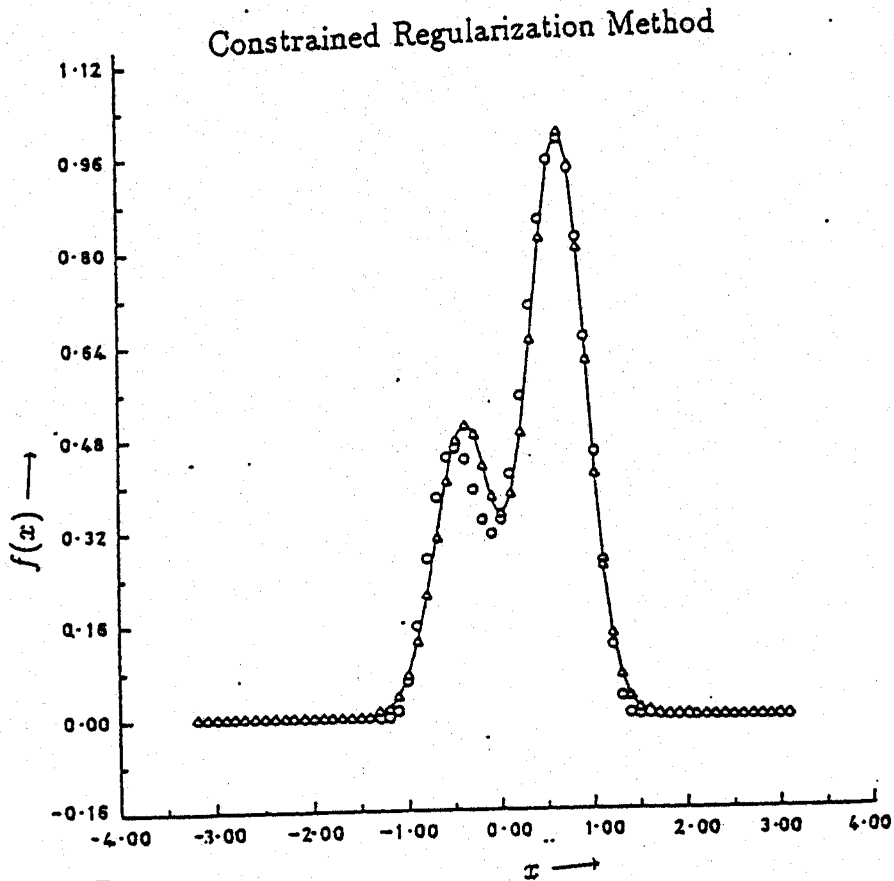

Fig (3) TRUE SOL. ——— NUM. SOL. CLEAN DATA △ △ △ SOL. FOR 1·7% ERROR ○ ○ ○

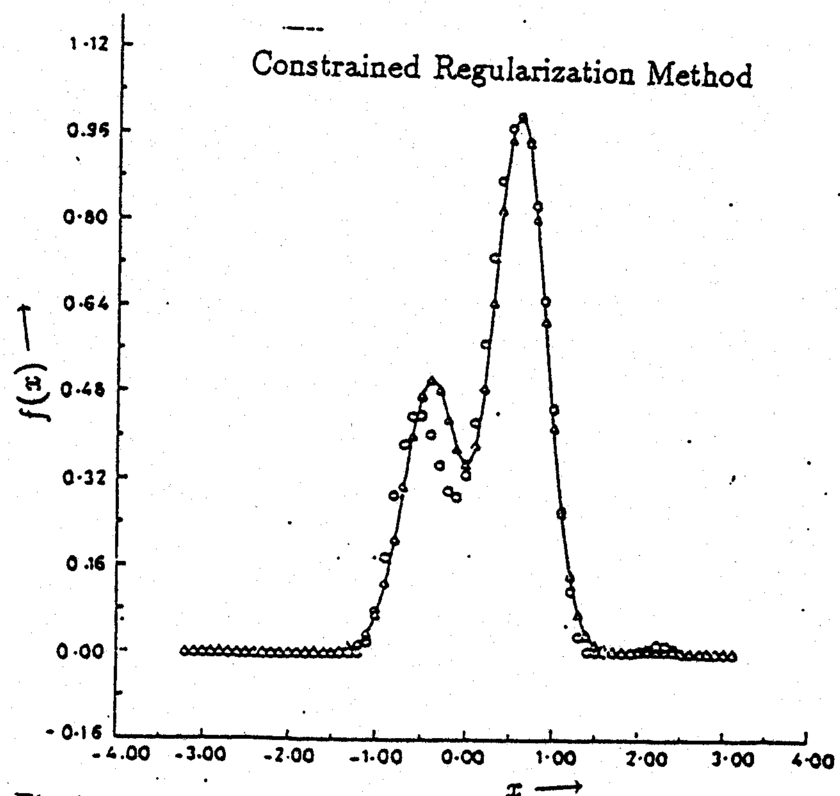

Fig (4) TRUE SOL. ——— NUM. SOL. △ △ △ SOL. FOR 3.3% ERROR = ○ ○ ○