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On the relation between order of accuracy, convergence rate and spectral slope for linear numerical methods applied to multiscale problems

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SUMMARY

The relation between order of accuracy and convergence rate for simple linear finite difference schemes for differentiation and advection is examined theoretically and empirically. For sufficiently smooth functions, i.e. those with sufficiently steep spectral slope, the convergence rate is given by the order of accuracy. For less smooth functions, with shallower spectral slope, differentiation and advection behave slightly differently: the convergence rate of a finite difference derivative is determined entirely by the spectral slope, while the convergence rate of a finite difference advection scheme is determined by an interaction between the spectral slope and the order of accuracy. © Crown copyright 2007. Reproduced with the permission of Her Majesty's Stationery Office. Published by John Wiley & Sons, Ltd.

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1. INTRODUCTION

A commonly used measure of the accuracy of a numerical scheme is its *order of accuracy*. For example, consider a function $\rho(x)$ with true derivative $\rho'_{\mathrm{tr}}(x)$, and let $\rho'_{\mathrm{fd}}(x)$ be a finite difference estimate of the derivative obtained by sampling ρ on a grid with spacing Δx. The *truncation error* ε is defined by

$$\rho'_{\mathrm{fd}}(x) = \rho'_{\mathrm{tr}}(x) + \varepsilon \tag{1}$$

The finite difference estimate is said to be mth order accurate if, for infinitely differentiable ρ, Taylor series analysis shows that $\varepsilon = O(\Delta x^m)$ as $\Delta x \to 0$. The *convergence rate* is the rate at which

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the truncation error (measured locally or in some global norm) actually does approach zero as $\Delta x \to 0$. Provided ρ has at least m continuous derivatives, ε does indeed decrease like $O(\Delta x^m)$: the convergence rate agrees with the order of accuracy. However, for many multiscale problems, such as numerical weather and climate prediction, the data have shallow spectral slopes, consistent with only a small number of continuous derivatives. Then the convergence rate may be slower than suggested by the order of accuracy. This raises the question: what is the relevance of order of accuracy, and how is it related to convergence rate, for multiscale problems? This question is addressed for a pair of one-dimensional model problems: differentiation of a function and advection of a function.

2. CONVERGENCE OF FINITE DIFFERENCE DERIVATIVES

A suitable test function is the isolated $\cos^n$ hill, given by

$$\rho(x) = \begin{cases} \cos^n \left[\dfrac{\pi(x-D)}{2d} \right] & \text{for } D-d \leqslant x \leqslant D+d \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where $0<d<D$, $x \in [0, 2D]$; $D=0.5$ and $d=\frac{7}{64}$ [1]. The shape of the isolated cosine hill can be seen in Figure 1. For integer n, this isolated $\cos^n$ hill has $n-1$ continuous derivatives, with the discontinuities occurring at $x = D \pm d$. The envelope of the spectrum $\hat{\rho}(k)$ decays as $k^{-(n+1)}$ as $k \to \infty$ [1]. The shape of the spectrum, calculated using the discrete fast Fourier transform, can be seen in Figure 1.

For the cases $n=1,2,\ldots,7$, we sample ρ pointwise on a uniform grid of N points, spacing $\Delta x = 2D/N$, and consider the convergence of linear finite difference schemes of order $m=1,2,\ldots,7$ for the spatial first derivative of ρ. The mth order scheme uses a stencil of $m+1$ points, centred

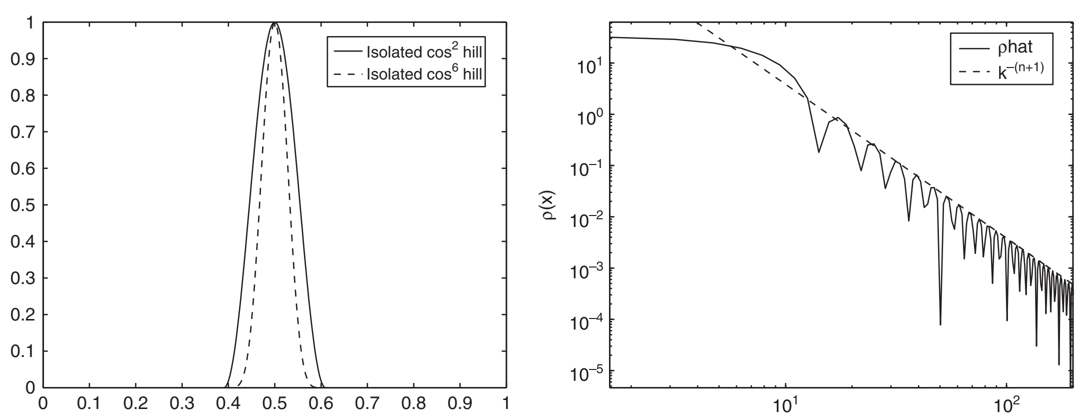

Figure 1. Left: the isolated cosine hill $\rho(x)$ for the cases $n=2$ and 6. Right: the spectral envelope $|\hat{\rho}(k)|$ of an isolated $\cos^2$ hill. A k^{-3} line has been added to show the spectral decay.

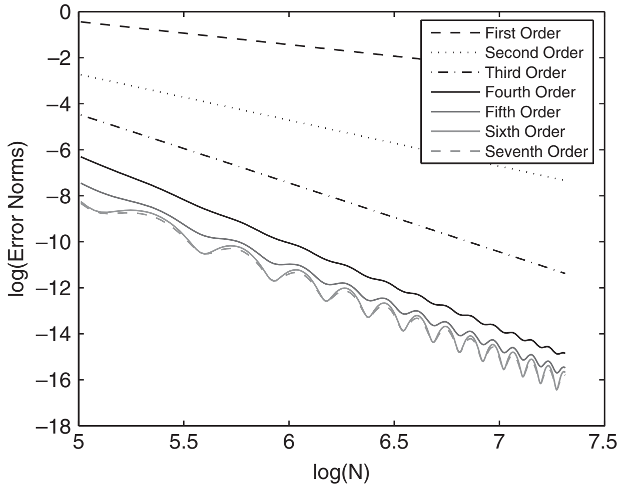

Figure 2. The l_1 normalized error for all the seven schemes with $n=4$. Moving from a fourth-order scheme to a fifth-order scheme gives the same convergence rate but offers significant reduction in the magnitude of the error; however, moving higher than fifth order offers less reduction.

for even m and biased half of one grid length to the left for odd m; this determines the scheme uniquely. Convergence with increasing resolution is measured in the l_1, l_2, and l_∞ norms.

Taylor series analysis gives predictions for the convergence rates:

$$l_1 \sim (\Delta x)^{\min(m,n)}, \quad l_2 \sim (\Delta x)^{\min(m,n-1/2)}, \quad l_\infty \sim (\Delta x)^{\min(m,n-1)} \tag{3}$$

These predictions depend only on the fact that ρ is infinitely differentiable except at a finite set of points where it has $n-1$ continuous derivatives, and not on any other details. Numerical testing confirms these predictions; an example is shown in Figure 2. For each n there is a maximum attainable convergence rate. Moving to a higher-order scheme will reduce the overall error, although eventually with diminishing returns; this can be seen in Figure 2.

The experiments were repeated using another function $\tilde{\rho}(x)$ constructed by randomizing the phases of the Fourier components $\hat{\rho}(k)$; $\tilde{\rho}$ has the same spectral shape as ρ, but does not have spatially localized discontinuities in the derivatives. In these numerical experiments l_1, l_2, and l_∞ all scale like $(\Delta x)^{\min(m,n-1/2)}$.

3. CONVERGENCE OF NUMERICAL ADVECTION SCHEMES

Now the same finite difference schemes, for $m=1,2,\ldots,6$, are used to evaluate ρ_x in the linear one-dimensional advection equation

$$\rho_t + U\rho_x = 0 \tag{4}$$

We take $U>0$ so that the spatial derivative schemes for odd m are upstream biased. A second-order scheme is used for the time derivative (centred difference for even m, Adams Bashforth for odd m), with the time step chosen sufficiently small that time truncation errors are negligible. The cosine

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Table I. l_2 Convergence rates for the advection of the isolated $\cos^n$ hill.

l_2	n in $\cos^n$						
Order (m)	1	2	3	4	5	6	7
1	0.8	0.9	0.9	0.8	0.8	0.8	0.8
2	1.0	1.8	2.0	2.0	2.0	2.0	2.0
3	1.1	1.9	2.8	3.0	3.0	3.0	3.0
4	1.2	2.0	2.8	3.9	4.1	4.1	4.1
5	1.3	2.0	2.9	3.8	4.8	5.0	5.0
6	1.3	2.1	3.0	4.0	4.9	6.0	6.1

hill is advected once around the domain with U kept constant. The convergence rates for the pointwise l_2 errors, determined empirically for various m and n, are shown in Table I. In particular (i) for $n>m$, the convergence rate is approximately equal to m; (ii) for $n\leqslant m$, the convergence rate is reduced below m.

These results can be explained theoretically as follows. Define the function $E(k,\Delta x,t)$ to be the error in the advected ρ divided by the initial ρ when ρ consists of single Fourier component proportional to e^{ikx}:

$$\rho_{\mathrm{fd}}(x,t)-\rho_{\mathrm{tr}}(x,t)=E(k,\Delta x,t)\rho_{\mathrm{tr}}(x,0) \tag{5}$$

Orthogonality of different Fourier components then allows l_2 to be expressed as

$$l_2=\left(\frac{1}{N}\sum_{j=1}^{N}|\varepsilon_j|^2\right)^{1/2}=\left(\sum_{l=-N/2+1}^{N/2}|E(k_l,\Delta x,t)|^2|\hat{\rho}(k_l)|^2\right)^{1/2} \tag{6}$$

where $k_l=\pi l/D$ is the lth resolved wavenumber. Let $R(k\Delta x)$ be the response function for the finite difference spatial derivative

$$\rho_{x,\mathrm{fd}}=R(k\Delta x)\rho_{x,\mathrm{tr}} \tag{7}$$

Then E can be expressed in terms of R by solving the spatially discretized version of (4) for a single Fourier component:

$$E(k,\Delta x,t)=\exp(-\mathrm{i}kUt)\{\exp[-\mathrm{i}kU(R-1)t]-1\} \tag{8}$$

For this problem $Ut=N\Delta x$. Defining $S(k\Delta x)\equiv(k\Delta x)(R-1)$ allows $|E|$ to be expressed as

$$|E|=|\exp[-\mathrm{i}kU(R-1)t]-1|=|\exp(-\mathrm{i}NS)-1| \tag{9}$$

For even m, R is real and $|E|$ is a function that oscillates between and 0 and 2; for odd m, R is complex and $|E|$ increases then quickly settles at 1, see Figure 3.

For a scheme of order m for the spatial derivative, $R(k\Delta x)=1+O[(k\Delta x)^m]$ for small $k\Delta x$. Therefore,

$$S=O[(k\Delta x)^{m+1}] \tag{10}$$

There are now two cases to consider. In the first case large scales (i.e. small k) dominate the error. The convergence rate is then controlled by the behaviour of E for small values of NS, where

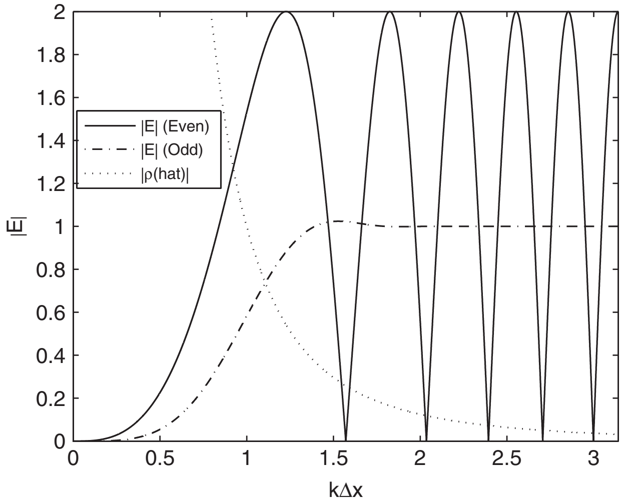

Figure 3. This plot shows $|E|$ for a second-order centred derivative and $|\hat{\rho}(k)|$ for an initial isolated $\cos^2$ hill; $N=11$.

$|E|$ is small. In this limit $|E|=O[N(k\Delta x)^{m+1}]$ while $\hat{\rho}(k)$ is independent of N for fixed k. Thus, substituting in (9) and (6), we obtain

$$l_2=[O(N^2(k\Delta x)^{2(m+1)})]^{1/2}$$

$$=O(N^{-m}) \tag{11}$$

In the second case, smaller scales (i.e. large k) dominate the error. The dominant contribution to the error will come from around the first peak in $|E|$, which occurs for $NS\sim$constant for both even and odd m. As N is increased, S at the peak must decrease, hence, the peak will move to small $k\Delta x$; therefore, the asymptotic behaviour of S is still given by (10). Thus, from (10), since S at the peak $\sim 1/N$ for large N, $k\Delta x$ at the peak $\sim(1/N)^{1/(m+1)}$, and k at the peak $\sim N^{m/(m+1)}$. The dominant errors thus come from small $k\Delta x$ but large k as $N\to\infty$. Using the fact that k at the peak grows with N, we may assume that the large k power law scaling $|\hat{\rho}(k)|\sim k^{-p}$. A scaling for the l_2 error can then be found most easily by introducing a change of variable $\lambda\equiv N^{-m}k^{m+1}$. In the asymptotic regime, E is approximately a function of λ, while the spectral amplitude, re-expressed in terms of λ, becomes $|\hat{\rho}(k)|\sim\lambda^{-p/(m+1)}N^{-pm/(m+1)}$. Thus, expression (6) for the l_2 error becomes

$$l_2\sim\left[\sum_{l=1}^{N}|E(\lambda_l)|^2\lambda_l^{-2p/(m+1)}N^{-2pm/(m+1)}\right]^{1/2} \tag{12}$$

where $\lambda_l=N^{-m}k_l^{m+1}$. The sum can be made to look like an integral by noting that

$$\delta k_l\equiv k_{l+1}-k_l=\pi/D \tag{13}$$

is constant, but also

$$\delta k_l \approx \frac{1}{m+1} N^{m/(m+1)} \lambda_l^{-m/(m+1)} \delta\lambda_l \tag{14}$$

Thus

$$l_2 \sim \left[\sum_{l=1}^{N} |E(\lambda_l)|^2 N^{(1-2p)m/(m+1)} \lambda_l^{-(2p+m)/(m+1)} \delta\lambda_l \right]^{1/2} \tag{15}$$

The N dependence can then be brought outside the sum, and $\delta\lambda_l \to 0$ for large N so that the sum approaches an integral independent of N. Therefore,

$$l_2 \sim N^{-(p-1/2)m/(m+1)} \tag{16}$$

Finally, for the isolated $\cos^n$ hill for which $p = n+1$,

$$l_2 \sim N^{-(n+1/2)m/(m+1)} \tag{17}$$

The two cases together are summarized as

$$l_2 = O(\Delta x^{\min[m, m(n+1/2)/(m+1)]}) \tag{18}$$

The values in the table are generally close to the predicted values, although with some differences. For $m=1$ asymptotic convergence rate was not reached for the values of N tested. Also, for large m the theory predicts that the peak in $|E|$ moves towards small $k\Delta x$ very slowly, ($k\Delta x$ at the peak $\sim (1/N)^{1/(m+1)}$), so that in practice roundoff errors start to dominate truncation errors before the asymptotic convergence rate is reached; the values shown are estimates taken just before roundoff errors become noticeable. In the case of $m=n$, the two powers in Equation (18) are sufficiently close to require greater resolution before the lower term dominates; the empirical convergence rates lie between these two values.

This derivation does not depend on the phases of the Fourier components of the initial data. Numerical experiments using the randomized phase function $\tilde{\rho}$ as initial data gave very similar convergence rates to those in Table I.

4. CONCLUSION

Convergence rates have been computed theoretically and numerically for differentiation and advection of the isolated $\cos^n$ hill. When n is sufficiently large, so that the function is sufficiently smooth and its spectrum is sufficiently steep, the convergence rate is given by the order of accuracy. For smaller n, n itself, through the spectral decay, controls the convergence rate of finite difference derivatives (3). For finite difference advection schemes, the convergence rate is determined by an interaction between the spectral decay and the order of scheme (18).

The spectral slope for atmospheric and oceanic quantities is very shallow, e.g. [2–4]. These shallow slopes apparently result from a combination of ubiquitous, effectively random, wave and turbulence fields and localized sharp features such as fronts. Although the results presented here are only for relatively simple one-dimensional cases, the examples using both the isolated $\cos^n$ hill ρ and its randomized phase version $\tilde{\rho}$ are nevertheless likely to be relevant. It would be valuable to know whether our conclusions can be extended to nonlinear and multidimensional problems.

Further tests have been completed with the isolated cosine hill adjusted to reflect observed atmospheric spectra. A further paper presenting these results, greater analysis of the work covered here, plus analytical and empirical convergence rates for interpolation and semi-Lagrangian advection, is in preparation.

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