Differential operators 2: The second derivative

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ABSTRACT

Differential operators are used in many seismic data processes such as triangle filters to reduce aliasing, finite difference solutions to the wave equation, and wavelet correction when modelling with diffractions or migrating with Kirchhoff algorithms. Short operators may be quite accurate when the data are restricted to low order polynomials, but may be inaccurate in other applications.

This is the second of three papers on differential operators and deals specifically with the second derivative. The first paper deals with the first derivative and the third paper deals with the square-root derivative.

The purpose of this paper is to evaluate visually the short operators that approximate a second derivative.

APPLICATIONS

The first paper in this series presents a number of applications for the different derivatives. They are:

1. The rho filter that applies corrections to the wavelet after diffraction modelling or Kirchhoff migration.

2. Fast filtering in the time domain that differentiates the filter operator to delta functions and is then applied to a trace that has been integrated. Convolving with the delta functions is equivalent to summing a few samples.

3. Finite difference solutions to the wave equation

ASSUMPTIONS

I assume an array of data f_n, that I call a trace, is sampled from a continuous function $f(t)$ defined in time. Its Fourier transform is in the frequency domain is F_n. The trace can be in either time or distance transforming into the frequency or wavenumber domains. I will assume the trace to be in the time domain and refer to the transform domain parameters as frequency.

The displayed results are created using MATLAB with code

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\2008-Matlab\DifferentialOperatorSecond.m
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INTRODUCTION

The second derivative is much easier to implement than the first derivative as the simplest implementation provides very good results, especially with the phase. The second derivative produces a 180 degree phase shift that is simple represented by a change in the sign. The amplitudes of the samples are even about time zero (i.e.

$f(-t_1) = f(+t_1)$). However, greater accuracy is usually required, especially when being applied many times when used with solutions to the wave-equation. A seismic trace is usually over sampled by a factor of three, or the maximum frequency is one third the Nyquist frequency. Operators usually have good accuracy at the lower frequencies and work well with the time sampled data.

In the spatial direction, the data is usually under sampled and is often aliased in areas with steep dip. This is a typical area where the second derivative is applied and knowing the frequency limits of the operator becomes essential in designing an accurate algorithm. In the time direction, a three point operator may be adequate, while in the spatial directions a five or larger operator may be required. Different approximations to the derivatives have lead to names of migration algorithms such as the fifteen forty-five and sixty degree algorithms.

SECOND DERIVATIVE

Since differentiation is a filtering process, the second derivative could be obtained by convolving twice with a first derivative. But the first derivative operator, in its simple forms as a forward and backward approximation, leads to phase errors. However, using one first, and the other second, an accurate second derivative can be approximated.

Assume the sequence f_n is differentiated to f'_n and the second derivative is f''_n. The forward difference derivative

$$\widehat{f}'_n = \frac{-f_n + f_{n+1}}{\delta t}, \tag{1}$$

and the backward difference

$$\widetilde{f}'_n = \frac{-f_{n-1} + f_n}{\delta t}, \tag{2}$$

when combined give the second derivative,

$$f''_n = \frac{-\widetilde{f}'_n + \widehat{f}'_n}{\delta t} = \frac{-\dfrac{-f_{n-1} + f_n}{\delta t} + \dfrac{-f_n + f_{n+1}}{\delta t}}{\delta t}. \tag{3}$$

or

$$\boxed{f''_n = \frac{f_{n-1} - 2f_n + f_{n+1}}{(\delta t)^2}}. \tag{4}$$

This is a well known result and is used extensively.

Consider another approach that uses the Taylor series:

$$f(t+\Delta t)= f(t)+(\Delta t)\frac{\partial f}{\partial t}(t)+\frac{(\Delta t)^2}{2!}\frac{\partial^2 f(t)}{\partial t^2}+\frac{(\Delta t)^3}{3!}\frac{\partial^3 f(t)}{\partial t^3}+\frac{(\Delta x)^4}{4!}\frac{\partial^4 f(t)}{\partial t^4}... \quad ,(5)$$

or with a negative increment

$$f(t-\Delta t)= f(t)-(\Delta t)\frac{\partial f}{\partial t}(t)+\frac{(\Delta t)^2}{2!}\frac{\partial^2 f(t)}{\partial t^2}-\frac{(\Delta t)^3}{3!}\frac{\partial^3 f(t)}{\partial t^3}+\frac{(\Delta x)^4}{4!}\frac{\partial^4 f(t)}{\partial t^4}-... \quad . (6)$$

Adding these two equations and reorganizing gives

$$\frac{f(t-\Delta t)-2f(t)+f(t+\Delta t)}{(\Delta t)^2}=\frac{\partial^2 f(t)}{\partial t^2}+\frac{(\Delta t)^2}{12}\frac{\partial^4 f(t)}{\partial t^4}+... \quad , \qquad (7)$$

where all the odd order derivative are now gone. The left side is identical to the first approximation to the second derivative in equation (3). We continue the rearrangement to give

$$\frac{\partial^2 f(t)}{\partial t^2}=\frac{f(t-\Delta t)-2f(t)+f(t+\Delta t)}{(\Delta t)^2}-\frac{(\Delta t)^2}{12}\frac{\partial^4 f(t)}{\partial t^4}+... \quad , \qquad (8)$$

where we now see an accurate representation of the second derivative that includes higher order derivatives. If our data is band limited, or smooth enough such the higher order derivatives are zero, then the approximation given by (4) become an exact solution.

If there are higher order derivatives, then we can include the fourth derivative by using

$$\frac{f(t-\Delta t)-2f(t)+f(t+\Delta t)}{(\Delta t)^2}=\frac{\partial^2 f(t)}{\partial t^2}\left(1+\frac{(\Delta t)^2}{12}\frac{\partial^2 f(t)}{\partial t^2}\right)+... \quad , \qquad (9)$$

where we now see only second order terms plus the sixth order and above. Solving for the second derivative we get a recursive form

$$\frac{\partial^2 f(t)}{\partial t^2}=\frac{f(t-\Delta t)-2f(t)+f(t+\Delta t)}{(\Delta t)^2\left(1+\frac{(\Delta t)^2}{12}\frac{\partial^2 f(t)}{\partial t^2}\right)}+... \quad . \qquad (10)$$

We can substitute a simple form of the second derivative from equation (4) into the denominator,

$$\frac{\partial^2 f(t)}{\partial t^2}=\frac{f(t-\Delta t)-2f(t)+f(t+\Delta t)}{(\Delta t)^2\left(1+\frac{f(t-\Delta t)-2f(t)+f(t+\Delta t)}{12}\right)}+... \quad , \qquad (11)$$

or in the discrete form we have

$$h_n = \frac{f_{n-1} - 2f_n + f_{n+1}}{(\Delta t)^2 \left[1 + \frac{1}{12}(f_{n-1} - 2f_n + f_{n+1}) \right]} + \ldots \quad (12)$$

Claerbout (1996) indicated that this truncated form can be further improved by modifying the 1/12 scaling term to 1/6.

$$\boxed{h_n = \frac{f_{n-1} - 2f_n + f_{n+1}}{(\Delta t)^2 \left[1 + \frac{1}{6}(f_{n-1} - 2f_n + f_{n+1}) \right]} + \ldots} \quad (13)$$

HIGHER ORDER APPROXIMATIONS

As with the first derivative, we can use the Taylor series to get higher order approximations. I will start with the sum of the two approximations in equation (7), but will continue in discrete form and assume the interval is unity, i.e.,

$$f_{n-1} - 2f_n + f_{n+1} = f_n'' + \frac{1}{12} f''''_n + \ldots \quad (14)$$

We do need an approximation to the fourth derivative and I will get that by taking the simple second derivative of the second derivative, i.e.,

$$f''_n = f_{n-1} - 2f_n + f_{n+1}, \quad (15)$$

to get

$$f''''_n = (f_{n-2} - 2f_{n-1} + f_n) - 2(f_{n-1} - 2f_n + f_{n+1}) + (f_n - 2f_{n+1} + f_{n+2}), \quad (16)$$

which simplifies to

$$f''''_n = f_{n-2} - 4f_{n-1} + 6f_n - 4f_{n+1} + f_{n+2}. \quad (17)$$

The fourth order approximation is substituted into (14) to get

$$f_{n-1} - 2f_n + f_{n+1} = f_n'' + \frac{1}{12}(f_{n-2} - 4f_{n-1} + 6f_n - 4f_{n+1} + f_{n+2}) + \ldots \quad (18)$$

and the second derivative becomes

$$f_n'' = f_{n-1} - 2f_n + f_{n+1} - \frac{1}{12}(f_{n-2} - 4f_{n-1} + 6f_n - 4f_{n+1} + f_{n+2}) + \ldots \quad (19)$$

$$\boxed{f_n'' \approx \frac{1}{12}(-f_{n-2} + 16f_{n-1} - 30f_n + 16f_{n+1} + -f_{n+2})} \quad (20)$$

This is the five point central difference equation for the second derivative. We can also solve for a second derivative at the first, second, fourth, or fifth point. The following figure contains many similar approximations to the second derivative and is taken from the internet.

Formula	Error T
$f''(x_i) \simeq \frac{-f(x_{i-3})+4f(x_{i-2})-5f(x_{i-1})+2f(x_i)}{h^2}$	$\frac{11}{12} h^2$
$f''(x_i) \simeq \frac{f(x_{i-1})-2f(x_i)+f(x_{i+1})}{h^2}$	$\frac{1}{12} h^2$
$f''(x_i) \simeq \frac{2f(x_i)-5f(x_{i+1})+4f(x_{i+2})-f(x_{i+3})}{h^2}$	$\frac{11}{12} h^2$
$f''(x_i) \simeq \frac{-10f(x_{i-5})+61f(x_{i-4})-156f(x_{i-3})+214f(x_{i-2})-154f(x_{i-1})+45f(x_i)}{12h^2}$	$\frac{137}{180} h^4$
$f''(x_i) \simeq \frac{f(x_{i-4})-6f(x_{i-3})+14f(x_{i-2})-4f(x_{i-1})-15f(x_i)+10f(x_{i+1})}{12h^2}$	$\frac{13}{180} h^4$
$f''(x_i) \simeq \frac{-f(x_{i-2})+16f(x_{i-1})-30f(x_i)+16f(x_{i+1})-f(x_{i+2})}{12h^2}$	$\frac{1}{90} h^4$
$f''(x_i) \simeq \frac{10f(x_{i-1})-15f(x_i)-4f(x_{i+1})+14f(x_{i+2})-6f(x_{i+3})+f(x_{i+4})}{12h^2}$	$\frac{13}{180} h^4$
$f''(x_i) \simeq \frac{45f(x_i)-154f(x_{i+1})+214f(x_{i+2})-156f(x_{i+3})+61f(x_{i+4})-10f(x_{i+5})}{12h^2}$	$\frac{137}{180} h^4$
$f''(x_i) \simeq \frac{-126f(x_{i-7})+1019f(x_{i-6})-3618f(x_{i-5})+7380f(x_{i-4})-9490f(x_{i-3})+7911f(x_{i-2})-4014f(x_{i-1})+938f(x_i)}{180h^2}$	$\frac{363}{560} h^6$
$f''(x_i) \simeq \frac{11f(x_{i-6})-90f(x_{i-5})+324f(x_{i-4})-670f(x_{i-3})+855f(x_{i-2})-486f(x_{i-1})-70f(x_i)+126f(x_{i+1})}{180h^2}$	$\frac{29}{560} h^6$
$f''(x_i) \simeq \frac{-2f(x_{i-5})+16f(x_{i-4})-54f(x_{i-3})+85f(x_{i-2})+130f(x_{i-1})-378f(x_i)+214f(x_{i+1})-11f(x_{i+2})}{180h^2}$	$\frac{47}{5040} h^6$
$f''(x_i) \simeq \frac{2f(x_{i-3})-27f(x_{i-2})+270f(x_{i-1})-490f(x_i)+270f(x_{i+1})-27f(x_{i+2})+2f(x_{i+3})}{180h^2}$	$\frac{1}{560} h^6$
$f''(x_i) \simeq \frac{-11f(x_{i-2})+214f(x_{i-1})-378f(x_i)+130f(x_{i+1})+85f(x_{i+2})-54f(x_{i+3})+16f(x_{i+4})-2f(x_{i+5})}{180h^2}$	$\frac{47}{5040} h^6$
$f''(x_i) \simeq \frac{126f(x_{i-1})-70f(x_i)-486f(x_{i+1})+855f(x_{i+2})-670f(x_{i+3})+324f(x_{i+4})-90f(x_{i+5})+11f(x_{i+6})}{180h^2}$	$\frac{29}{560} h^6$
$f''(x_i) \simeq \frac{938f(x_i)-4014f(x_{i+1})+7911f(x_{i+2})-9490f(x_{i+3})+7380f(x_{i+4})-3618f(x_{i+5})+1019f(x_{i+6})-126f(x_{i+7})}{180h^2}$	$\frac{363}{560} h^6$

FIG. 1. Examples of various approximations to the second derivative.

`http://documents.wolfram.com/mathematica/Built-inFunctions/AdvancedDocumentation/DifferentialEquations/NDSolve/PartialDifferentialEquations/TheNumericalMethodOfLines/SpatialDerivativeApproximations.html`

As in the first-derivative paper, the above equations are suitable for insertion into a matrix.

The above approximations all assume that the higher order derivatives are zero and that we should only be applying these operators for correspondingly smooth data. This will become more evident when viewing the following spectral properties of the different approximations.

GRAPHICAL EXAMPLES

Figure 2a contains the amplitude spectrum of the second derivative defined by $(j\omega)^2 = -\omega^2$ with N_{fft} = 64. The phase is zero (or 180°) and the amplitude is seen to be increasing with the square of the sample number. The negative frequencies are plotted on the right side of the figure to illustrate what happens in the center at the Nyquist frequency. The inverse transform is plotted in (b).

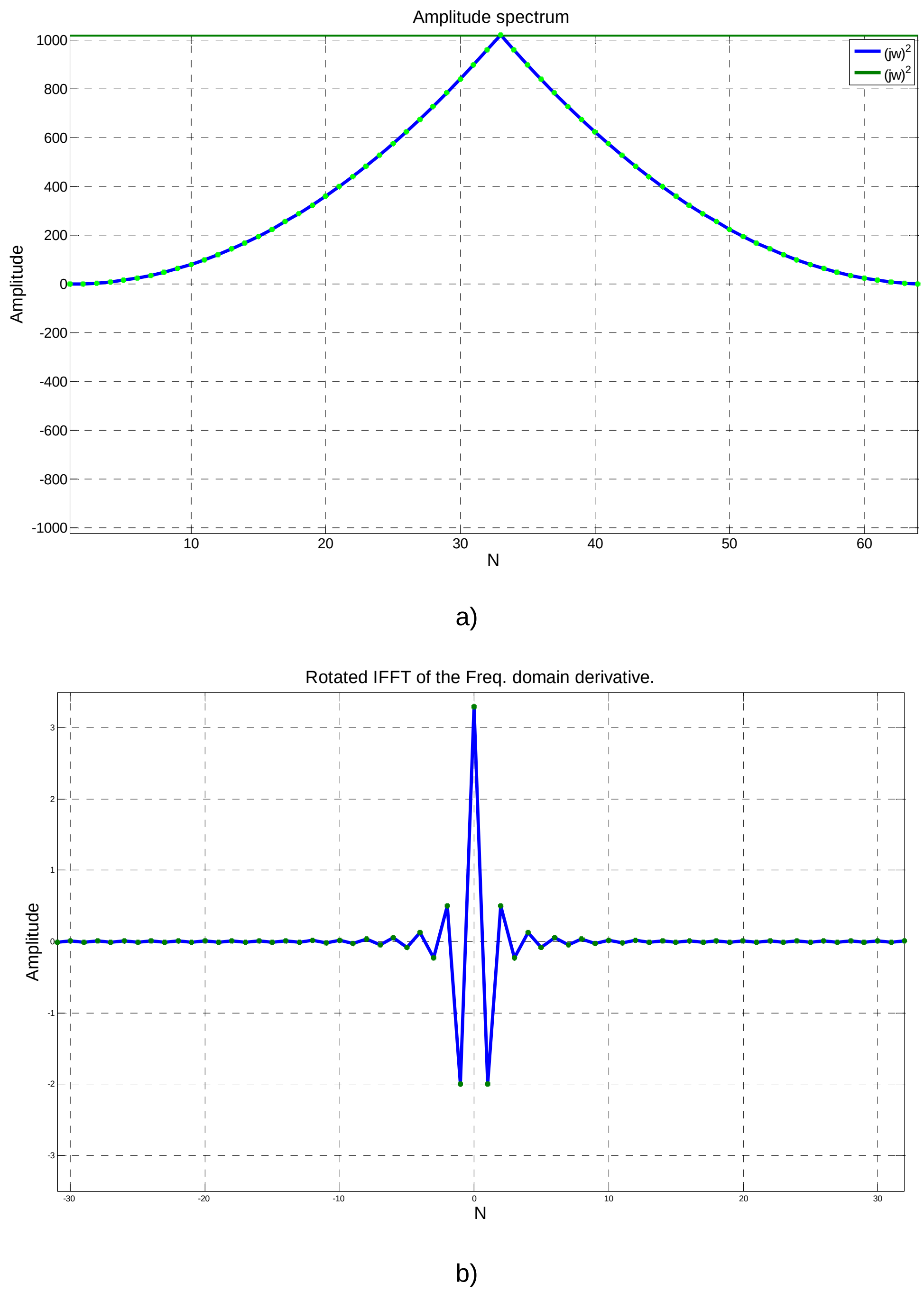
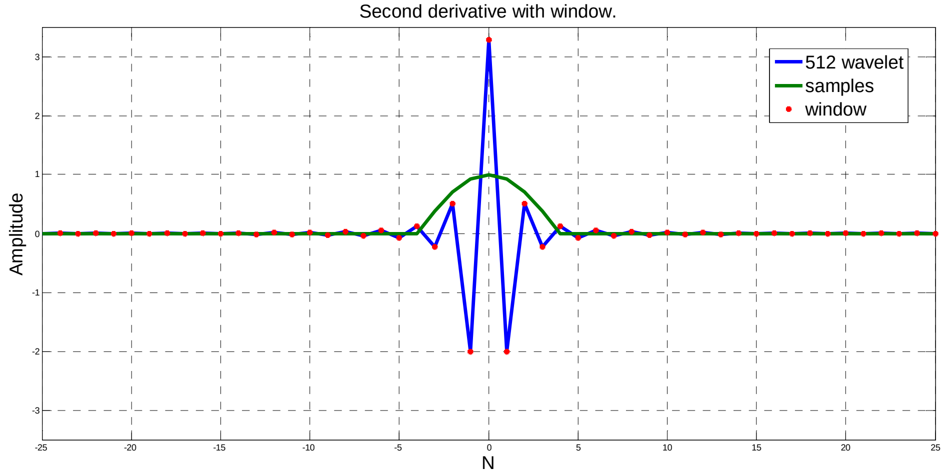
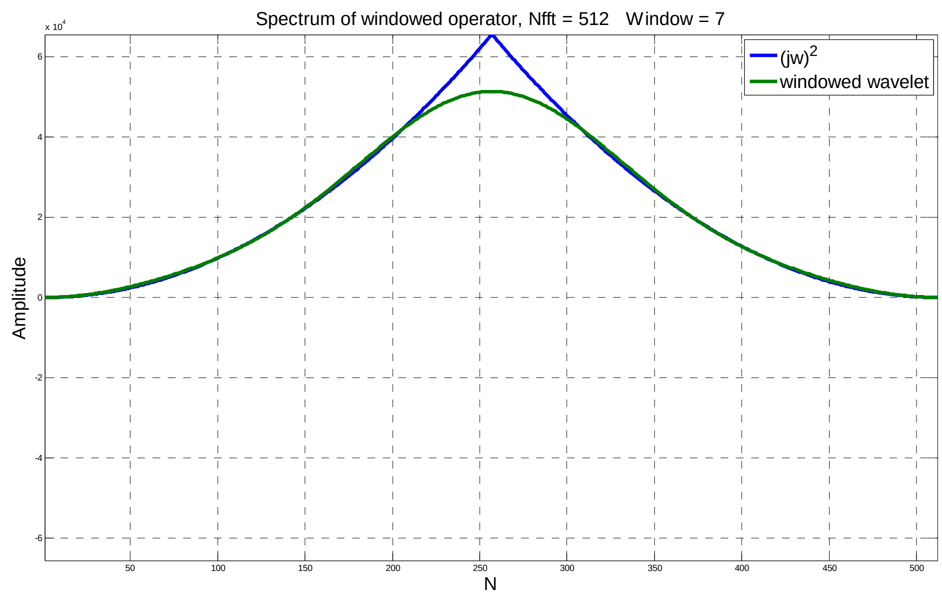


FIG. 2. Amplitude spectrum a) and the inverse transform b) of the second derivative.

The data in Figure 2b shows that a small operator will be effective as most of the energy of the wavelet is concentrated towards the center. To avoid wrap around effects a larger value for N_{fft} will be used (512) and the data zoomed to view the wavelet. A seven point operator is created by windowing with a cosine shown in Figure 3a with the corresponding amplitude spectrum in (b).



a)



b)

FIG. 3. A windowed wavelet a) and b) it spectrum.

The amplitude spectrum looks OK in Figure 3b, but its relative error in Figure 4 appears quite large. The error is due to a slight change in the DC value of the time domain operator. It is really quite small as the amplitudes are small. We can greatly reduce this error by using a raised cosine window as illustrated in Figure 5. This also reduces the bandwidth of the operator as illustrated in Figure 6.

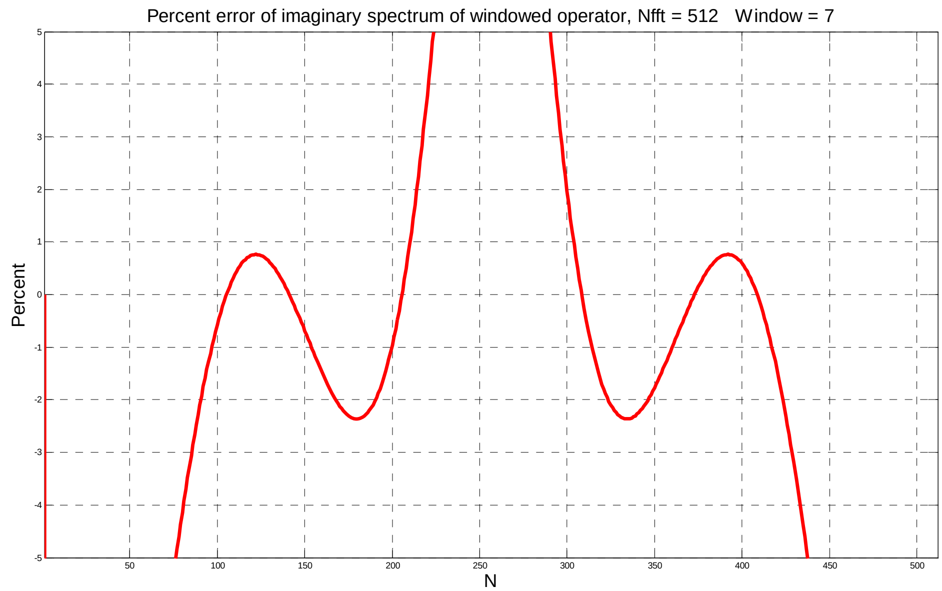


FIG. 4. Error of a seven point operator when using a cosine window.

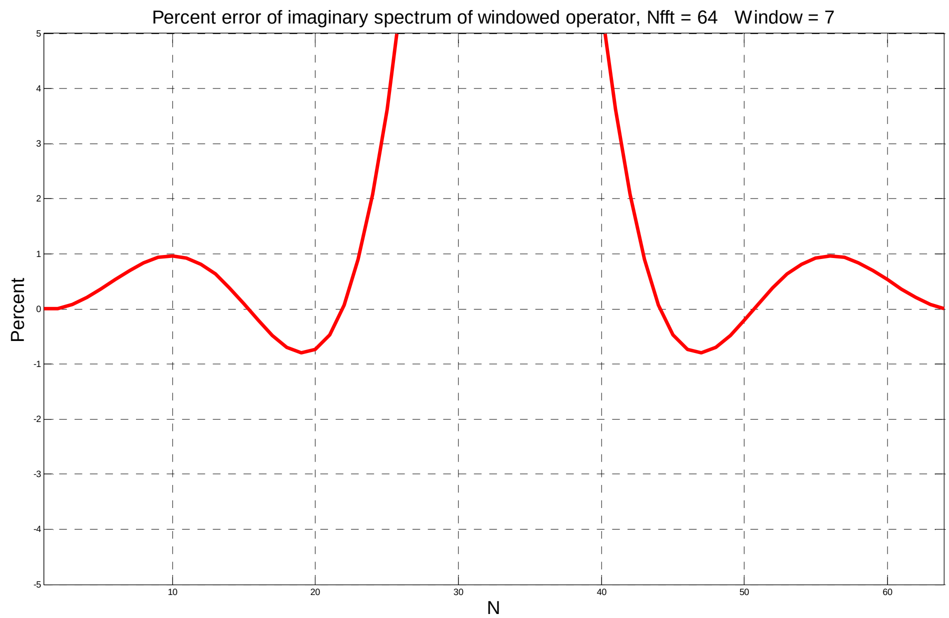


FIG. 5. Error of a seven point operator when using a raised cosine window.

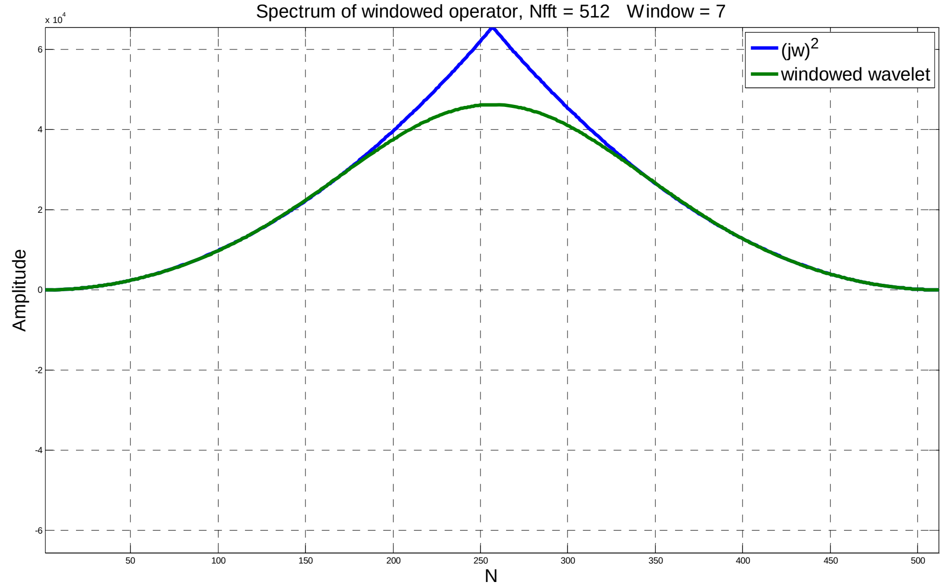


FIG. 6. Amplitude spectrum of the seven point operator when a raised cosine window is used in the time domain.

The amplitudes of this latest seven point window are shown below.

```
0.0325    -0.2500   1.7071   -2.9793   1.7071   -0.2500   0.0325
```

The corresponding seven point polynomial operators are:

```
0.0111    -0.1500   1.5000   -2.7222   1.5000   -0.1500   0.0111
```

COMPARISON OF AMPLITUDES SPECTRUMS

Three central difference operators of size 3, 5, and 7, using the polynomial method are plotted in Figure 7. Spectrally derive operators using the raised cosine are plotted for size 3, 5, 7, and 9, and displayed in Figure 8.

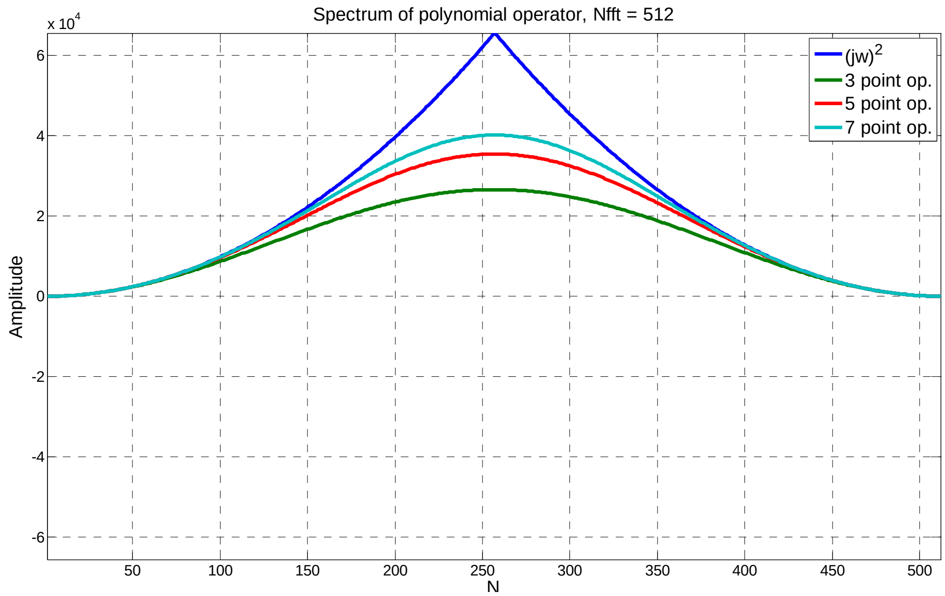


FIG. 7. Amplitude spectrum for operators derived using the Taylor series.

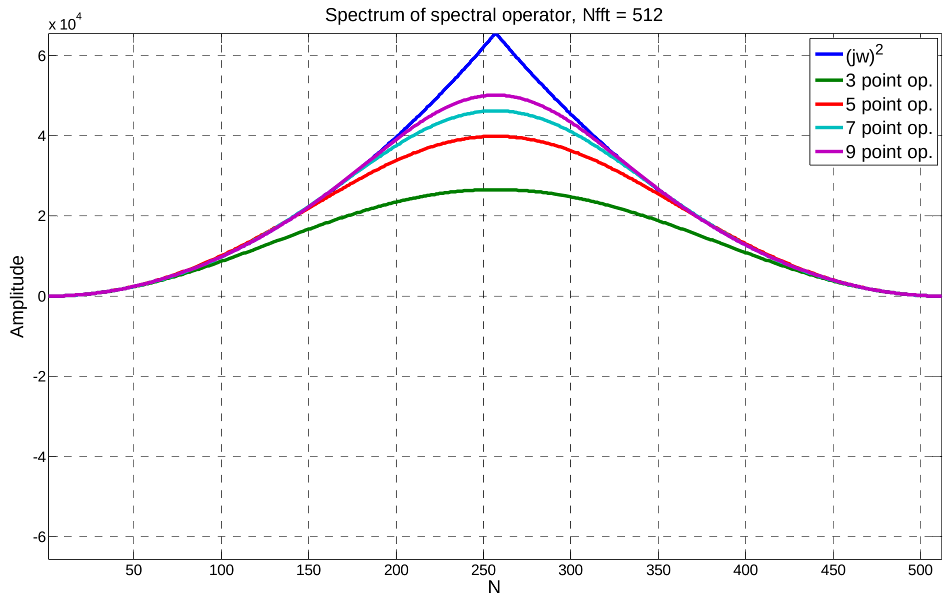


FIG. 8. Amplitude spectrum for operators derived using time domain windowing.

Amplitudes of the spectral errors are shown in Figure 9 for the polynomial operators and in Figure 10 for the spectral operators.

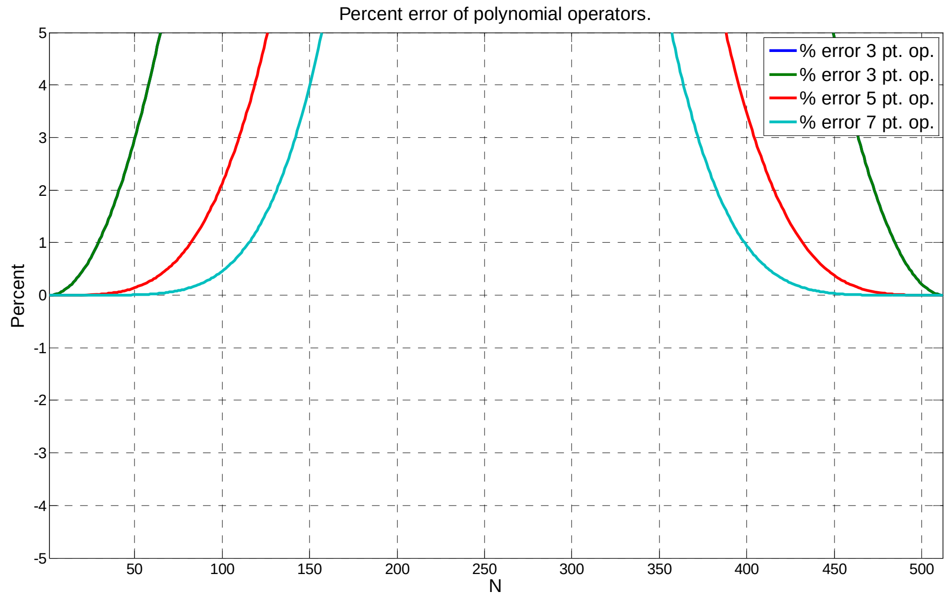


FIG. 9. Percent errors for the Taylor series operators.

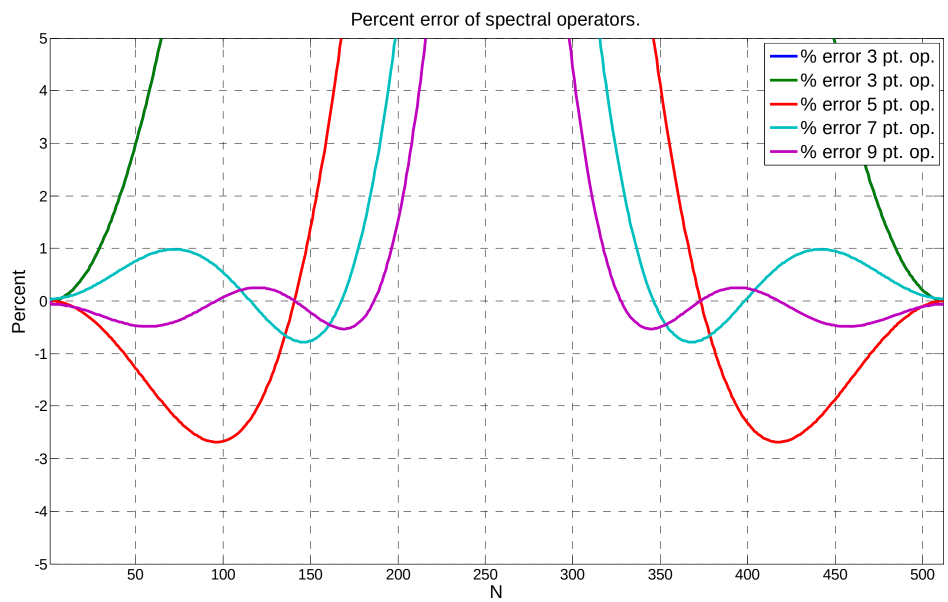


FIG. 10. Percent errors for the time domain windowing operators.

A plot comparing the two seven point operators is shown in Figure 11. The polynomial operator has a 1% bandwidth to approximately 115 hz, while the spectrally derived operator has a bandwidth of approximately175 Hz.

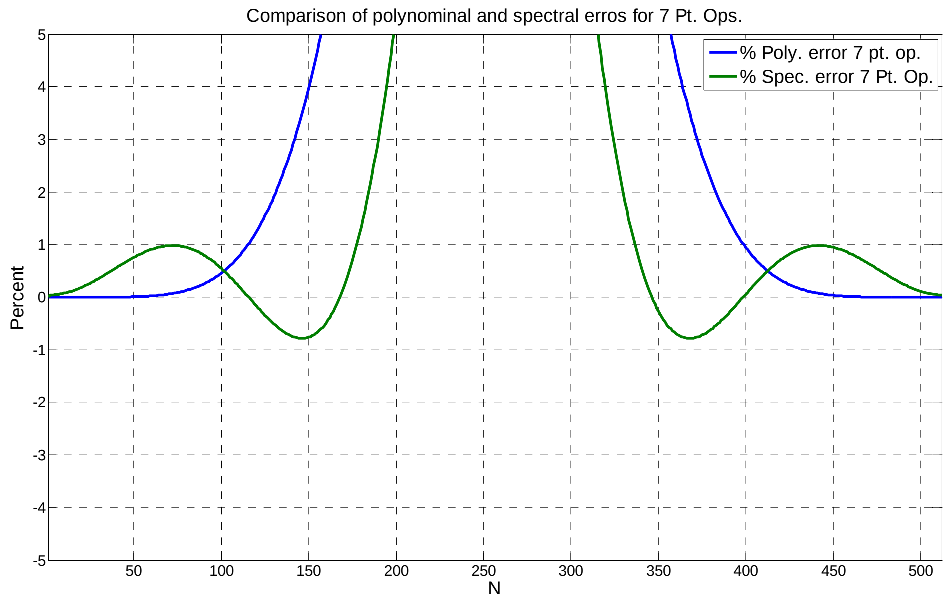


FIG. 11. Comparison of spectrum errors for seven point operators.

CONCLUSIONS

Numerous short approximations to the second derivative were presented. The best solution for a seven point operator was found from the inverse Fourier transform of a windowed $(j\omega)^2$ function.

Operators were defined using polynomial approximations and truncated Taylor series. These short operators do assume a low order polynomial and can define the derivative at any location within the locally smoothed area. This aids in defining second derivatives at the beginning and end of an array (the boundary conditions).

Spectrally derived operators have a larger bandwidth for an equivalent seven point operator.

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