A SQUARE ROOT RECURRENCE FOR CAUSAL BRANCH-CUT FUNCTIONS

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Attempts to find extrapolation equations for elastic waves have led to techniques that are applicable to a variety of physical problems other than scalar waves. In chapters 9.1 and 9.6 of my book, ***Fundamentals of Geophysical Data Processing,*** we find a useful mathematical representation of many physical problems:

$$\frac{d}{dz}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & A \\ B & 0 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} \tag{1}$$

where A and B (1) may be scalars or block matrices and (2) may be functions of ∂_x or of its Fourier representation ik_x. Inserting either one into the other and neglecting z-derivatives of A and B we have useful starting points for the development of a wave extrapolation theory:

$$\frac{d^2u}{dz^2} = ABu \tag{2a}$$

$$\frac{d^2v}{dz^2} = BAv \tag{2b}$$

Proceeding with only (2a) we wish to find a representation of $(AB)^{\frac{1}{2}}$ which will be the negative of an impedance function. An impedance function R has a positive real part which is necessary for the stability of the desired extrapolation equation

$$\frac{du}{dz} = (AB)^{\frac{1}{2}} u = -Ru \tag{3}$$

As a mechanism for obtaining the desired square root, consider the recurrence

$$S_{n+1} = \lambda + \frac{AB - \lambda^2}{\lambda + S_n} \tag{4}$$

Assuming convergence we may solve (4) for S_∞ obtaining

$$S_\infty^2 = AB = (-R)^2 = R^2 = -k_z^2 \tag{5}$$

The major questions are (1) whether or not convergence will occur, (2) how to choose λ and S_0 so that convergence is rapid, and (3) how to ensure that the intermediate approximations S_n are themselves impedance functions. Before launching into a general theory, which I don't understand anyway, let us consider some examples.

Scalar Waves

Try

$$ab = -k_z^2 = k_x^2 - \frac{\omega^2}{v^2} \tag{6a}$$

$$\lambda = \frac{-i\omega}{v} \tag{6b}$$

$$S_0 = \frac{-i\omega}{v} \tag{6c}$$

We find the familiar 15-degree scalar result

$$S_1 = \frac{-i\omega}{v} + \frac{vk_x^2}{-2i\omega} \tag{7}$$

Laplace Equation

Try

$$ab = -k_z^2 = k_x^2 \tag{8a}$$

$$\lambda = 1 \tag{8b}$$

$$S_0 = 0 \tag{8c}$$

We find

$$S_1 = k_x^2 \tag{9a}$$

$$S_2 = 1 + \frac{k_x^2 - 1}{1 + k_x^2} \tag{9b}$$

Looking at (8a) you might at first think that the square root of k_x^2 would turn out to be $\pm\, k_x$. But the answer as graphed in figure 1 turns out to be $|k_x|$ which is positive for either positive or negative values of k_x as it must be in order to be an impedance function. So the downward continuation equation for Laplace's equation is

$$\frac{du}{dz} = -|k_x|u \tag{10}$$

Speed of Convergence

Inspecting the recurrence

$$S_{n+1} = \lambda + \frac{AB - \lambda^2}{\lambda + S_n} \tag{4}$$

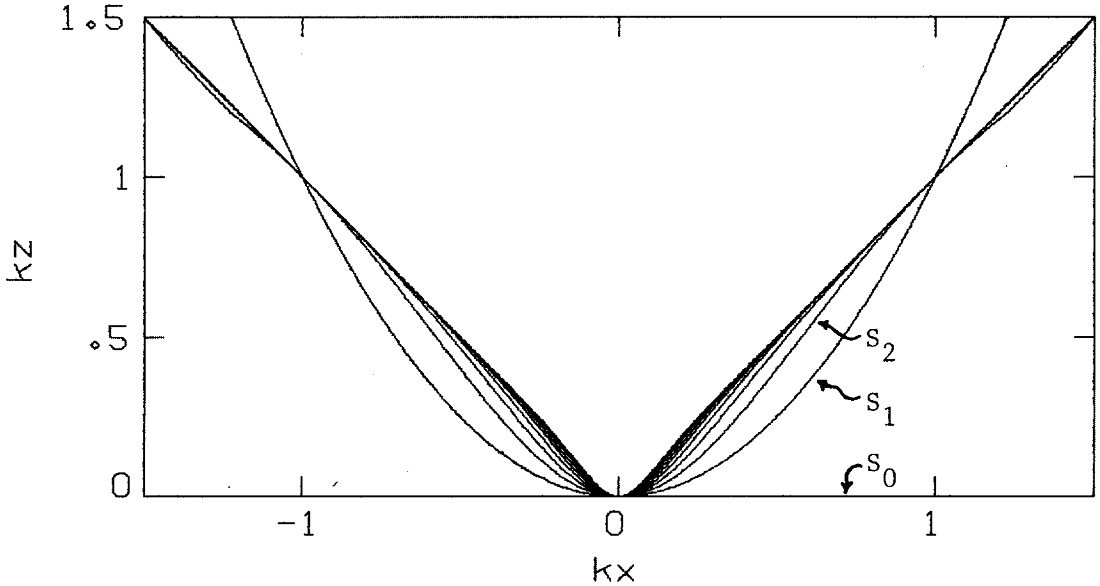

FIG. 1. The square root for Laplace's equation is the absolute value function.

we note that if $\lambda = S_\infty$ where $S_\infty^2 = AB$, then from any starting point S_0 we have convergence in one step. Likewise, if S_n is close to S_∞, then insensitivity to a poor choice of λ is apparent from writing the recurrence as

$$S_{n+1} = \frac{\lambda S_n + AB}{\lambda + S_n} \tag{11}$$

It turns out that if λ is chosen equal to S_n our recurrence reduces to Newton's square root recurrence which is well-known to have quadratic convergence about the starting point. A disadvantage of $\lambda = S_n$ is that it rapidly increases the number of powers of AB in the operator S_n. Another approach is to start the square root recurrence for Laplace's equation at $\lambda = S_0 = 1$ as shown in figure 2. Clearly, better convergence about $k_x = 1$ has come at the cost of poorer convergence at $k_x = 0$.

Causality

Consider again the recurrence (4) where λ is thought of as the causal differentiation operator [say $\lambda = -i\omega + \epsilon$ or $\lambda = (-i\omega)^{1-\epsilon}$ as $\epsilon \to 0$]. We could also take λ to be the causal integration operator.

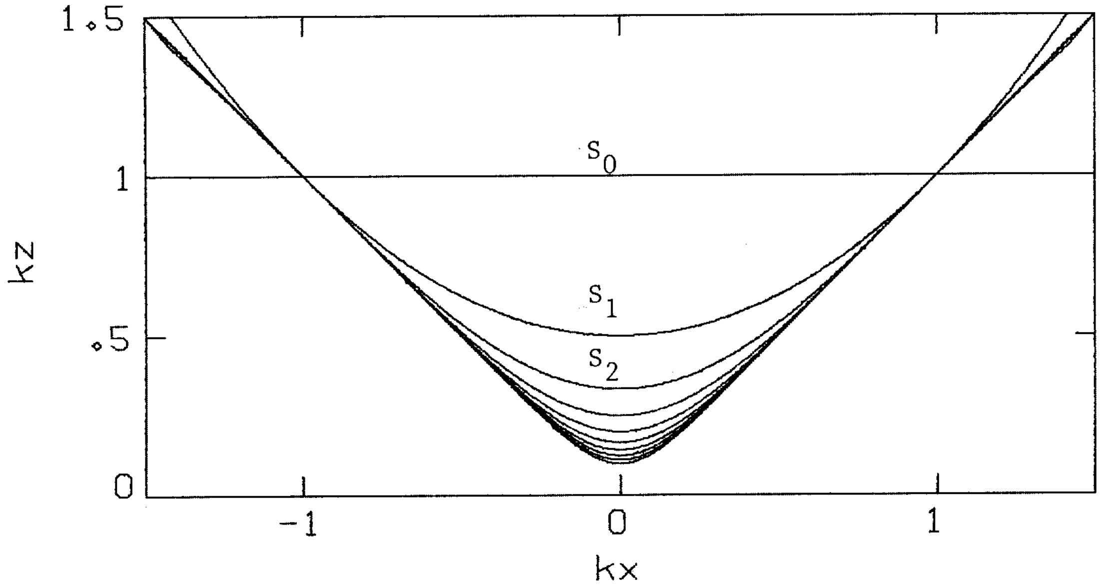

FIG. 2. Extrapolation equation for Laplace equation. Approximations converge quadratically about $k_x = 1$.

$$S_{n+1} = \lambda + \frac{AB - \lambda^2}{\lambda + S_n} \tag{4}$$

We intend to show that S_n is an impedance function for any n, not just at $n = \infty$. An impedance function has just two properties: first, it is causal, and second, its frequency domain representation has a positive real part. We will assume that these properties are possessed by S_n and then show that they are also possessed by S_{n+1}. Naturally, we will also be assuming that the AB we are given is of the form of a squared impedance function. Such a function may be called a ***causal branch-cut*** function (or cbc function) because it is permitted to lie everywhere in the complex plane except on the negative real axis (since its phase angle is double that of the impedance function). An impedance function squared in the frequency domain is one convolved with itself in the time domain; hence the numerator $AB - \lambda^2$ is obviously causal. The denominator $\lambda + S_n$ is the sum of two impedances, so it is an impedance. Likewise its inverse is an impedance, so we can combine everything to see that S_{n+1} is causal.

Positivity

I have not yet been able to show analytically that the recurrence preserves positivity. However, a simple numerical test case was convincing. Take $AB = \exp(i176\pi/180)$ which has an exact square root near the imaginary axis. This should be a hard case, and a poor choice of λ and S_0 should be able to cause one of the S_n to jump over 90 degrees. When starting values for λ and S_0 were taken at various places along the positive imaginary axis, convergence to 88 degrees always resulted; and none of the approximations ever exceeded 90 degrees. Taking negative imaginary values for λ and S_0 resulted in convergence at -92 degrees with all approximations along the way having negative real parts.

It was interesting that convergence was ***always*** achieved although sometimes slowly. This leads me to the assertion that for any cbc function AB the square root recurrence will converge to the positive square root if the sign of the imaginary part of AB is in agreement with the sign of the imaginary part of λ and of S_0 for all frequencies ω. The Laplace equation was a degenerate case in which AB did not have either frequency dependence or an imaginary part, so it was appropriate to take λ and S_0 to be real.

Elastic Waves

For simplicity take the elastic wave problem to have been transformed from physical variables to p-wave, s-wave variables. Then we have

$$AB = -k_z^2\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = k_x^2\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} - \omega^2\begin{bmatrix}\alpha^{-2} & 0\\ 0 & \beta^{-2}\end{bmatrix} \qquad (12)$$

Taking

$$S_0 = \frac{-i\omega}{\alpha}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \quad \text{and} \quad \lambda = \frac{-i\omega}{\beta}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \qquad (13a,b)$$

The matrices are all diagonal and things proceed rather simply. First order forms are

$$S_\alpha = \frac{-i\omega}{\alpha} + \frac{k_x^2}{-i\omega\left(\frac{1}{\beta} + \frac{1}{\alpha}\right)} \tag{14a}$$

$$S_\beta = \frac{-i\omega}{\beta} + \frac{k_x^2}{-i\omega\left(\frac{1}{\beta} + \frac{1}{\alpha}\right)} \tag{14b}$$

Graphs of these and higher order forms are shown in figure 3.

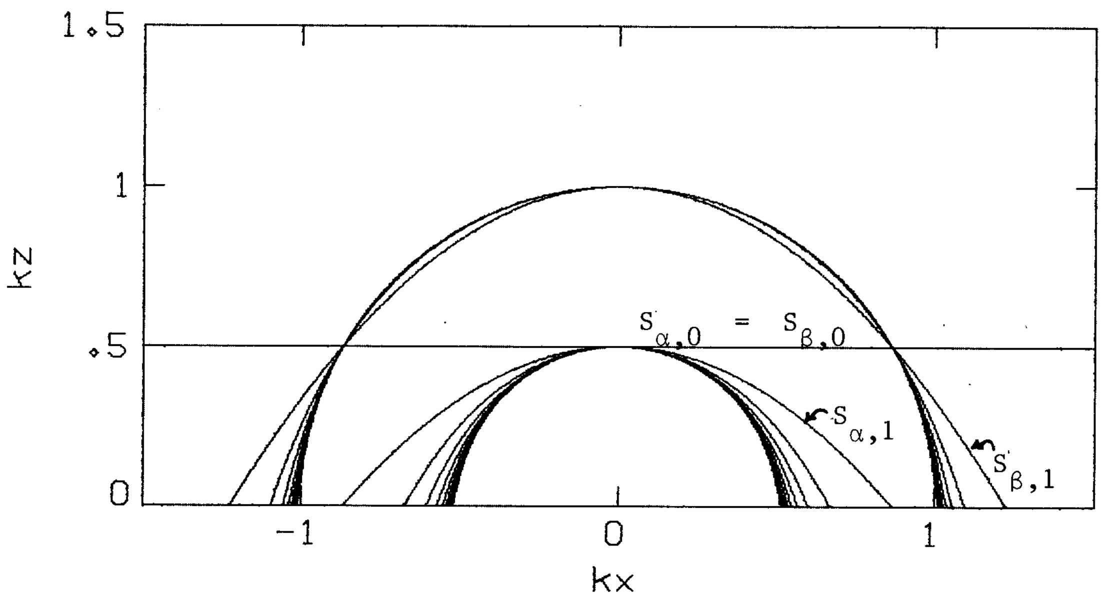

FIG. 3. Dispersion relations for elastic waves.

It is notable that S_β fits exactly not only when $\omega^2 = k_z^2\alpha^2$ but also when $\omega^2 = k_z^2\beta^2$. The forms (14) do not fit as well as the 15-degree equation in the small k_x region but they should fit better elsewhere.

Bullet-proofing

In acoustics the ab function for pressure is

$$ab \;=\; -k_z^2 \;=\; \frac{-\omega^2}{v^2} - \rho \,\frac{\partial}{\partial_x}\,\frac{1}{\rho}\,\frac{\partial}{\partial_x} \qquad (15)$$

which may be written as

$$ab \;=\; \frac{\rho^{\frac{1}{2}}}{v}\left[(-i\omega)^2 + v\left(\rho^{\frac{1}{2}}\,\frac{\partial}{\partial_x}\,\rho^{-\frac{1}{2}}\right)\left(\rho^{\frac{1}{2}}\,\frac{\partial}{\partial_x}\,\rho^{-\frac{1}{2}}\right)^T v\right]\frac{1}{\rho^{\frac{1}{2}}v} \qquad (16)$$

Letting D_1 and D_2 denote diagonal matrices and the positive symmetric x differential operator be denoted by T we have

$$\frac{\partial^2}{\partial z^2}\,u \;=\; D_1[I + T]D_2 u \qquad (17)$$

We are experienced at finding $[I + T]^{\frac{1}{2}}$ with the Muir expansion and we could obviously find other expansions by means of (4). When asked to find a square root representation for (17) what we do is let $D_1D_2 = D^2$ and solve

$$\frac{\partial}{\partial z}\,w \;=\; D^{\frac{1}{2}}[I + T]^{\frac{1}{2}}D^{\frac{1}{2}}w \qquad (18)$$

Substituting (18) into itself does not reduce to a form which may obviously be identified with (17) because the diagonal matrices do not commute with T. Physically we know that D_1 and D_2 will commute with T over regions in which there is no lateral material variation. In SEP-16 we showed that equation (18) dissipates the function w^*w, so we regard w as an energy flux variable. The justification for this is still not completely understood but it seems to begin as follows. Recall (2a) and (2b)

$$\frac{\partial^2}{\partial z^2}\begin{bmatrix} u \\ v \end{bmatrix} \;=\; \begin{bmatrix} ab & 0 \\ 0 & ba \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} \qquad (19)$$

In acoustics this takes the form

$$\frac{\partial^2}{\partial z^2}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}\begin{bmatrix} I+T & 0 \\ 0 & I+T \end{bmatrix}\begin{bmatrix} D_2 & 0 \\ 0 & D_1 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} \tag{20}$$

Defining new variables

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} D_2 & 0 \\ 0 & D_1 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} \tag{21}$$

we obtain

$$\frac{\partial^2}{\partial z^2}\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} D_1 D_2 & 0 \\ 0 & D_1 D_2 \end{bmatrix}\begin{bmatrix} I+T & 0 \\ 0 & I+T \end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \tag{20}$$

Both equations are now the same so we can abandon one of them. Bringing a diagonal $D^2 = D_1 D_2$ to the left side we have

$$D^{-2}\frac{\partial^2}{\partial z^2} w' = [I + T]\, w' \tag{21}$$

The square of equation (18) is still not quite the same as (21). It is known (see for example Hildebrand, ***Methods of Applied Mathematics***, p. 74-80) that there exists a transformation which simultaneously diagonalizes [I + T] and converts the quadratic form $(w')^* D^{-2} w'$ to the form $w^* w$. Also, most of the book ***Discrete and Continuous Boundary Problems***, by F. V. Atkinson, seems to relate to this type of problem.