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Numerical evaluation of inverse integral transforms: dynamic response of elastic materials

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Abstract

This study discusses the use of numerical integration in evaluating the improper integrals appearing as inverse integral transforms of non-analytic functions. These transforms appear while studying the response of various sources in an elastic medium through integral transform method. In these studies, the inverse Fourier transforms are solved numerically without bothering about the singularities and branch points in the corresponding integrands. References on numerical integration cited in relevant papers do not support such an evaluation but suggest contrary. Approximation of inverse Laplace transform integral into a series is used without following the essential restrictions and assumptions. Volume of the published papers using these dubious procedures has reached to an alarming level. The discussion presented aims to draw the attention of researchers as well as journals so as to stop this menace at the earliest possible.

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1. Introduction

The use of numerical integration in computing the inverse integral transforms sounds fascinating and can be thought to be a very useful numerical procedure. For the last nearly two decades, few research groups are claiming the use of Romberg integration to compute the inverse Fourier transforms as improper integrals. However, none of these researchers ever discussed the branch points or the singularities present in the corresponding integrands. Sharma (2010a) has discussed the errors deliberately committed by these researchers while going for this numerical adventure. The relevant studies mainly consider calculating the response of elastic materials to various sources of deformation. Nearly fifty of such papers are listed in Sharma (2010a), which have appeared in reputed international journals devoted to mechanics of solids. Irony is that even after this publication (Sharma, 2010a), these authors did not stop their erroneous numerical adventure on inverse Fourier transforms. In most of these papers, the inverse Laplace transforms are also calculated numerically. It has been claimed that the procedure and computer programs used for this numerical inversion are taken from Honig and Hirdes (1984). Unfortunately, in none of these studies, authors have bothered to discuss any of the restrictions, which are essential to apply the said procedure (Honig and Hirdes, 1984). One such restriction is to ensure the absence of singularities from the integration scene. This requires the translation of the imaginary axis to the right so that all the singularities of function under transform lies on the left half-plane. Obviously, this can be possible only after locating all the singularities of the integrand. In the studies under scanner, such singularities happen to be the zeroes of a non-algebraic complex expression, which may not be solved through any obvious technique or using a standard method. But, the tradition of ignoring the singularities in numerical evaluation of integral transforms is continued unabated, as can be checked in Ailawalia and Kumar (2019), Kumar et al. (2018), Kumar et al. (2017a,b) and Kumar et al. (2016a,b,c).

A survey of relevant literature indicates that this adventure was perhaps started with a research paper of Sharma and Kumar (1996) published in Journal of Thermal Stresses. This publication success encouraged Sharma and co-authors to use the same procedure in other similar studies. In the next five years, they published nearly a dozen papers in various reputed journals. Then, sometime around the start of the 21st century, this procedure of J.N. Sharma's camp seems to have infected few other research groups (R Kumar, MIA Othman, MA Ezzat, P Ailawalia plus co-authors). The result is hundreds of papers in various regional and international journals since then. Surprisingly, all these papers claim the use of the same techniques for inverse integral transforms with ditto text. But, restrictions attached to the procedure of Honig and Hirdes (1984) for Laplace transform are not discussed in any of these studies. Suitability of this method to the integrands in their studies is never ensured. Few dozens of such papers are cited in the study (Kumar et al., 2016a) chosen to discuss. This study is also using the numerical integration to evaluate inverse integral transforms so as to compute the thermomechanical interactions in transversely isotropic magneto-thermoelastic medium.

The present author has chosen to discuss the various aspects of numerical procedure (Honig and Hirdes, 1984), which is used to calculate the inverse Laplace transforms. This procedure demands to follow few restrictions along with some manipulations. The aim is not to target a particular paper but to expose the dubious numerical procedures, which have been ditto repeated in each of the papers under scanner. The paper of Kumar et al. (2016a) (referred as paper-A, hereafter) is chosen to explain the abuse of this procedure by ignoring all the essential restrictions. In this paper, the integral transforms are inverted numerically to calculate displacement, stresses, temperature change and induced magnetic field in the physical domain. It is claimed that the inverse Fourier transforms are computed through Romberg integration and the procedure of Honig and Hirdes (1984) is used to compute the inverse Laplace transforms.

Frequency and volume of the studies using this erroneous procedure have reached to an alarming level. So, any delay in exposing this erroneous procedure may cause an irreparable loss to an important aspect of mathematics dealing with numerical computations. The present discussion aims to draw the attention of the corresponding researchers towards the sanctity of the mathematical procedures. It is further expected that the editors of the journals as well as readers should be more cautious while dealing with the papers involving this erroneous procedure and the research groups frequently using it.

2. Integral Transforms

Purpose of the numerical part in paper-A is to calculate displacement, stresses, temperature change and induced magnetic field in the physical domain. That means to calculate a function $f(x,z,t)$ from $\hat{f}(\xi,z,s)$ through $\bar{f}(x,z,s)$, where $\hat{f}(\xi,z,s)$ represents any of the expressions (44)-(49) in paper-A. With few printing corrections in paper-A, the inverse Fourier transform is written as follows.

$$\bar{f}(x,z,s)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{-i\xi x}\,\hat{f}(\xi,z,s)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}[\cos(\xi x)\,\hat{f}_e-i\sin(\xi x)\,\hat{f}_0]d\xi, \tag{1}$$

where $\hat{f}_e$ and $\hat{f}_0$ denote even and odd parts of function $\hat{f}(\xi,z,s)$, respectively. Then, the inverse Laplace transform of $\bar{f}(x,z,s)$ yields

$$f(x,z,t)=\frac{1}{2\pi i}\int_{C-i\infty}^{C+i\infty}\bar{f}(x,z,s)e^{st}ds, \tag{2}$$

which represents the deformation characteristics (displacements, stresses, temperature change and induced magnetic field) in space-time domain.

In reverse order, each of the expressions (44)-(49) in paper-A is designated, in turn, as a function $\hat{f}(\xi,z,s_k)$ but with a chosen value of z. This function of ξ and s is used in the inverse Fourier transform (1) to calculate the function $\bar{f}(x,z,s)$ for a chosen value of x. Then, $\bar{f}(x,z,s)$, as a function of s, is used in the inverse Laplace transform (2) to evaluate the function $f(x,z,t)$, for a chosen value of t. Finally, the values of function $f(x,z,t)$ could be calculated for any given values of the triplet (x,z,t). In the numerical evaluation of inverse Laplace transform, as proposed in Dubner and Abate (1968) and modified in Durbin (1973), the function $f(x,z,t)$ in (2) is approximated as

$$f(x,z,t)\approx g_N(x,z,t)-e^{-2CL}g_{\dot{N}}(x,z,2L+t),\ 0\le t\le 2L,\ \ \dot{N}<N; \tag{3}$$

$$g_N(x,z,t) = \frac{1}{2}C_0 + \sum_{k=1}^{N} C_k,\ C_k = \frac{1}{L}e^{Ct}\,\mathrm{Re}[e^{\frac{ik\pi t}{L}}\ \bar{f}(x,z,c+\frac{ik\pi t}{L})]. \quad (4)$$

Note that the function values $\bar{f}(x,z,c+\frac{ik\pi t}{L})$ constituting C_k's are to come from the inverse Fourier transforms of $\hat{f}(\alpha,\beta,z,s)$ at $s = C + \frac{ik\pi}{L}$. That means, from relation (1) above, we have to solve the integral

$$\bar{f}(x,z,s) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} e^{-i\beta x}\,\hat{f}(\alpha,\beta,z,s)\,d\beta \quad (5)$$

and to evaluate it for $s = C + \frac{ik\pi}{L}$ with integer k varying from 0 to N. Here the function $\hat{f}$ represents, in turn, the physical entities defined through the expressions (44)-(49) of paper-A.

3. Evaluation of Inverse Fourier Transforms

"*The last step is to calculate the integral in Eq. (54). The method for evaluating this integral is described in Press et al. (1992). It involves the use of Romberg's integration with adaptive step size. This also uses the results from successive refinements of the extended trapezoidal rule followed by extrapolation of the results to the limit when the step size tends to zero.*"

It is obvious that the most part of this text on page 6567 of paper-A is just the definition of Romberg integration. But, there seems to some blind faith attached to this text as whole of this is ditto repeated in almost all the papers using this numerical adventure. However, to calculate the said integral, i.e. inverse Fourier transform (5), is not the last but first step in the process to compute $f(x,z,t)$ from $\hat{f}(x,z,s)$ through $\bar{f}(\alpha,\beta,z,s)$. Anyway, the purpose is to calculate the improper integral (5) with integrand $\hat{f}(\alpha,\beta,z,s_k)e^{-i\beta x}$ (or its alternate form), for $s_k = C + \frac{ik\pi}{L}$, ($k$= 0,1,2,…,$N$).

So, we have an expression for $\hat{f}(\alpha,\beta,z,s_k)$ in (44)-(49) of paper-A with $s_k(= C + \frac{ik\pi}{L})$ replacing s. Clearly, for any s_k, the integrand has singularities at the points where it is unbounded. In general, these singularities arise with the vanishing of the determinant Δ, which appears as denominator in each of the expressions (44)-(49) in paper-A. It is noted that Δ, is calculated to be a non-algebraic complex expression, which involves radicals as well. Then, some specific method from complex analysis will be required to locate its zeroes. It seems that instead of locating the zeroes of Δ, Kumar et al. (2016a) have preferred to look away from these trouble-making singularities of $\hat{f}(\alpha,\beta,z,s_k)$.

In addition to the above, the roots of complex cubic equation (31) in paper-A cannot be all real. That means, the corresponding roots α_i are going to be complex. Then, in expressions (33)-(36), choosing $e^{-\alpha_i z}$ does not make sense as radiation requirement unless all the α_i have positive real parts. Moreover, the relevant expressions involve the square root of various complex quantities, which may encounter bifurcation (branch cuts) as β varies continuously. Hence, a miracle numerical method is expected, which could evaluate an improper integral in the presence of unknown singularities and unknown branch points in its range of integration. Kumar et al. (2016a) have chosen for numerical integration using the Romberg method. The reference of Press et al. (1992) is cited in support of this choice. But, it has been explained very clearly in Sharma (2010a) that Romberg integration cannot be used for such integrals and the cited reference (Press et al., 1992) never supported this adventure. Moreover, on the evaluation of such integrals, a relevant reference (Ewing et al., 1957) suggests to use the contour integration rather than numerical integration (Sharma, 2010a).

In the relevant literature, one can find some earlier references dealing with the Romberg integration of singular integrands (Hunter, 1967; Fox, 1967; Fox and Hayes, 1970; El-Tom, 1971). However, in each case, the Romberg integration could be applied only for singularities of very specific kinds. Details are found in Press et al. (1992) and relevant discussion is available in Sharma (2010a). Moreover, it involves a lot of analytical manipulation. For example, Fourier transforms (when any range of integration is infinite) are done by splitting the infinite branch of the integral when the function falls quickly along it.

The above discussion poses many questions to all those researchers who are evaluating the Fourier transform numerically through the Romberg integration method. Have their numerical results been obtained by satisfying the necessary requirements and using the suggested way-outs? Else, any procedure they adopted must have been approximating the integral with a series sum. The

terms in this series must be ignoring the singularities (El-Tom, 1971). But, how could one be able to ignore the singularities without locating them? Then, was the convergence obtained always with an acceptable convergence rate? Which, if any, were the situations where convergence could not be achieved and how were these handled? The most important question is, did they ever verify their own procedures for a known pair of Fourier transforms involving functions with singularities and branch points?

4. Evaluation of Inverse Laplace Transforms

In the twin-transform procedure, the inverse Laplace transform part, given by

$$f(x,z,t) = \frac{1}{2\pi i}\int_{C-i\infty}^{C+i\infty} \bar{f}(x,z,s)e^{st}ds\,, \tag{6}$$

is calculated approximately through the expression (3). The required function values $\bar{f}(x,z,C+\frac{ik\pi}{L})$ in (4) come from the Romberg integration of a singular integrand with singularities and branch points at unknown locations.

The numerical procedure used to compute the inverse Laplace transform (6) is claimed to be that of Honig and Hirdes (1984), which is an improvement to the procedures suggested by Dubner and Abate (1968) and Durbin (1973). For ease of discussion, let $f(t)$ and $F(s)$ represent the functions $f(x,z,t)$ and $\bar{f}(x,z,s)$ respectively.

Following Honig and Hirdes (1984), the real constant C in (6) is to be chosen so that it is greater than the real parts of all the singularities of $F(s)$. There is no singularity of $F(s)$ with $\mathrm{Re}(s) > 0$ is the required assumption. This is to be ensured by a suitable translation of the imaginary s-axis. Then the following points are notable.

a) The procedure proposed yields a good result through the choice of a particular contour (a vertical line with abscissa $C > 0$).

b) The absence of singularities of $F(s)$ in the right half-plane ensures that there exist $c > 0$, $m \geq 0$ and $t_0 \geq 0$, such that $|f(t)| \leq ct^m$, for all $t \geq t_0$. This helps to estimate the discretization error resulting from the approximation of infinite integral by an infinite series. This error can be made small if the product CL (i.e. τT in Honig and Hirdes (1984)) is sufficiently large.

c) An infinite series can be summed up only for finite number (N) of terms. Hence there occurs a truncation error which may diverge for large values of CL.

d) From b) and c) above, it is clear that both errors may not be reduced simultaneously for an arbitrary increase or decrease of CL. 'Korrektur'-method allows a reduction of discretization error without enlarging the truncation error. But this requires non-zero m to satisfy the condition $\frac{m!}{2^m} \leq 1 + 2CL$ else the method is not applicable.

e) An adequate reduction of total error can be obtained by the 'Korrektur'-method only if (for fixed N and L) the parameter C is suitable. There may exist a value τ_0 such that successful application of the 'Korrektur'-method requires $C < \tau_0$. But, acceleration of convergence (i.e. reduction of truncation error) may hold only for $C > \tau_0$. However, a simultaneous application of acceleration of convergence method and 'Korrektur'-method is recommended if parameters (N, L, C) are optimally chosen.

f) In Honig and Hirdes (1984), two situations are specified to obtain the optimized parameters. One is the equality of discretization error and truncation error that decides an optimized value of C (of the method of Durbin (1973)) for fixed values of N and L. The other one minimizes the sum of the absolute values of the two errors to decide an optimized value of C (in accordance to 'Korrektur'-method and acceleration of convergence method) for fixed N and L.

The final word is that any study using the method of Durbin (1973) and the procedure of Honig and Hirdes (1984) for the evaluation of Laplace transform must ensure the following points.

i) The value of C is fixed to ensure that all the singularities of $F(s)$ lies on the left half-plane. This requires to find all the singularities of the function $F(s)$, and an appropriate translation of the imaginary axis to the right. Unfortunately, in all the studies using this techniques, none has bothered to specify the singularities involved. For example, in paper-A, the singularities for integrand come from the values of S for which denominator (Δ) in (44)-(49) vanishes. Note that the roots (α_i) of the complex cubic equation (31) in paper-A and hence l_j as well as d_j are functions of S. Consequently, Δ is a non-algebraic complex function of s, which must be solved to locate its zeroes. But, no standard method is available to find the zeroes of such an irrational complex function.

ii) A value of m to satisfy $|f(t)| \leq ct^m$, for all $t \geq t_0$ is used to ensure the applicability of 'Korrektur'-method. For non-zero m, the application of the method is subject to the condition $\frac{m!}{2^m} \leq 1 + 2CL$, which puts a restriction on the product (CL) of two parameters C and L.

iii) 'Korrektur'-method and convergence of acceleration method can only be applied simultaneously if parameter C is optimized for values of *N* and *L* chosen according to i) and ii) above.

The hundreds of papers under scanner claim the use of the procedure of Honig and Hirdes (1984) in solving the inverse Laplace transform numerically. Such a solution has been used mainly in the numerical examples solved to calculate and exhibit the response of elastic materials to various kinds of sources. But not a single such study could afford a little space to mention about the values chosen or calculated for any of the *C*, *m*, *L*, *N* or $^{3}{}_{0}$. This cannot be a coincidence or some kind of a miracle. The bare fact is that, in all these studies, the authors have not bothered to ensure any of the requirements mentioned above. So this is some kind of insensitivity towards the sanctity of mathematical techniques.

5. Concluding Remarks

From Sharma (2010a), it is clear that Romberg integration cannot evaluate the inverse Fourier transforms appearing in paper-A unless

i) locations of all the singularities are known;
ii) all these singularities are integrable;
iii) branch points are identified to define the branch line integrals with (single-valued) uniform functions as integrands.

Another perspective may put forward a question that what is wrong in employing the numerical (Romberg) integration to integrals ignoring the singularities and branch points? Such a question can be answered with the application of this bye-pass technique (Kumar et al., 2016a) in calculating the integrals appearing in the solutions of classical Lamb problems (Ewing et al., 1957). These results should be verified with the corresponding results calculated in Ewing et al. (1957) using the procedures of complex analysis. Unfortunately, not a single reference could be found in the relevant literature, where this black-box technique has been verified or even tested on a known pair of Fourier transforms. Moreover, if the improper integrals as in paper-A can be evaluated using Romberg integration and bye-passing the branch points and any number of singularities then it may not be possible to find an example of a non-integrable function.

For numerical integration of inverse Laplace transform, the procedure and computer programs of Honig and Hirdes (1984) can be used only with many restrictions. It starts with choosing the value of *C* in equation (2). This requires to locate all the singularities of $F(s)$ so that imaginary axis in complex plane could be shifted to carve a region where $F(s)$ becomes analytic. This requires solving a complex transcendental equation for all its complex solutions. There cannot be a general method for solving such an equation and numerical methods are not beyond doubt (Sharma, 2010b). While studying the dynamic response of an elastic layer or plate, the resulting transcendental equation involve periodic functions (Sharma et al., 2004). Then, any shifting of imaginary axis will not be sufficient to carve a region free from singularities. That means, no finite value of *C* is possible. Then, what is being evaluated in the computer programs and exhibited in the plots in all the papers using Honig and Hirdes (1984) as a gate-pass? This is not simply a question but a big mystery. The present author wishes if this mystery could ever open.

It is obvious that readers may expect to see the losses coming from the incorrect procedure questioned in the present study. In this regard, authors are working on to solve the problem studied in Sharma et al. (2000) again, but keeping in mind all the limitations discussed above as well as in Sharma (2010a, b). This involves finding the singularities for source problem in thermoelastic medium with stress-free isothermal or insulated boundary. These singularities are obtained as the zeroes of thermoelastic Rayleigh function, which is analogous to solve the frequency equation for thermoelastic Rayleigh waves (Sharma, 2014). So, the focus of future publications will be to demonstrate the effects of ignored limitations on the dynamic response of elastic materials.

The presented discussion aims to draw the attention of the researchers working on the response of elastic media to the disturbance generated by various kinds of sources. These people are urged to ensure the requirements and follow the actual procedures specified for the numerical implementation of mathematical techniques. The relevant research journals are expected to be cautious while dealing with the papers involving this technique and the research groups frequently using this technique. The ultimate concern is the insensitivity in using the mathematical techniques to such an extent that it starts emanating a scent of an academic fraud.

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