Taylor series derivation of nonstationary wavefield extrapolators

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Summary

A Taylor series approach is used to derive two elemental and complementary wavefield extrapolators directly from the Helmholtz equation (i.e. the wave equation after a temporal Fourier transform). These extrapolators are for vertical propagation when velocity varies arbitrarily in the horizontal direction. The Helmholtz equation provides two alternative and exact pseudodifferential operator forms for the second derivative with respect to the vertical coordinate. These lead to alternative but approximate pseudodifferential operators for the nth vertical derivative as required in the Taylor series. When these approximate operators are substituted into the Taylor series, the series can be summed to give the two alternative extrapolators: PSPI (*phase shift plus interpolation*) and NSPS (*nonstationary phase shift)*. The resulting extrapolators are Fourier integral operators and are approximate unless velocity is constant when they both simplify to ordinary phase shift.

An investigation of the accuracy of these approximations is done using the *composition theorem* of pseudodifferential operators. The result suggests that NSPS and PSPI produce errors that are complementary in that they tend to cancel when the extrapolations are averaged together. A numerical example supports this conclusion.

Introduction

Explicit one-way wavefield extrapolators can be conveniently formulated as phase-shift operators in the Fourier domain. We take the extrapolation direction to be the vertical coordinate (z) and, for a particular extrapolation step, allow the velocity to depend only upon the transverse coordinates. Gazdag (1978) applied the phase-shift method to the vertical extrapolation of waves through a constant-velocity step which allowed a v(z) medium to be handled. Berkhout (1981) showed that the phase-shift method can be regarded as an infinite order Taylor series extrapolation.

Gazdag and Squazzero (1984) extended phase shift to lateral velocity variation through the PSPI algorithm. Stoffa et al. (1990) proposed the *spilt-step Fourier* technique that applied the vertical phase delay (thin-lens term) exactly in the (x, ω) domain and used a single reference velocity for the angle-dependent delay (focusing term) in the (k_x, ω) domain. Better approximations to the above method were developed by Wu (1992) and Wu and Wu (1998) as the phase-screen method that extended the split-step method by improving focusing. Margrave and Ferguson (1997 and 1999a) used nonstationary filter theory to derive two alternative extensions of phase-shift to lateral velocity variations. They gave explicit, analytic integral forms for these

extensions that can be identified as Fourier integral operators (Stein, 1993). One form was shown to be a generalization of PSPI in the limiting case of very rapid lateral velocity variations. The other, called NSPS, has been shown to be the (x, ω) domain transpose of PSPI (Margrave and Ferguson, 1999b).

In related developments, Fishman and McCoy (1985) gave a general algorithm for factoring the Helmholtz operator, for arbitrary lateral velocity variations, into upgoing and downgoing operators and derived several approximate factorizations. One of their approximations is equivalent to the generalized PSPI expression of Margrave and Ferguson (1999a). Grimbergen et al. (1998) used eigenvalue decomposition to numerically factor the Helmholtz equation. For arbitrary lateral velocity variations, they approximated the lateral derivatives with finite difference operators and achieved a high-quality though computationally intensive factorization. Yao and Margrave (2000) demonstrate that a similar eigenvalue factorization may be performed in the Fourier domain that affords a better lateral derivative.

In this paper, we show that a Taylor series approach can be used to derive the PSPI and NSPS integral operators from the Helmholtz equation for laterally varying media. The derivation shows precisely how both operators are approximate but in complementary ways. We show that first order error terms from both operators tend to be similar but opposite in sign. This suggests that using them alternately in a multi-step extrapolation will lead to higher accuracy.

Exact second derivatives from the Helmholtz equation

A seismic wavefield $\psi(z)$ at depth z is predictable from a wavefield $\psi(0)$ recorded at $z = 0$ by Taylor series (Berkhout, 1981). All orders of the depth derivatives of ψ must be known at $z = 0$. However, from the Helmholtz equation, only the second-depth derivative is easily found. Two equivalent forms of the second derivative, derived from the Helmholtz equation, are classifiable as *pseudo differential operators* or *nonstationary filters*. The two equivalent second derivatives yield two approximate forms for the nth-depth derivative, and thus to two elemental, but not equivalent, extrapolators. (These forms are elemental in that they are simple, complementary and can be combined to get higher-order extrapolators.)

The Taylor series expansion of a monochromatic wavefield, $\psi(x, z, \omega)$, in the z coordinate, gives an expression for the wavefield at depth z in terms of the wavefield at the reference depth 0, and is

$$\psi(x,z) = \psi(x,0) + \sum_{j=1}^{\infty} \frac{z^j}{j!} \left[\frac{\partial^j}{\partial z^j} \psi(x,z) \right]_{z=0} \qquad (1)$$

where the ω dependence is suppressed. In the constant velocity case, Berkhout (1981) showed that all orders of derivatives can be obtained exactly from the wave equation (in

the (k_x, ω) domain and the resulting series can be summed to give the phase-shift operator.

An expression for the second depth derivative is found using the Helmholtz equation

$$\frac{\partial^2}{\partial z^2}\psi(x,z) = -\left[\frac{\partial^2}{\partial x^2}+\left(\frac{\omega}{v(x)}\right)^2\right]\psi(x,z) \qquad (2)$$

where $v(x)$ is the wave propagation velocity. The Fourier transform of equation (2) over x gives

$$\frac{\partial^2}{\partial z^2}\hat{\psi}(k_x,z) = -\int k_z^2(x,k)\psi(x,z)\exp(ik_x x)dx \quad (3)$$

where the spectrum $\hat{\psi}$ of ψ is

$$\hat{\psi}(k_x,z) = \int \psi(x,z)\exp(ik_x x)dx \qquad (4)$$

and the vertical wave number k_z is defined through

$$k_z^2(x,k_x) = \left(\frac{\omega}{v(x)}\right)^2 - k_x^2 . \qquad (5)$$

Equation (3) is an exact expression for the second z derivative of ψ and is an *adjoint-form pseudodifferential operator* that maps a wavefield ψ to the second-depth derivative of a spectrum $\hat{\psi}$, and whose *symbol* is $-k_z^2$. It is also a nonstationary *convolution* filter. As a nonstationary filter, equation (3) is in *mixed-domain* form, the input being a wavefield and the output a spectrum (Margrave, 1998).

An alternative, exact prescription for the second depth derivative is found by substituting for ψ on the right-hand side of equation (2) with the inverse Fourier transform of $\hat{\psi}$

$$\psi(x,z) = \frac{1}{2\pi}\int \hat{\psi}(k_x,z)\exp(-ik_x x)dk_x . \qquad (6)$$

The operator contained by the square brackets in equation (2) can be moved inside the Fourier integral with the result

$$\frac{\partial^2}{\partial z^2}\psi(x,z) = -(2\pi)^{-1}\int k_z^2(x,k_x)\hat{\psi}(k_x,z)\exp(-ik_x x)\,dk_x .$$

Equation (7) is a *standard-form pseudodifferential operator* (Stein, 1993: 231) that maps a spectrum $\hat{\psi}$ to the second depth derivative of a wavefield ψ, and whose *symbol* is also $-k_z^2$. It is also a *nonstationary combination filter* (Margrave, 1998). Like the convolution filter in equation (3) the combination filter is a mixed-domain filter; the input and output are in different domains. These two expressions for the second derivative are exact, and therefore, equivalent.

Estimation of all depth derivatives

By inspection, the nonstationary convolution filter of equation (3) suggests that the nth depth derivative is approximately

$$\frac{\partial^n}{\partial z^n}\hat{\psi}(x,z) \approx \left[\hat{D}_\pm^n \psi\right](k_x,z) \equiv \int \left[\pm ik_z\right]^n \psi(x,z)\exp(ik_x x)dx \qquad (8)$$

where the hat over the operator $\hat{D}_\pm^n$ indicates that a forward Fourier integral is applied.

Similarly, from the combination filter of equation (7)

$$\frac{\partial^n}{\partial z^n}\psi(x,z) \approx \left[D_\pm^n \hat{\psi}\right](x,z)$$

$$\equiv (2\pi)^{-1}\int \left[\pm ik_z\right]^n \hat{\psi}(k_x,z)\exp(-ik_x x)dk_x \qquad (9)$$

where the derivative operator $D_\pm^n$ applies an inverse Fourier transform.

The operators $D_\pm^n$ and $\hat{D}_\pm^n$ provide the exact second derivatives but are only approximate for all other orders. In the limit of constant velocity they become exact for all n. When $D_\pm^n$ and $\hat{D}_\pm^n$ are used in the Taylor series expansion, the results are the two elemental extrapolation methods PSPI and NSPS.

Returning to equation (1), the required n^{th} depth derivatives can be replaced by $D_\pm^n$ to give

$$\psi(x,z) \approx \psi(x,0) + \sum_{j=1}^\infty \frac{z^j}{j!}\left[D_\pm^j \hat{\psi}\right](x,0) \qquad (10)$$

or, using the integral form for $D_\pm^n$ and interchanging the order of summation and integration leads to

$$\psi(x,z) \approx (2\pi)^{-1}\int \sum_{j=0}^\infty \frac{(\pm izk_z)^j}{j!}\hat{\psi}(k_x,0)\exp(-ik_x x)dk_x \quad (11)$$

where the first term in equation (10) is included through the 0th term in the summation. Recognizing the series expansion for the exponential function allows this to be written as

$$\psi(x,z) \approx (2\pi)^{-1}\int \alpha(x,k_x,\pm z)\hat{\psi}(k_x,0)\exp(-ik_x x)dk_x \quad (12)$$

where the symbol of this pseudo-differential operator is

$$\alpha(x,k_x,\pm z) = \exp(\pm izk_z(x,k_x)), \qquad (13)$$

and k_z is given by equation (5).

Equation (12) is the nonstationary wavefield extrapolator identified as the limiting form of PSPI by Margrave and Ferguson (1999a). Fishman and McCoy (1985) developed the same expression as an approximate factorization of the Helmholtz equation when v depends only on the transverse coordinates. They characterize it as a *high frequency approximation*.

The development of a second expression for wavefield extrapolation using $\hat{D}_\pm^n$ (equation (8)) follows in a similar fashion but starts with the Fourier transform of the Taylor series in equation (1)

$$\hat{\psi}(k_x,z) = \hat{\psi}(k_x,0) + \sum_{j=1}^\infty \frac{z^j}{j!}\left[\frac{\partial^j}{\partial z^j}\hat{\psi}(k_x,0)\right]_{z=0} . \qquad (14)$$

After replacing the derivatives with the approximation $\hat{D}_\pm^n$ and performing similar manipulations as before, this becomes

$$\hat{\psi}(k_x,z) \approx \int \alpha(x,k_x,\pm z)\psi(x,0)\exp(ik_x x)dx \qquad (15)$$

with α given by equation (13). This result is the NSPS extrapolator identified by Margrave and Ferguson (1999a).

Assessing the accuracy of the approximations

The wavefield extrapolators given by equations (12) and (15) have been well described in Margrave and Ferguson (1999a). They are equivalent to ordinary phase shift when

velocity is constant but can give dramatically different results with rapid lateral gradients. In the (x,ω) domain, they can be shown to be the transpose of one another (Margrave and Ferguson 1999b). Here we investigate the accuracy of the approximations made in the preceding derivation. For this purpose, we compare the exact second derivatives (equations (3) and (7)) to the result of two applications of the approximate first derivatives $\hat{D}_{\pm}^{1}$ and $D_{\pm}^{1}$. This comparison reveals error terms in both approximations that are complex valued, and have opposing trends.

Beginning with $\hat{D}_{\pm}^{1}$, the approximate second derivative is

$$\frac{\partial^2}{\partial z^2}\hat{\psi} \approx \left[\hat{D}_{\pm}^{1}\hat{D}_{\pm}^{1}\psi\right](k_x) = -\int \gamma_z\,(y,k_x)\psi(y)\exp(ik_x y)dy \qquad (16)$$

where symbol γ_z is

$$\gamma_z = (2\pi)^{-1}\iint k_z\,(x,k_x)k_z\,(y,m)\exp\big(i[m-k_x][y-x]\big)dmdx. \qquad (17)$$

From $D_{\cdot}^{1}$ the approximate second derivative is

$$\frac{\partial^2}{\partial z^2}\psi \approx \left[D_{\pm}^{1}D_{\pm}^{1}\hat{\psi}\right](x) = -(2\pi)^{-1}\int \gamma_z^{*}(x,m)\hat{\psi}(m,z)\exp(-imx)dm \qquad (18)$$

where γ_z^{*} is the complex conjugate of γ_z.

Equations (16) and (18) are pseudo-differential equations that map the wavefield ψ (equation (16)) or the spectrum $\hat{\psi}$ (equation (18)) to their approximate second depth derivatives simultaneous with a change in Fourier domain. The symbol γ_z is the *composition* of symbols $k_z\,(x,k_x)$ and $k_z\,(y,m)$. A general theorem for a composition of symbols (Stein, 1993: 237-238) can be used to provide an asymptotic formula for γ_z with the result

$$\gamma_z\,(x,m) = k_z^{2}(x,m) - i\frac{\partial}{\partial m}k_z\,(x,m)\frac{\partial}{\partial x}k_z\,(x,m)$$
$$-\frac{1}{2}\frac{\partial^2}{\partial m^2}k_z\,(x,m)\frac{\partial^2}{\partial x^2}k_z\,(x,m)+\cdots \qquad (19)$$

Since the even terms are real, γ_z^{*} will have the opposite sign for every other term. The first term in this asymptotic series reproduces the action of the exact second-depth derivative. Higher order terms represent error, and the odd numbered terms are complex. Generation of complex terms by application of $\hat{D}_{\pm}^{n}$ or $D_{\pm}^{n}$ may explain the instability of PSPI observed by Etgen (1994) and demonstrated for NSPS by Margrave and Ferguson (1999b). Unconstrained complex values in the exponent, k_z, of α (equation 13) can lead to instability during recursive application.

This result suggests, though it falls short of a proof, that the first-order errors in the PSPI and NSPS extrapolators tend to cancel one another. NSPS uses $\hat{D}_{\pm}^{n}$ while PSPI uses $D_{\pm}^{n}$ and these derivative operators have been shown to have complementary errors. However, the extrapolators also use all other orders of the D operators so the complete story is much more complex than we present here.

The validity of the asymptotic series (equation (19) requires the existence of all orders of spatial and wavenumber derivatives of k_z. The wavenumber derivatives will exist to all orders except possibly at the evanescent boundary. The spatial derivatives impose a smoothness condition on v(x). This condition is not necessarily required for the NSPS and PSPI extrapolators themselves, but it is needed for this form of error analysis.

These investigations, together with the fact that NSPS and PSPI are the (x,ω) domain transposes of one another, suggest that a symmetric combination of these elemental extrapolators may be more accurate. This does indeed seem to be the case as was reported by Margrave and Ferguson (1999b) but there are many possible symmetric forms. Also, either NSPS or PSPI is as accurate as the best explicit finite difference technique and accuracy increases as the extrapolation step size decreases. So the need for higher-order symmetric forms may be academic.

As an illustration, consider an initial wavefield consisting of nine bandlimited impulses arranged symmetrically from -1500 m to +1500 at .52 seconds. Let a velocity model be defined such that v=5000 m/s if x<0 and v=2000 m/s if x>0. Figure 1 shows the result of the extrapolation of the initial wavefield 200 m upward using NSPS while Figure 2 shows the result from using PSPI. The PSPI result shows characteristic wavefield discontinuities where the velocity model is discontinuous. While the NSPS result looks more pleasing it is also incorrect since the hyperbolae should change slope where they cross the velocity boundary. (The PSPI result does change slope but is discontinuous.) Figure 3 shows the simple arithmetic average of the results in Figures 1 and 2. The result in Figure 3 is more physical than either of the others because it has minimal discontinuities and events tend to change slope at velocity boundaries. The arithmetic average is a type of symmetric extrapolator. Another possibility is the alternating cascade of NSPS and PSPI. Even though this example violates the conventions of the derivation in that k_z is discontinuous, the expected complementary behavior is still seen. This suggests that the result is more general than the limitations of our derivation might indicate.

Conclusions

The NSPS and PSPI wavefield extrapolators can be derived from the Helmholtz equation for laterally varying media. The Taylor series approach relies on the development of approximate pseudodifferential operators for the nth order wavefield derivatives taken in the extrapolation direction. Two alternative forms for such operators were developed from the Helmholtz equation. Both forms have the same kernel but one applies it with a change from the Fourier wavenumber domain to the space domain and the other changes domains in the reverse direction. When these approximate derivatives are used in the Taylor series, the series can be summed to generate two alternative wavefield extrapolators of the familiar exponential form.

The effectiveness of the approximate derivative operators was assessed using the composition theorem of pseudodifferential operators. The result suggests that the two elementary extrapolators are complementary in that their errors tend to oppose one another. A numerical example supports this by showing that the average of NSPS and PSPI extrapolations is superior to either alone.

Acknowledgements

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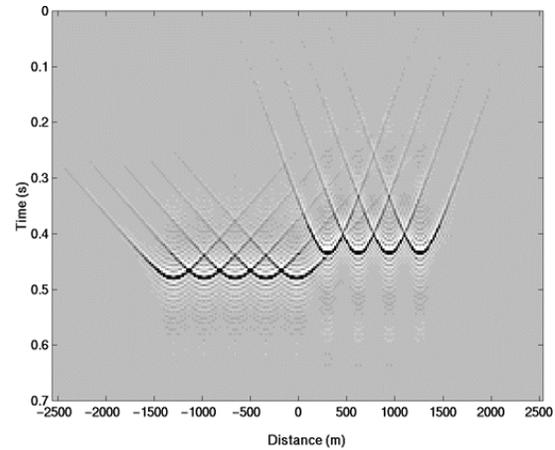
Figure 1. A horizontal alignment of 9 bandlimited impulses have been upward extrapolated 200 m using NSPS through a velocity model that is discontinuous at x=0. On the left, the velocity was 5000 m/s and on the right it was 2000 m/s.
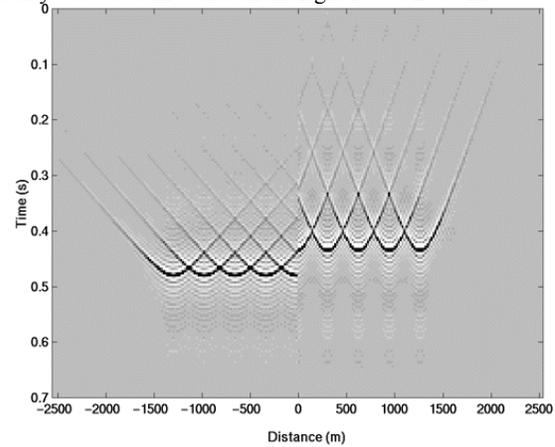

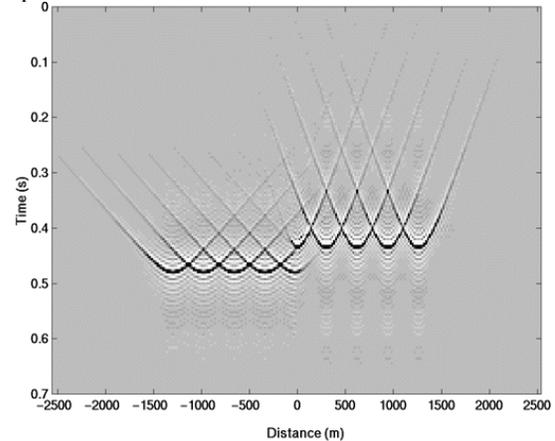Figure 2. A similar result to Figure 1 except that the PSPI extrapolator has been used.

Figure 3. The wavefield of Figures 1 and 2 have been arithmetically averaged.