King Fahd University of Petroleum & Minerals

DEPARTMENT OF MATHEMATICAL SCIENCES

Technical Report Series

TR 155

November 1993

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On the Spline Regularized Inversion of the Laplace Transform

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Abstract

In this paper we have discussed an algorithm to convert the Laplace transform into an integral equation of the first kind of convolution type, which is an ill–posed problem and used a spline regularization method to solve it.

The algorithm is applied to several examples taken from [2, 4, 5, 6, 10, 23], and in general, it gives a good approximation to the true solution. We investigated the behavior of the optimal regularization parameter and results are shown in the table and the diagrams.

AMS(MOS) Subject Classification 65R20, 65R30
Key Words Inversion of Laplace transform, ill–posed problem, convolution equation, cross validation, spline regularization, filter function.

1. Introduction.

There are many problems whose solution may be found in terms of a Laplace transform which is then, however too complicated for inversion using different methods. However, no single method gives optimum results for all purposes and all occasions. For a detailed bibliography, the reader should consult Piessens [14] and Piessens and Branders [15].

The problem of the recovery of a real function $f(t)$ $t \geq 0$, given its Laplace transform

$$\int_0^\infty e^{-st} f(t) dt = g(s) \tag{1.1}$$

for real values of s, is an ill–posed problem in the sense of Hadamard and is therefore affected by numerical instability. This difficulty is not very serious when $g(s)$ is also known for complex values of s. In such a case, several methods have been developed [4, 9, 10, 15, 16, 25] which, in general, work rather well even if they require a large computational cost and high precision arithmetic. For example, the Weeks method [25] and its variants [9, 15] use an expansion of $f(t)$ in terms of Laguerre polynomials and the analyticity properties of Laplace transform.

The ill–posedness of Laplace transform inversion in the case where $f \in L^2(R_+)$ and $g(s)$ is known for all real and positive values of s, can be investigated by means of the Mellin transform [1, 7, 10]. In practice, however, $g(s)$ is known only in a finite set of points. The case of an infinite set of equidistant points was investigated by Papoulis [12]. Several other methods have been proposed, and a review and comparison is given in Davies [4] and Talbot [21].

The previous methods do not include regularization techniques. Regularization methods have been discussed by Varah [23], Essah and Delves [6] and Davies [3]. The results of Varah are quite pessimistic. Regularization by means of truncated singular function expansion is investigated in Bertero [1]. Numerous methods are available in the literature for the numerical evaluation of the Laplace transform inversion which have been described by Schmittroth [18], Norden [11], Salzer [17], Shirtliffe and Stephenson [19].

2. Description of the Method

In (1.1) given $g(s)$, $s \geq 0$ we wish to find $f(t)$, $t \geq 0$ and $f(t) = 0$ for $t < 0$, so that (1.1) holds.

Frequently, $g(s)$ is measured at certain points. We assume $g(s)$ is given analytically with known $f(t)$, so that we can measure the error in the numerical solution.

We shall convert the Laplace transform into the first kind integral equation of convolution type. We make the following substitution in equation (1.1).

$$s = a^x \quad \text{and } t = a^{-y} \quad \text{where } a > 1 \tag{2.1}$$

Then

$$g(a^x) = \int_{-\infty}^{\infty} \log a e^{-a^{x-y}} f(a^{-y}) a^{-y} dy \tag{2.2}$$

Multiplying both sides of (2.2) by a^x we obtain the convolution equation

$$\int_{-\infty}^{\infty} K(x-y)F(y)dy = G(x), \quad -\infty \leq x \leq \infty \tag{2.3}$$

where

$$\left.\begin{array}{l} G(x) = a^x g(a^x) = sg(s) \\ K(x) = \log a a^x e^{-a^x} = \log a s e^{-s} \\ F(y) = f(a^{-y}) = f(t) \end{array}\right\} \tag{2.4}$$

In order that we can apply our deconvolution method to equation (2.3), it is necessary that $G(x)$ has essentially compact support, i.e., $G(x) \to 0$ as $x \to \pm\infty$ which is a property, we demand from our data function $G(x)$.

Let $B_j(H;x)$ be the n–th order cardinal B–spline (n even) with knots $(j - \frac{1}{2}n)H, \ldots, (j + \frac{1}{2}n)H$, i.e., $B_j(H;x) = Q_n(\frac{x}{H} - j + \frac{n}{2})$ where

$$Q_n(x) = \frac{1}{(n-1)!} \sum_{j=0}^{n} (-1)^j \binom{n}{j} ((x-j)_+^{n-1}. \tag{2.5}$$

In addition let $MH = 1$ where $M \leq N$ is an integral power of 2. We assume that $B_j(H;x)$ is periodically continued outside the interval $(0,T)$, with period T. Then $B_j(H;x)$ has a Fourier series

$$B_j(H;x) = \sum_{q=-\infty}^{\infty} \hat{B}_{jq} \exp(iw_q x) \tag{2.6}$$

where

$$\hat{B}_{jq} = \int_0^T B_j(H;x) \exp(-iw_q x) dx \tag{2.7}$$

and $w_q = \frac{2\pi q}{T}$.

Since $B_j(H;x)$ is simply a translation of $B_0(H;x)$ by an amount jH, we have

$$\hat{B}_{jq} = \hat{B}_{oq} \exp(-iw_q H)$$

where

$$\hat{B}_{oq} = H \left[\frac{\sin \frac{w_q H}{2}}{\frac{w_q H}{2}} \right]^4 \tag{2.8}$$

Tikhonov Regularization Using Cardinal Cubic B–splines

We shall approximate the convolution equation (2.3) by

$$\int_0^T K_N(x-y) F_M(y) dy = G_N(x) \tag{2.9}$$

where we assume that F, G and K have essentially finite support in $[0, T)$, F_M is a cubic spline ($n = 4$) of the form

$$F_M(x) = \sum_{j=1}^{M-1} \alpha_j B_j(H; x), \quad M \leq N \tag{2.10}$$

The real M dimensional vector

$$\underline{\alpha} = (\alpha_0, \ldots, \alpha_{M-1})^T$$

of unknown coefficients will be determined, the spline in equation (2.10) has the Fourier series

$$F_M(x) = \sum_{q=-\infty}^{\infty} \hat{F}^B_{M,q} \exp(i w_q x) \tag{2.11}$$

where

$$\begin{aligned} \hat{F}^B_{M,q} &= \sum_{j=0}^{M-1} \alpha_j \hat{B}_{jq} && (2.11a) \\ &= \hat{B}_{oq} \sum_{j=0}^{M-1} \alpha_j \exp\left(-\frac{2\pi i}{M} jq\right) \\ &= \sqrt{M} \hat{B}_{oq} \hat{\alpha}_s, \quad s = q (\operatorname{mod} M), && (2.12) \end{aligned}$$

where

$$\underline{\hat{\alpha}} = \psi^H_M \underline{\alpha} \tag{2.13}$$

We find it advantageous to determine $\underline{\hat{\alpha}}$ rather than $\underline{\alpha}$, because of the simple properties available in discrete Fourier spaces. The vector $\underline{\alpha}$ in equation (2.10) may then be determined from the inverse M-dimensional FFT

$$\underline{\alpha} = \psi_M \underline{\hat{\alpha}} \tag{2.14}$$

where ψ is the unitary matrix with elements

$$\psi_{rs} = \frac{1}{\sqrt{N}} \exp\left(\frac{2\pi i}{N} rs\right), \quad r, s = 0, 1, 2, \ldots, N-1$$

P–th Order Tikhonov Regularization [22].

Consider the smoothing functional

$$C(F_M;\lambda) = C(\underline{\alpha},\lambda) = \|K_N(x) * F_M(x) - G_N(x)\|_2^2 + \lambda\|F_M^{(P)}\|_2^2 \tag{2.15}$$

using Plancherel's theorem we have

$$\|K_N * F_M - G_N\|_2^2 = \frac{1}{N^2}\sum_{q=-\frac{1}{2}N}^{\frac{1}{2}N} |\hat{K}_{N,q}\hat{F}^B_{M,q} - \hat{G}_{N,q}|^2$$

Hence using equation (2.12)

$$\|K_N{*}F_M{-}G_N\|_2^2 = \frac{1}{N^2}\sum_{q=-\frac{1}{2}N}^{\frac{1}{2}N}\left[\left(\sqrt{M}\hat{B}_{oq}\hat{K}_{N,q}\hat{\alpha}_s - \hat{G}_{N,q}\right)\left(\sqrt{M}\,\hat{B}_{oq}\overline{\hat{K}}_{N,q}\overline{\hat{\alpha}}_s - \overline{\hat{G}}_{N,q}\right)\right] \tag{2.16}$$

where

$$s \equiv q(\operatorname{mod} M)$$

Also, Plancherel's theorem applied to the regularizing functional in equation (2.15) gives

$$\begin{aligned}\|F_M^{(P)}\|^2 &= \sum_{q=-\infty}^{\infty} w_q^{2p}|\hat{F}^B_{M,q}|^2 = 2\sum_{q=1}^{\infty} w_q^{2p}|\hat{F}^B_{M,q}|^2 \\ &= 2M\sum_{q=1}^{\infty} w_q^{2p}\hat{B}^2_{oq}|\hat{\alpha}_s|^2 \qquad \text{where } s \equiv (\operatorname{mod} M)\end{aligned} \tag{2.17}$$

The simplification of expression (2.17) requires the use of an attenuation factor τ_q. For cubic cardinal splines ($n = 4$) it is shown by Stoer [20] and Gautschi [8] that

$$\tau_q = \left[\frac{\sin\frac{\pi q}{M}}{\frac{\pi q}{M}}\right]^4 \frac{3}{1+2\cos^2(\frac{\pi q}{M})}. \tag{2.18}$$

In expression (2.17) we wish to arrange the summation over q to summation over s, where $s \equiv q(\bmod M)$. Define the matrix

$$W^{(1)} = \begin{bmatrix} \operatorname{diag} \sqrt{M}\hat{B}_{o,s}\hat{K}_{N,s} \\ \cdots\cdots\cdots \\ \operatorname{diag} \sqrt{M}\hat{B}_{0,M-s}\overline{\hat{K}}_{N,M-s} \end{bmatrix} \quad \begin{matrix} \text{order } N \times M \\ s = 0, 1, \ldots, M-1 \end{matrix} \tag{2.19}$$

From the property $\hat{K}_{N,q} = \overline{\hat{K}}_{N,N-q}$ of discrete FTs it then follows that expression (2.16) simplifies to

$$\|(K_N * F_M - G_N\|_2^2 = \|W^{(1)}\underline{\hat{\alpha}} - \underline{\hat{G}}_N\|_2^2 \tag{2.20}$$

and (2.17) can be written as

$$\begin{aligned} \|F_M^{(P)}\|^2 &= 2M \sum_{s=1}^{M-1} \left\{ |\hat{\alpha}_s|^2 \sum_{n=0}^{\infty} w_{Mn+s}^{2p} \hat{B}_{0,Mn+s}^2 \right\} \\ &= 2M \sum_{s=1}^{M-1} \tau_s |\hat{\alpha}_s|^2 \end{aligned} \tag{2.21}$$

where

$$\tau_s = \sum_{n=0}^{\infty} w_{Mn+s}^{2p} \hat{B}_{0,Mn+s}^2 \tag{2.22}$$

$$\begin{aligned} &= (2\pi)^{2p} \sum_{n=0}^{\infty} (Mn+s)^{2p} H^2 \left[\frac{\sin \frac{\pi(Mn+s)}{M}}{\frac{\pi(Mn+s)}{M}} \right]^8 \\ \tau_s &= (2\pi)^{2p} H^2 s^8 \left[\sin \frac{\frac{\pi s}{M}}{\frac{\pi s}{M}} \right]^8 \sum_{n=0}^{\infty} (Mn+s)^{2p-8} \\ &= (2\pi)^{2p} s^8 \hat{B}_{0,s}^2 \sum_{n=0}^{\infty} (Mn+s)^{2p-8} \end{aligned} \tag{2.23}$$

Since $\hat{\alpha}_s = \overline{\hat{\alpha}}_{M-s}$, equation (2.21) further simplifies to

$$\|F_M^{(P)}\|_2^2 = 2M \sum_{s=1}^{\frac{1}{2}M} (\tau_s + \tau_{M-s}) |\hat{\alpha}_s|^2 \tag{2.24}$$

In particular, when $p = 2$, from (2.23) it follows that

$$\tau_s = (2\pi)^4 s^4 \hat{B}_{0,s}^2 \sum_{n=0}^{\infty} \left(\frac{s}{Mn+s} \right)^4$$

while

$$\tau_{M-s} = (2\pi)^4 s^4 \hat{B}_{0,s}^2 \sum_{n=1}^{\infty} \left(\frac{s}{Mn - s} \right)^4$$

so that

$$\begin{aligned}
\tau_s + \tau_{M-s} &= (2\pi)^4 s^4 \hat{B}_{0,s}^2 \sum_{n=-\infty}^{\infty} \left(\frac{s}{Mn + s} \right)^4 \\
&= \frac{(2\pi)^4 s^4 \hat{B}_{0,s}^2 \left[1 + 2\cos^2\left(\frac{\pi s}{M}\right)\right]}{3\left[\frac{\sin\frac{\pi s}{M}}{\frac{\pi s}{M}}\right]^4} \\
&\qquad\qquad (\text{ see Pennisi [13]}) \\
&= \frac{16}{3} M^2 \sin^4\left(\frac{\pi s}{M}\right)\left[1 + 2\cos^2\left(\frac{\pi s}{M}\right)\right] \qquad (2.25)
\end{aligned}$$

Defining the $M \times M$ matrix

$$W^{(2)} = \operatorname{diag}\left\{\left[M\left(\tau_s + \tau_{M-s}\right)\right]^{1/2}\right\} \qquad (2.26)$$

it follows from (2.24) that

$$\left\| F_M^{(P)} \right\|_2^2 = \left| W^{(2)} \underline{\hat{\alpha}} \right\|^2 \qquad (2.27)$$

Thus, from equations (2.20) and (2.27) we may express the smoothing functional (2.15) as

$$C(\underline{\alpha}, \lambda) = \left\| W^{(1)} \underline{\hat{\alpha}} - \underline{\hat{G}}_N \right\|_2^2 + \lambda \left\| W^{(2)} \underline{\hat{\alpha}} \right\|_2^2 \qquad (2.28)$$

The minimizer of (2.28) is clearly

$$\underline{\hat{\alpha}} = (W + \lambda V)^{-1} W^{(1)H} \underline{\hat{G}}_N \qquad (2.29)$$

where

$$\left.\begin{aligned} W &= W^{(1)H} W^{(1)} \\ V &= W^{(2)H} W^{(2)} \end{aligned}\right\} \qquad (2.30)$$

It is not necessary to invert the matrix $W + \lambda V$ directly because it is diagonal. From equations (2.19), (2.26), (2.29) and (2.30) it follows that

$$\hat{\alpha}_s = \frac{1}{\sqrt{M}} \frac{\hat{B}_{0,s}\overline{\hat{K}}_{N,s}\hat{G}_{N,s} + \hat{B}_{0,M-s}\hat{K}_{N,M-s}\overline{\hat{G}}_{N,M+s}}{\left[\hat{B}_{0,s}^2\left[\left|\hat{K}_{N,s}\right|^2 + \hat{B}_{0,M-s}^2\left|\hat{K}_{N,M-s}\right|^2\right] + N^2\lambda\left(\tau_s + \tau_{M-s}\right)\right]}$$

$$\hat{\alpha}_s = \frac{1}{\sqrt{M}} \frac{\hat{B}_{0,s}\left[\overline{\hat{K}}_{N,s}\hat{G}_{N,s} + \left(\frac{s}{M-s}\right)^4 \hat{K}_{N,M-s}\overline{\hat{G}}_{N,M+s}\right]}{\hat{B}_{0,s}^2\left[\left|\hat{K}_{N,s}\right|^2 + \left(\frac{s}{M-s}\right)^8\left|\hat{K}_{N,M-s}\right|^2\right] + N^2\lambda\left(\tau_s + \tau_{M-s}\right)} \tag{2.31}$$

since

$$\hat{B}_{0,M-s} = \left(\frac{s}{M-s}\right)^4 \hat{B}_{0,s} \tag{2.32}$$

We can easily verify that $\hat{\alpha}_s = \overline{\hat{\alpha}}_{M-s}$ so that the inverse $FFT\underline{\alpha} = \psi_M\hat{\underline{\alpha}}$ is a real vector as required.

The Filter for Cardinal B–Spline Regularization

The Fourier coefficients of the regularized (filtered) solution $F_M(x) \in B_M(0,T)$ clearly depends on λ through equations (2.11a), (2.13) and (2.31). In equation (2.31), we denote the dependence of $\hat{\alpha}_s$ on λ by writing $\hat{\alpha}_s = \hat{\alpha}_s(\lambda)$. Thus the Fourier coefficients of the filtered solution are

$$\hat{F}_{M,q}^B(\lambda) = \sqrt{M}\hat{B}_{0,q}\hat{\alpha}_s(\lambda), \quad s \equiv q \pmod{M}$$

whereas those of the unregularized (unfiltered) solution are

$$\hat{F}_{M,q}^B(0) = \sqrt{M}\hat{B}_{0,q}\hat{\alpha}_s(0).$$

Clearly the underlying filter $Z_{q;\lambda}$ must satisfy

$$\hat{F}_{M,q}^B(\lambda) = Z_{q;\lambda}\hat{F}_{M,q}^B(0)$$

so that we can deduce

$$Z_{q;\lambda} = \frac{\hat{\alpha}_s(\lambda)}{\hat{\alpha}_s(0)} \tag{2.33}$$

$$= \frac{\hat{B}_{0,s}^2[|\hat{K}_{N,s}|^2 + (\frac{s}{M-s})^8|\hat{K}_{N,M-s}|^2]}{\hat{B}_{0,s}^2[|\hat{K}_{N,s}|^2 + (\frac{s}{M-s})^8|\hat{K}_{N,M-s}|^2] + N^2\lambda(\tau_s + \tau_{M-s})} \tag{2.34}$$

The filter will of course apply to every Fourier coefficients $q = 0, \pm 1, \pm 2, \ldots$, but will have only M possible values depending on q modulo M. The regularization parameter λ is still to be determined.

Determination of Regularization Parameter λ

Let the filtered solution $F_M(x) \in B_M\ (0, T)$, which minimizes $\|K_N * F_M - G_N\|_2^2 + \lambda\|F_M''\|_2^2$ be given by (we have $p = 2$)

$$F_M(x) = \sum_{q=-\infty}^{\infty} \hat{F}_{M,q}^B \exp(iw_q x) \tag{2.35}$$

Consider

$$\hat{G}_{N,\lambda,q} = \hat{K}_{N,q}\hat{F}_{M,q}^B \quad , \quad q = 0, 1, \ldots, N-1 \tag{2.36}$$

$$= \begin{cases} \sqrt{M}\hat{B}_{0,q}\hat{K}_{N,q}\hat{\alpha}_s & , \quad s \equiv q(\bmod M) \\ 0 & , \quad \text{otherwise} \end{cases} \quad q = 0, 1, \ldots, N-1$$

We now introduce the $N \times N$ influence matrix

$$A(\lambda) = \psi_N \hat{A}(\lambda) \psi_N^H$$

where

$$\underline{\hat{G}}_{N,\lambda} = \hat{A}(\lambda)\underline{\hat{G}}_N \tag{2.37}$$

$\hat{A}(\lambda)$ is block diagonal with the following structure

$$\hat{A}(\lambda) = \left[\begin{array}{c|c} \text{diag } \underline{a}_1 & \text{diag } \underline{a}_2 \\ \hline \text{diag } \underline{a}_3 & \text{diag } \underline{a}_4 \end{array}\right] \tag{2.38}$$

where $\underline{a}_k \in \mathscr{C}^M$, $\quad K = 1,2,3,4$ and

$$a_{1,s} = \begin{cases} \frac{\sqrt{M}(\hat{B}_{0,s})^2|\hat{K}_s|^2}{D_s} & s=0 \\ \frac{\sqrt{M}(\hat{B}_{0,s})^2|\hat{K}_s|^2}{2D_s} & 1 \le s \le M-1 \end{cases}$$

$$a_{2,s} = \begin{cases} 0 & s=0 \\ \frac{\sqrt{M}(\hat{B}_{0,s})^2(\frac{s}{M-s})^4\hat{K}_s\overline{\hat{K}}_{M+s}}{2D_s}, & 1 \le s \le M-1 \end{cases}$$

$$a_{3,s} = \begin{cases} \frac{\sqrt{M}\hat{K}_{M+s}\hat{B}_{0,M+s}\hat{B}_{0,s}\overline{\hat{K}}_s}{D_s}, & s=0 \\ \frac{\sqrt{M}\hat{K}_{M+s}\hat{B}_{0,M+s}\hat{B}_{0,s}\overline{\hat{K}}_s}{2D_s}, & 1 \le s \le M-1 \end{cases}$$

$$a_{4,s} = \begin{cases} 0 & s=0 \\ \frac{\sqrt{M}\hat{B}_{0,M+s}\hat{B}_{0,s}(\frac{s}{M+s})^4|\hat{K}_{M+s}|^2}{2D_s}, & 1 \le s \le M-1 \end{cases}$$

where

$$D_s = M\hat{B}_{0,s}^2[|\hat{K}_s|^2 + (\frac{s}{M-s})^8|\hat{K}_{M-s}|^2] + \lambda N^2(\tau_s + \tau_{M-s}).$$

For simplicity of notation we have written $\hat{K}_s$ for $\hat{K}_{N,s}$ in $a_{1,s}, a_{2,s}, a_{3,s}, a_{4,s}$ and D_s. The optimal λ as defined by GCV method may be found (in Davies [3] and Wahba [24]) by minimizing the expression

$$V(\lambda) = \frac{\frac{1}{N}\|(I - \hat{A}(\lambda))\underline{\hat{G}}_N\|_2^2}{[\frac{1}{N}\text{ Trace }(I - \hat{A}(\lambda))]^2} \tag{2.39}$$

which from equation (2.38) simplifies to

$$V(\lambda) = \frac{\frac{1}{N}\{\sum_{s=0}^{M-1}|(1-a_{1,s})\hat{G}_s - a_{2,s}\overline{\hat{G}}_{M-s}|^2 + \sum_{s=0}^{M-1}|(1-a_{4,s})\overline{\hat{G}}_{M-s} - a_{3,s}\hat{G}_s|^2\}}{[1 - \frac{1}{N}\sum_{s=0}^{M-1}(a_{1,s} + a_{4,s})]^2} \tag{2.40}$$

In order to minimize $V(\lambda)$ in equation (2.40) we have used a subroutine which uses a quadratic interpolation technique to obtain a minimum.

3. Numerical Results

In this section we tabulate the results of the above method applied to the test examples taken from Varah [23], McWhirter and Pike [10], Essah and Delves

[6] and Brianzi [2]; only optimal results have been quoted in the table and the diagrams. All data functions have the property $g(s) = 0(s^{-1})$ and no noise is added apart from machine rounding error.

Example 1 ([2, 6, 23])

$$\begin{aligned} f(t) &= 1 - e^{-t/2} \\ g(s) &= \frac{0.5}{s(s+0.5)} \end{aligned}$$

The optimal result is shown in diag (1).

Example 2 ([5])

$$\begin{aligned} f(t) &= 2 - e^{-t} \\ g(s) &= \frac{2}{s} - \frac{1}{s+1} \end{aligned}$$

The optimal result is shown in diag (2).

Example 3 ([2, 23])

$$\begin{aligned} f(t) &= t^2 e^{-t/2} \\ g(s) &= \frac{2}{(s+1/2)^3} \end{aligned}$$

The optimal result is shown in diag (3).

Example 4 ([2, 10])

$$\begin{aligned} f(t) &= te^{-t} \\ g(s) &= \frac{1}{(1+s)^2} \end{aligned}$$

The optimal result is shown in diag (4).

Table

Problem	A	T	H	λ	$V(\lambda)$	$\|f - f_\lambda\|_\infty$	diag
1	10.0	10.5	0.16406	7.021×10^{-8}	0.561023	2.8×10^{-2}	1
2	10.0	11.6	0.18125	2.999×10^{-8}	0.55818	2.7×10^{-3}	2
3	15.0	12.0	0.18750	1.100×10^{-11}	1.342×10^{-8}	1.3×10^{-2}	3
4	10.0	12.0	0.18750	1.100×10^{-11}	3.6094×10^{-12}	4.8×10^{-4}	4

Acknowledgement

The author acknowledges the excellent research and computer facilities availed at King Fahd University of Petroleum and Minerals during the preparation of this paper.

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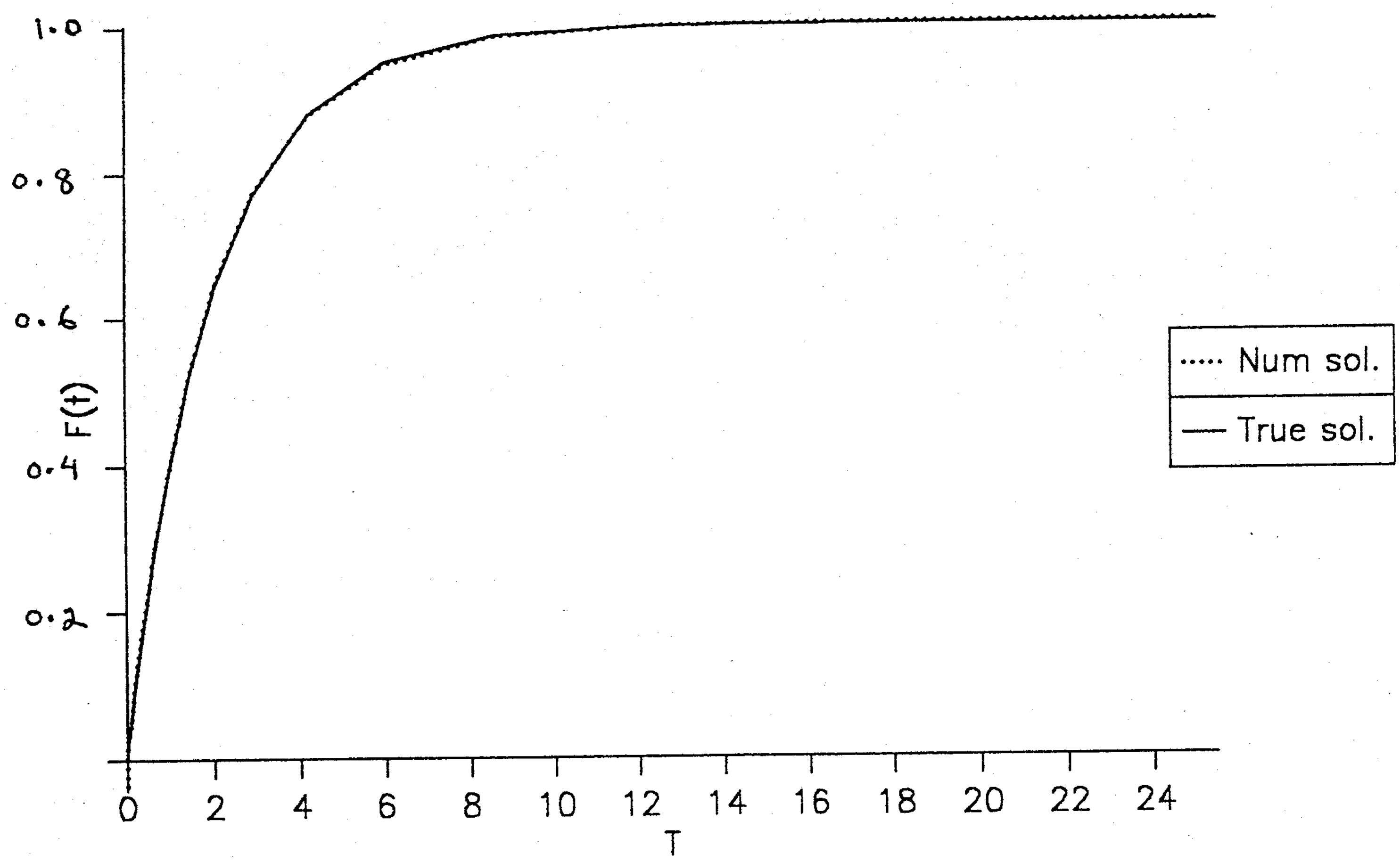
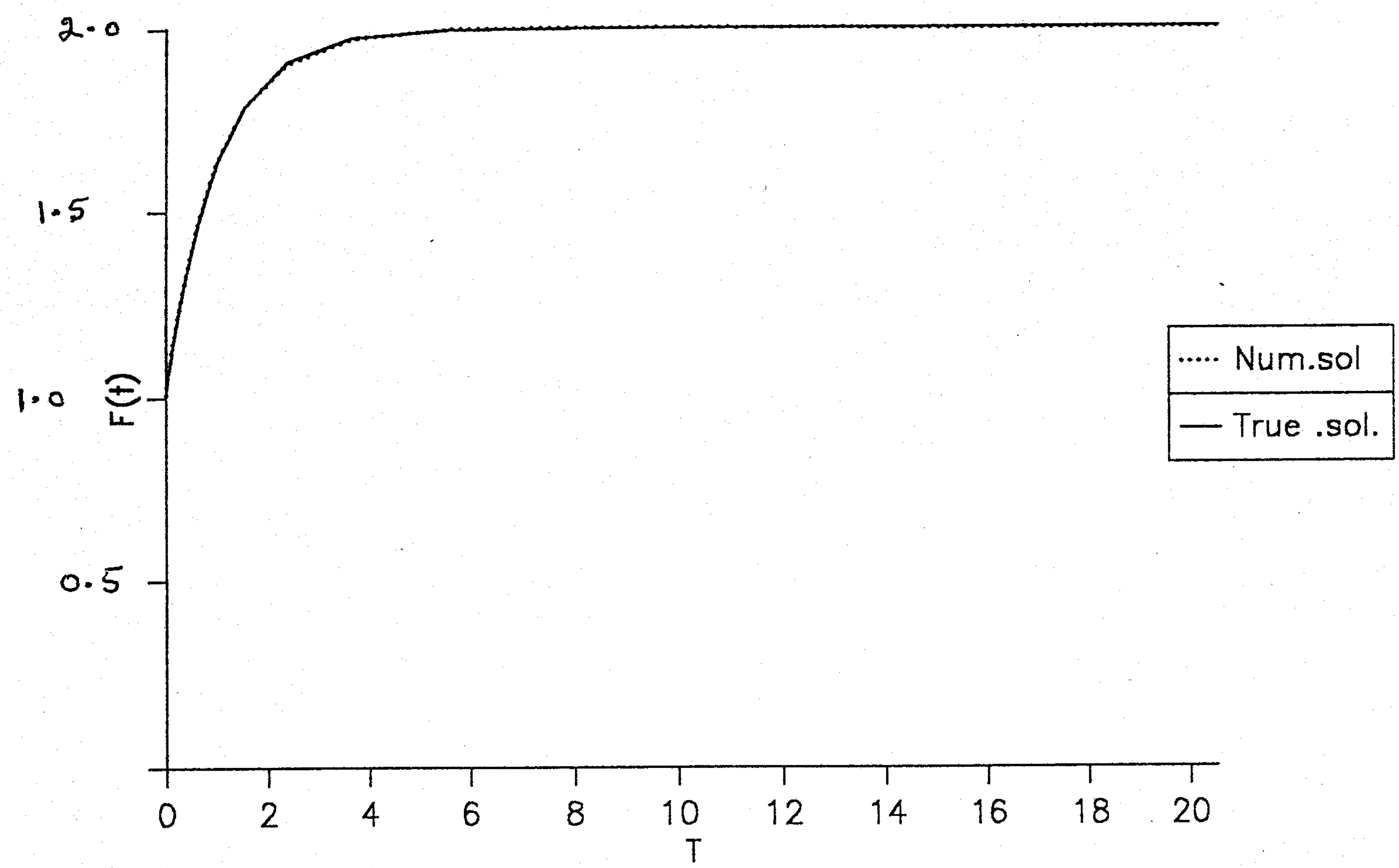
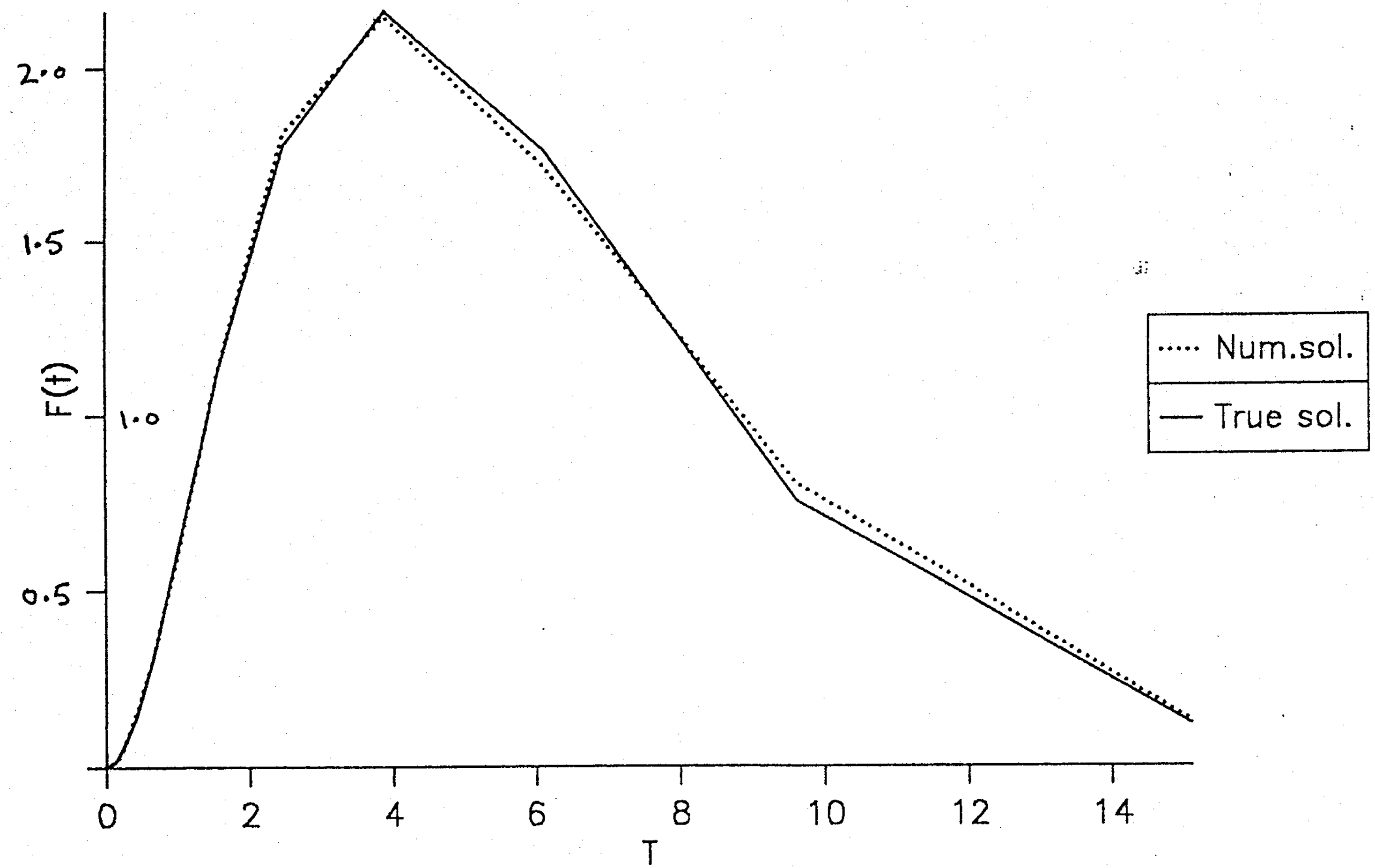
Diag(1) Gcv Spline Method



Diag(2) Gcv Spline Method



Diag(3) Gcv Spline Method



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Diag(4) Gcv spline method