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Supra-Convergent Schemes on Irregular Grids

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Abstract. As Tikhonov and Samarskiĭ showed for $k = 2$, it is not essential that kth-order compact difference schemes be centered at the arithmetic mean of the stencil's points to yield second-order convergence (although it does suffice). For stable schemes and even k, the main point is seen when the kth difference quotient is set equal to the value of the kth derivative at the middle point of the stencil; the proof is particularly transparent for $k = 2$. For any k, in fact, there is a $\lfloor k/2 \rfloor$-parameter family of symmetric averages of the values of the kth derivative at the points of the stencil which, when similarly used, yield second-order convergence. The result extends to stable compact schemes for equations with lower-order terms under general boundary conditions. Although the extension of Numerov's tridiagonal scheme (approximating $D^2y = f$ with third-order truncation error) yields fourth-order convergence on meshes consisting of a bounded number of pieces in which the mesh size changes monotonically, it yields only third-order convergence to quintic polynomials on any three-periodic mesh with unequal adjacent mesh sizes and fixed adjacent mesh ratios. A result of some independent interest is appended (and applied): it characterizes, simply, those functions of k variables which possess the property that their average value, as one translates over one period of an arbitrary periodic sequence of arguments, is zero; i.e., those bounded functions whose average value, as one translates over arbitrary finite sequences of arguments, goes to zero as the length of the sequences increases.

1. Some Supra-Convergent Schemes. The ordinary differential equation $D^k y = f$ with initial conditions $D^p y = b_p$ at $x = 0$, $p = 0, 1, \ldots, k-1$, can be approximated by the finite-difference equation $\Delta^k Y = F$ with appropriate initial conditions on Y, where Δ^k is the kth-order difference quotient, i.e., $k!$ times the divided difference on $k+1$ points. For even k and a uniform grid with spacing h, as long as F is within $O(h^2)$ of f at the middle point of the stencil, the truncation error $\Delta^k y - F$ is $O(h^2)$, and so is the solution error $\Delta^p(y - Y)$, $p < k$. For odd k or nonuniform grids with maximum interval h, the truncation error may or may not be $O(h^2)$. Nevertheless, we will show that for a class of F's the solution error remains $O(h^2)$. We call such enhancement of truncation error *supra*-convergence.

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An easy special case occurs when we set $F = f(\bar{x}^{(k)}) + O(h^2)$, where we define $\bar{x}^{(p)}_{i+p/2} := (x_i + \cdots + x_{i+p})/(p+1)$, and we henceforth shall write $\bar{x}$ for $\bar{x}^{(k)}$. It is sufficient to take $y(x) = x^{k+1}$, whence $f(x) = (k+1)!x$. Let $q(x)$ be the polynomial of degree k interpolating x^{k+1} at $x_i, \ldots, x_{i+k}$. By definition, $(\Delta^k y)_{i+k/2} := D^k q$. But $q(x) = x^{k+1} - \prod_{j=0}^{k}(x - x_{i+j})$; therefore, $(\Delta^k y)_{i+k/2} = (k+1)!\bar{x}_{i+k/2}$, so that in this case the truncation error is $O(h^2)$ where, with $h_i := (x_{i+1} - x_i)$, $h := \max_i h_i$. The truncation error in the k initial difference quotients $(\Delta^p Y)_{p/2}$ will be $O(h^2)$ if we set them equal to $D^p y(\bar{x}^{(p)}_{p/2}) + O(h^2)$, e.g., to $D^p y(0) + \bar{x}^{(p)}_{p/2} D^{p+1} y(0)$. So we shall use

$$(\Delta^p Y)_{p/2} = b_p + \bar{x}^{(p)}_{p/2} b_{p+1}, \qquad p < k-1;$$

and

$$(\Delta^p Y)_{p/2} = b_p + \bar{x}^{(p)}_{p/2} f(0), \qquad p = k-1.$$

For other F's, the truncation error is not $O(h^2)$, for example, if k is even and $F_{i+k/2} = f(x_{i+k/2})$. Nevertheless, in this case also, the solution error is $O(h^2)$. To see this, let

$$\Delta^k Y_{i+k/2} = D^k y(x_{i+k/2}) \quad \text{and} \quad \Delta^k \bar{Y}_{i+k/2} = D^k y(\bar{x}_{i+k/2}).$$

Given the previous result, it suffices to show that $\Delta^{k-1}(Y - \bar{Y}) = O(h^2)$, since then we can recur down to $Y - \bar{Y} = O(h^2)$. Indeed, using this recursion for the difference quotients, we have

$$\begin{aligned}\Delta^k(Y - \bar{Y})_i &= \frac{\Delta^{k-1}_{i+1/2} - \Delta^{k-1}_{i-1/2}}{(x_{i+k/2} - x_{i-k/2})/k}(Y - \bar{Y}) = D^k y(x_i) - D^k y(\bar{x}_i) \\ &= (x_i - \bar{x}_i) D^{k+1} y(\bar{x}_i) + O(h^2).\end{aligned}$$

Noting next that the width of the stencil is

$$x_{i+k/2} - x_{i-k/2} = \sum_{c<k/2} (h_{i+c} + h_{i-c-1}),$$

while

$$\begin{aligned}(k+1)(\bar{x}_i - x_i) &= \sum_{m=1}^{k/2} [(x_{i+m} - x_i) - (x_i - x_{i-m})] \\ &= \sum_{m=1}^{k/2} \sum_{d<m} (h_{i+d} - h_{i-d-1}),\end{aligned}$$

we must show that finite sums of the form

$$S := \sum_i (h_{i+c} + h_{i-c-1})(h_{i+d} - h_{i-d-1}) g(\bar{x}_i),$$

c and d integers, $\sum_i h_i$ bounded, are $O(h^2)$ for smooth $g(x)$. For this, recall that the shift operator $(Tf)_i := f_{i+1}$ is unitary on the space H of real doubly infinite sequences whose norm is finite under the usual inner product:

$$(f, T^{-1}g) = (Tf, g) = (f, T^* g) \qquad \left(:= \sum_{i=-\infty}^{\infty} f_i (T^* g)_i\right).$$

For finite sums $[f, g] := \sum_{i=I}^{J} f_i g_i$, however, we have only $T^* \simeq T^{-1}$, where, if A and B are linear operators on H,

$$A \simeq B \quad \text{means} \quad |[f, Ag] - [f, Bg]| \leqslant \text{const} \|f\|_\infty \|g\|_\infty$$

independent of f, g, and the limits of the sum. We can write

$$S = \sum_i (Ch)_i (Dh)_i g(\bar{x}_i) = [Ch, (Dh)\bar{g}],$$

where

$$C := T^c + T^{-c-1}, \quad D := T^d - T^{-d-1}, \quad \bar{g}_i := g(\bar{x}_i).$$

The operators C and D satisfy

$$C^* \simeq TC, \quad D^* \simeq -TD, \quad CD \simeq DC.$$

Finally, let

$$r \approx s \quad \text{mean} \quad r - s = O(h^2).$$

Now, $[T^a h, (T^b h)\bar{g}]$ is

$$\sum_i h_{i+a} h_{i+b} g(\bar{x}_i) = [T^a h, T^b(h\bar{g})] + \sum_i h_{i+a} h_{i+b}(g(\bar{x}_i) - g(\bar{x}_{i+b}))$$
$$\approx [T^a h, T^b(h\bar{g})],$$

since $g(\bar{x}_i) - g(\bar{x}_{i+b}) = O(|\bar{x}_{i+b} - \bar{x}_i|)$ and $\sum_i h_i$ is finite. Therefore,

$$S = [Ch, (Dh)\bar{g}] \approx [Ch, D(h\bar{g})] \approx -[TDCh, h\bar{g}]$$
$$\approx -[TCDh, h\bar{g}] \approx -[Dh, C(h\bar{g})] \approx -[Dh, (Ch)\bar{g}] = -S;$$

so $S = O(h^2)$.

It is easily seen that second-order convergence will obtain also (for k even *or* odd) if

$$F_{i+k/2} = f(\tilde{x}_{i+k/2}) + O(h^2),$$

where, with $\lfloor m \rfloor :=$ "the greatest integer in m", the symmetric average $\tilde{x}$ is defined by

$$\tilde{x}_{i+k/2} := \sum_{j=0}^{\lfloor k/2 \rfloor} \theta_j (x_{i+j} + x_{i+k-j})/2,$$

with the constraint

$$\sum_{j=0}^{\lfloor k/2 \rfloor} \theta_j = 1,$$

and the θ_j are presumed essentially independent of i; i.e., they change at most a finite number of times fixed independent of the mesh.

We illustrate for odd $k =: 2m - 1$. Hence, we consider

$$\Delta^k (Y - \bar{Y})_{i+1/2} = \frac{(\Delta_{i+1}^{k-1} - \Delta_i^{k-1})}{(x_{i+m} - x_{i-m+1})/k}(Y - \bar{Y}) = D^k y(\tilde{x}_{i+1/2}) - D^k y(\bar{x}_{i+1/2})$$
$$= (\tilde{x}_{i+1/2} - \bar{x}_{i+1/2}) D^{k+1} y(\bar{x}_{i+1/2}) + O(h^2).$$

Now, the width of the stencil can be expressed as a symmetric sum:

$$(x_{i+m} - x_{i-m+1}) = \left[\sum_{c<m} (h_{i+c} + h_{i-c}) \right] - h_i.$$

And, since

$$2(\tilde{x}_{i+1/2} - \bar{x}_{i+1/2}) = \sum_{j<m} \theta_j (x_{i+m-j} + x_{i-m+j+1} - 2\bar{x}_{i+1/2}) \quad \left(\sum_{j<m} \theta_j = 1 \right),$$

it suffices, in order to exhibit a corresponding *anti*symmetric sum, to consider

$$2\bar{x}_{i+1/2} - (x_{i+a} + x_{i-a+1}) = \left[\sum_{j=1}^{m} (x_{i+j} + x_{i-j+1})/m\right] - (x_{i+a} + x_{i-a+1}),$$

with $1 < a \leqslant m$. Multiplying by m, we note

$$\sum_{j=1}^{m} \left[(x_{i+j} - x_{i+a}) - (x_{i-a+1} - x_{i-j+1})\right]$$
$$= \sum_{a<j\leqslant m} \sum_{a<d<j} (h_{i+d} - h_{i-d}) - \sum_{1\leqslant j<a} \sum_{j\leqslant d<a} (h_{i+d} - h_{i-d}).$$

Thus, it remains only to show that finite sums of the form

$$S := \sum_i (h_{i+c} + h_{i-c})(h_{i+d} - h_{i-d}) g(\bar{x}_{i+1/2})$$

are $O(h^2)$ for smooth $g(x)$. But this follows as before, now using $C := T^c + T^{-c} \simeq C^*$ and $D := T^d - T^{-d} \simeq -D^*$.

Finally, we note that if $f^{(2)}$ is bounded,

$$f(\tilde{x}) = \tilde{f} + O(h^2) \qquad \left(\tilde{f}_{i+k/2} := \sum_{j=0}^{\lfloor k/2 \rfloor} \theta_j \left[f(x_{i+j}) + f(x_{i+k-j})\right]/2\right),$$

since symmetric averaging is a particular instance of local averaging.

Appendix 3 proves that symmetric averaging of the source term is the only mesh-*independent* averaging allowable to supra-convergent compact difference schemes involving Δ^k.

2. More General Equations. The effect of lower-order terms in the differential operator can be reduced to considerations of more ordinary stability by means of a standard device. Let

$$L := \sum_{p<k} a_p D^p, \quad \hat{L} := \sum_{p<k} \hat{a}_p \hat{\Delta}^p, \quad (D^k + L)y = f, \quad (\Delta^k + \hat{L})Y = \hat{f},$$

with truncation error

$$\hat{t} := \Delta^k y + \hat{L}y - \hat{f}.$$

Second-order accurate initial difference quotients are specified as before, except that $D^k y(0)$ is now calculated as $(f - Ly)(0)$.

Now, we *could* simply suppose that each $(\hat{a}_p \hat{\Delta}^p U)_{i+k/2}$ is centered, along with $\hat{f}$, at $\bar{x}_{i+k/2}$ (this can easily be done with $O(h^2)$ truncation error and, for $p < k - 1$, can be done in many ways, e.g., by evaluating derivatives of local polynomial interpolants there). Then $\hat{t}$ would already be $O(h^2)$.

But, more generally, we suppose that each $(\hat{a}_p \hat{\Delta}^p U)_{i+k/2}$ is some uniformly bounded combination of $(\Delta^p U)_{i+p/2}, \ldots, (\Delta^p U)_{i+k-p/2}$, such that its principal truncation error is similar in form to that already analyzed:

$$\left(\hat{a}_p \hat{\Delta}^p y\right) - \left(a_p D^p y\right)(\bar{x}) \approx \sum_{m=1}^{M(p)} (\tilde{x}^{(p,m)} - \bar{x}) g_{p,m}(\bar{x}),$$

where each $\tilde{x}^{(p,m)}$ is some symmetric average and the $g_{p,m}(x)$ are smooth functions, while, similarly, $f(\bar{x}) - \hat{f} \approx \sum_{m=1}^{M(k)} (\tilde{x}^{(k,m)} - \bar{x}) g_{k,m}(\bar{x})$. Then,

$$\hat{t} \approx \left(D^k y\right)(\bar{x}) + \hat{L}y - \hat{f} \approx \sum_{p\leqslant k} \sum_{m=1}^{M(p)} (\tilde{x}^{(p,m)} - \bar{x}) g_{p,m}(\bar{x}).$$

Now, define W by $\Delta^k W = \hat{t}$, $W_0 = \cdots = \Delta W^{k-1}_{(k-1)/2} = 0$. As in the first section, $\Delta^p W = O(h^2)$, $p < k$. Then, since $(\Delta^k + \hat{L})[W - (y - Y)] = \hat{L}W = O(h^2)$, the solution error $\Delta^p(Y - y)$, $p < k$, is $O(h^2)$, because the operator $\Delta^k + \hat{L}$ is stable for the ordinary difference quotient initial value problem in the usual sense: for h small enough,

$$\max_{p<k} \|\Delta^p U\|_\infty \leqslant \text{const}\left[\|(\Delta^k + \hat{L})U\|_\infty + \max_{p<k} |(\Delta^p U)_{p/2}|\right]$$

(see Appendix 1).

Perhaps the simplest, most compact difference schemes in this family are, with $a_i := a(x_i)$,

$$k \text{ even:} \quad (\hat{a}\hat{\Delta}^p Y)_i := \begin{cases} (a\Delta^p Y)_i, & p \text{ even;} \\ a_i[(\Delta^p Y)_{i+1/2} + (\Delta^p Y)_{i-1/2}]/2, & p \text{ odd;} \end{cases}$$

$$k \text{ odd:} \quad (\hat{a}\hat{\Delta}^p Y)_{i+1/2} := \begin{cases} [(a\Delta^p Y)_{i+1} + (a\Delta^p Y)_i]/2, & p \text{ even;} \\ (a_{i+1} + a_i)(\Delta^p Y)_{i+1/2}/2, & p \text{ odd.} \end{cases}$$

These schemes are a special instance of those defined by

$$(\hat{a}\hat{\Delta}^p Y)_i := [\tilde{a}_{i+c}(\Delta^p Y)_{i+d} + \tilde{a}_{i-c}(\Delta^p Y)_{i-d}]/2,$$

$$\tilde{g}_{i+r/2} := \sum_{j=0}^{\lfloor r/2 \rfloor} \theta_j [g(x_{i+j}) + g(x_{i+r-j})]/2$$

(i, c, d appropriately integral or half-integral), whose truncation error is within second order of that of

$$[a(\tilde{x}_{i+c})(\Delta^p Y)_{i+d} + a(\tilde{x}_{i-c})(\Delta^p Y)_{i-d}]/2.$$

To analyze the latter we use the Leibniz-like identity

$$\begin{aligned} f_+ g_+ - 2f_0 g_0 + f_- g_- = {} & (f_+ - 2f_0 + f_-)g_0 + (g_+ - 2g_0 + g_-)f_0 \\ & + (f_+ - f_0)(g_+ - g_0) + (f_0 - f_-)(g_0 - g_-). \end{aligned}$$

Then, with $f_\pm := a(\tilde{x}_{i\pm c})$, $g_\pm := (\Delta^p y)_{i\pm d}$, $f_0 := a(\bar{x}_i)$, and $g_0 := D^p y(\bar{x}_i)$, we conclude that the truncation error has the right form:

$$\begin{aligned} & [a(\tilde{x}_{i+c})(\Delta^p y)_{i+d} + a(\tilde{x}_{i-c})(\Delta^p y)_{i-d}]/2 - (aD^p)y(\bar{x}_i) \\ & \quad \approx (\tilde{x}_i^{(1)} - \bar{x}_i) Da(\bar{x}_i) D^p y(\bar{x}_i) + (\tilde{x}u(2)_i - \bar{x}_i) a(\bar{x}_i) D^{p+1} y(\bar{x}_i), \end{aligned}$$

where

$$\tilde{x}_i^{(1)} := (\tilde{x}_{i+c} + \tilde{x}_{i-c})/2, \qquad \tilde{x}_i^{(2)} := (\bar{x}_{i+d}^{(p)} + \bar{x}_{i-d}^{(p)})/2$$

are symmetric averages as required.

All this can be extended to boundary value problems (b.v.p.'s) using the following argument. Let the boundary conditions be expressed as $B\lambda y = b$, where B is a k by $2k$ matrix, and $\lambda g := (g(a), \ldots, D^{k-1}g(a), g(b), \ldots, D^{k-1}g(b))^T$. We suppose both the initial-value problem and the b.v.p. are nonsingular. Hence, on the null-space of $D^k + L$, the boundary values can in principle be obtained linearly and invertibly from the initial values. That is to say, there is some nonsingular matrix Λ such that $B\lambda = [\Lambda \,|\, 0]\lambda$ on that null-space. But compact boundary conditions may be expressed similarly: with the left boundary at x_0 and the right at x_n,

$\hat{B}\lambda Y = \hat{b}$,

$$\text{where } \hat{\lambda}U := \left(U_0, \Delta U_{1/2}, \ldots, \Delta^{k-1}U_{(k-1)/2}, U_n, \Delta U_{n-1/2}, \ldots, \Delta^{k-1}U_{n-(k-1)/2}\right)^T.$$

And, given the stability we assumed above for the initial difference quotient problem along with the consistency we have demonstrated, given also a suitable consistency and structure for the approximate boundary conditions, one can show the same kind of relationship holds between them and the initial-difference quotients, this time on the k-dimensional null-space of $\Delta^k + \hat{L}$, and with $\hat{\Lambda}$ bounded and uniformly invertible as $h \to 0$. (For more details, see, e.g., Swartz [1980]).

Now let y solve the b.v.p.; and Y, the approximate b.v.p.; and suppose Y_{in} solves the approximate i.v.p. for y. According to the first part of this section, $E_{in} := y - Y_{in}$ satisfies $\Delta^p E_{in} = O(h^2)$, $p < k$. For $y - Y =: E$ to behave likewise, it suffices that $\Delta^p(E - E_{in}) = O(h^2)$, $p < k$. But $E - E_{in}$ lies in the null-space of $\Delta^k + \hat{L}$, and an additional assumption of $O(h^2)$ truncation error on the boundary conditions (for realizations, see, e.g., Swartz [1980]) means $\hat{B}\hat{\lambda}(E - E_{in})$ is $O(h^2)$. $\hat{\Lambda}$ being uniformly invertible now implies that the *initial* difference quotients of $E - E_{in}$ are also $O(h^2)$. So, finally, our presumed stability for the initial-difference-quotient problem yields the desired result for $E - E_{in}$, hence for E.

3. Numerov's Method: A Counterexample. The results so far impel one to wonder: Given a difference scheme defined for nonuniform meshes, a scheme that possesses higher-order truncation error when the mesh is uniform; does one always attain that higher-order convergence even when the mesh is not uniform? We show now how Numerov's scheme provides a qualified counterexample.

To do this, we first recast the results of the first section for the differential equation

$$D^2 y = f, \qquad y(0) = Dy(0) = 0,$$

as approximated by the second-order difference quotient scheme

$$(\Delta Y_{i+1/2} - \Delta Y_{i-1/2})/[(h_i + h_{i-1})/2] = f(x_i), \quad Y_0 = 0, \quad \Delta Y_{1/2} = h_0 f(0)/2,$$

in the manner of Samarskiĭ [1971, pp. 26–27]. Plugging in the first monomial the scheme fails to handle exactly, namely $y(x) = (x - x_i)^3$, we see that the first-order part of the truncation error is $2(h_i - h_{i-1})$, i.e., $(h_i - h_{i-1})y^{(3)}(x_i)/3$. In general, then, multiplying by the average local mesh size, and recurring the equation for the first difference quotient of the error ΔE back to $i = 1$, we have

$$\begin{aligned}\Delta E_{j+1/2} - \Delta E_{1/2} &= \frac{1}{6}\sum_{i=1}^{j}\left(h_i^2 - h_{i-1}^2\right)y^{(3)}(x_i) + O(h^2)\\ &= -\frac{1}{6}\sum_{i=1}^{j-1} h_i^2\left(y^{(3)}(x_{i+1}) - y^{(3)}(x_i)\right) + O(h^2),\end{aligned}$$

using summation by parts. But, that final sum is itself $O(h^2)$; thus ΔE (and E, also) is $O(h^2)$.

Now, extensions of Numerov's scheme to this problem result when seeking linear, tridiagonal combinations of both Y and mesh-point values of f so that the order of the truncation error is as high as possible. Uniqueness results with the imposition of two constraints on the scheme: that the tridiagonal combination of the f's be an average, and that the scheme be exact for quartic polynomials $y(x)$. One obtains

$$\begin{aligned}&(\Delta Y_{i+1/2} - \Delta Y_{i-1/2})/[(h_i + h_{i-1})/2]\\ &\quad = \alpha_i f_{i+1} + (1 - \alpha_i - \gamma_i)f_i + \gamma_i f_{i-1} =: (Af)_i,\end{aligned}$$

where $f_i := f(x_i)$, and

$$\alpha_i := \left(h_i^2 - h_{i-1}^2 + h_i h_{i-1}\right)/\left[6h_i(h_i + h_{i-1})\right],$$
$$\gamma_i := \left(h_{i-1}^2 - h_i^2 + h_i h_{i-1}\right)/\left[6h_{i-1}(h_i + h_{i-1})\right];$$

in principle, the same as one of Osborne's schemes [1967, associated with (4.10)]. Plugging in $y(x) = (x - x_i)^5$ this time, we find that

$$3\left[(h_i + h_{i-1})/2\right]\left[A(D^2y) - \Delta^2 y\right]_i = 2\left(h_i^4 - h_{i-1}^4\right) + 5h_i h_{i-1}\left(h_i^2 - h_{i-1}^2\right).$$

It follows, if $y^{(6)}$ is smooth, that ΔE is given by

$$\Delta E_{j+1/2} - \Delta E_{1/2} = c_1\Sigma_1 + c_2\Sigma_2 + O(h^4),$$

where

$$\Sigma_1 := \sum_{i=1}^{j}\left(h_i^4 - h_{i-1}^4\right)y^{(5)}(x_i), \qquad \Sigma_2 := \sum_{i=1}^{j} h_i h_{i-1}\left(h_i^2 - h_{i-1}^2\right)y^{(5)}(x_i),$$

and neither c_1 nor c_2 is zero. Now, Σ_1 sums by parts to $O(h^4)$; what about Σ_2? If one fixes on some index interval $I \leqslant i \leqslant J$ where the factors in its summand have constant sign (such as would occur in index intervals where the sequence (h_i) is monotone), then

$$\left|\sum_I^J h_i h_{i-1}\left(h_i^2 - h_{i-1}^2\right)y^{(5)}(x_i)\right| \leqslant \|y^{(5)}\|_\infty \left|\sum_I^J \left(h_i^2 + h_{i-1}^2\right)\left(h_i^2 - h_{i-1}^2\right)/2\right|,$$

using the geometric-arithmetic mean inequality; and the last sums to $O(h^4)$. Hence, most algorithms that recursively *adapt* the mesh to attain an approximate solution using Numerov's method for this problem would benefit from the efficiencies associated with fourth-order convergence, assuming the error in Y_0 and $\Delta Y_{1/2}$ were $O(h^4)$.

On the other hand, suppose that the mesh is three-periodic, i.e., that the mesh spacing is h, rh, sh, h, rh, $sh, \ldots$, with $0 < r$, $s \leqslant 1$. And suppose that $y^{(5)}(x) \equiv 1$. Then, after the jth period,

$$\Sigma_2 = (1 - r)(1 - s)(s - r)(1 + r + s)jh^4,$$

which, when jh is order one, is not $O(h^4)$ unless $(1 - r)(1 - s)(s - r) = O(h)$. With this exception, then, ΔE will not be $O(h^4)$; and, as ΔE is eventually of one sign, E will not be, either.

4. General Comments. C. de Boor has pointed out to us that the essential point, in the second paragraph of Section 1, is a special case of the result that the kth divided difference of x^{k+n} is given by

$$\sum_{|a|=n} x^a, \qquad x^a := x_i^{a_0} x_{i+1}^{a_1} \cdots x_{i+k}^{a_k};$$

and he has mentioned reference to Steffensen [1927, p. 19] or Milne-Thomson [1933, p.8] (see, also, Schumaker [1981, p 47]). We can offer no excuse that its present application is news to us.

We find that the recurrence relation for the difference quotients, namely

$$\Delta^j U_i = \frac{\Delta^{j-1}U_{i+1/2} - \Delta^{j-1}U_{i-1/2}}{(x_{i+j/2} - x_{i-j/2})/j}, \quad i \text{ integral (half-integral) when } j \text{ is even (odd)},$$

is more memorable once one realizes that the denominator represents both (a) the mean mesh size in the stencil for $\Delta^j U_i$, and (b) the distance between the points $\bar{x}_{i\pm 1/2}^{(j-1)}$ at which the difference quotients $\Delta^{j-1}U_{i\pm 1/2}$ attain their extra polynomial exactness as derivative approximations.

The literature already contains many references to *super*convergence, a notion originally associated with unanticipated accuracy—at special points—of approximate solutions obtained by Galerkin and collocation methods. In these contexts, proofs of such results use the fact that here the approximate solution Y is defined for all x; and the residual error $(D^k + L)(Y - y)$ is defined well enough so that its integrals against derivatives of the appropriate Green's function for $D^k + L$ can be used for error estimates, and sometimes shown especially small at certain locations.

Although less apparent in this present paper than in its precursors (Manteuffel and White [1986], Samarskiĭ [1971, pp. 130–139], and, especially, Tikhonov and Samarskiĭ [1962]—the last two concern second-order convergence associated with a large variety of conservative difference schemes for selfadjoint, second-order problems), the analysis we have applied is the analog of this on the discrete side of things. For, the truncation error is $(\Delta^k + \hat{L})(Y - y)$ instead, and the cancellation occurs in weighted sums of this against what amounts to difference quotients of the appropriate Green's matrix of $\Delta^k + \hat{L}$.

We choose to emphasize this distinction by associating the term supra-convergence with the latter.

However, it must be said immediately that there are at least two phenomena of unanticipated accuracy which, off hand, appear covered by neither approach: that in Thomée and Wendroff [1974] (although it seems closer to ordinary truncation error analysis once one uses Swartz and Wendroff's [1974] observation); and the unusual accuracy associated with a special class of difference schemes (Osborne [1967]), considered concurrently by Lynch and Rice [1980] and Doedel [1978, 1980]. But this too, given the stability the latter prove, is covered by ordinary analysis; for they attain unexpectedly high-order truncation error using the following device.

As in Lynch and Rice [1980] (or, in effect, Osborne [1967, p. 136]), and for the O.D.E. $D^k y = f$: take the kth difference quotient of the $(k-1)$st degree Taylor expansion of y about x_i to find that

$$\begin{aligned}\Delta^k y_{i+k/2} &= 0 + \int_{x_i}^{x_{i+k}} \Delta^k_{i+k/2}(\cdot - s)_+^{k-1} D^k y(s)\, ds/(k-1)! \\ &= \int_{x_i}^{x_{i+k}} B_{i,k}(s) D^k y(s)\, ds,\end{aligned}$$

where $B_{i,k}$ is the B-spline of degree $k-1$ with knots $x_i, \ldots, x_{i+k}$, normalized to integrate to one. This is to be approximated by an average of $f(\xi_1), \ldots, f(\xi_r)$, where the r evaluation points ξ_j may be chosen at will (so Lynch, Rice, and Doedel presume) from the interval $[x_i, x_{i+k}]$. Now, the B-spline being positive on (x_i, x_{i+k}), Lynch and Rice regard this average as an approximate weighted quadrature. So,

selecting the ξ_j as the zeros of an appropriate orthogonal polynomial with respect to this weight, they attain higher-order polynomial exactness (thus, truncation error) than one would normally expect. But, taking $D^k y(x) := x - \bar{x}_{i+k/2}$ above, it follows from our second paragraph (of Section 1) that the first moment of the B-spline, about the mean $\bar{x}_{i+k/2}$ of its knots, is zero—a fact also apparent from Schumaker's book [1981, pp. 128–129]—giving an alternate view of our associated second-order truncation error. Lynch and Rice extend this idea to more general equations using a relatively deep argument showing that the polynomial exactness can then be enforced if the ξ_j are appropriately perturbed to new positions in (x_i, x_{i+k}), positions that must be found numerically, and for each i; and they prove stability for general equations under certain restrictions on the mesh and mesh size. Doedel, for the compact scheme $(D^k + L)p(\xi_1) = f(\xi_1)$ (where p is the polynomial interpolating $Y_i, \ldots, Y_{i+k}$), proves stability for all small h [1980], having already [1978] noted second-order accuracy when ξ_1 is the zero of $D^k \prod_{j=0}^{k}(\cdot - x_{i+j})$ (now known as $\bar{x}_{i+k/2}$).

Just as superconvergence can yield various orders of enhancement over the ordinary errors one expects in its context, so it seems for supra-convergence. For example, we mention the conservative cell-centered (or "block-centered") difference schemes first analyzed in modern times by Levermore [1982], cf. Larsen, Levermore, Pomraning, and Sanderson [1985]; but previously considered by Tikhonov and Samarskiĭ [1962] (and for certain P.D.E.'s by Samarskiĭ [1963a, b]); more recently by Wheeler [1983], cf. Weisert and Wheeler [1984] (also for certain P.D.E.'s); and perhaps most thoroughly by Manteuffel and White [1986]. Not based completely on polynomial approximation, O.D.E. schemes of this ilk are exemplified by an *in*consistent tridiagonal approximation to $D^2 y$. Yet this truncation error, which is bounded only if local mesh ratios remain bounded, converts to $O(h^2)$ convergence upon application of factors of the corresponding Green's matrix. (Neither of the proofs that the solution of the *first*-order cell-centered scheme

$$(Y_{i+1/2} - Y_{i-1/2})/[(h_i + h_{i-1})/2] = Dy(x_i), \qquad Y_{1/2} = y(\bar{x}_{1/2}) + O(h^2),$$

gives an $O(h^2)$ approximation to $y(\bar{x})$, namely, the analog of the first proof of Section 3 or the application of the trapezoidal rule's known accuracy, suggest the details covering second-order equations.) There also exist *vertex*-centered, compact approximations to D^k, $k > 2$, with order h^{3-k} truncation error, that yield $O(h^2)$ supra-convergence (Manteuffel and White [1985]).

Nevertheless, we have yet to see supra-convergence for compact schemes that yields more than one order higher convergence than the truncation error for the polynomial-based schemes.

We point out that we have not tried to prove that the *positive* aspects of the example in Section 3 hold in practical application. For, although analogs of Numerov's tridiagonal method can be defined when lower-order terms are present (as in Swartz [1974, Section 7], Lynch and Rice [1980, p. 369], or Doedel [1978, Example 5.2]), one still must prove the truncation error decomposes into analogs of Σ_1 and Σ_2; and that a finite number of sign-changes in the factors in that Σ_2 will yield only a fourth-order contribution. Also: Fourth-order compact approximation of non-Dirichlet boundary data needs to be more explicitly considered—although

this is a less serious problem, as it only means involving an additional fixed number of mesh-point values of f (not Y) near the two boundaries (as could have been done in Swartz [1980]).

In 1982, A. White rediscovered, numerically, the phenomenon we have called supra-convergence for second-order boundary value problems; and he and T. Manteuffel constructed the proofs, based on the linear algebra involved, in their [1986] paper. The present paper represents an attempt to explain the phenomenon in terms more familiar to some, and to explore one of its limitations. On the other hand, Grigorieff's [1983] response to Manteuffel and White's work is that, after all, there is no surprise if the truncation error in such schemes can be measured (stably) as suitably small. Thus, suppose one uses discrete analogs of $\max_x |\int^x f(\xi)\, d\xi|$ in a generalization of the "Spijker norm" (Tikhonov and Smaraskiĭ [1962], Spijker [1968], Stetter [1973, pp. 81–87]); in particular, the one that sums the kth difference quotient to yield the $(k-1)$st. Then truncation errors *we* regarded as $O(h)$ in size are now only $O(h^2)$, as Grigorieff shows in an example ($\theta = (1, 0, \ldots, 0)$). Primarily, though, he argues that the lower-order difference quotients are stable with respect to such measures of the size of $\Delta^k + \hat{L}$ (plus boundary conditions, assuming both they and $\hat{L}$ are consistent). It was his example which suggested we describe the $\lfloor k/2 \rfloor$-parameter family of special evaluation points (in Section 1) as symmetric averages.

It may be worth noting the role that numerical computation played in the evolution of this paper. The slope of log-log plots of the maximum error against maximum mesh size is the traditional method of extracting the convergence rate for a numerical scheme; and it was the 63° tilt of the least-squares line fitting clusters of 200 such points, the ith point being associated with a mesh with i points chosen at random in $(0, 1)$, which convinced us that there was something worth proving for commonly used schemes approximating second-order boundary value problems. Yet, the same experiments for Numerov's method yielded slopes close to four; and it was only after some weeks of unsuccessful proofs that we noticed that the hypothesis of $O(h^4)$ convergence to $y(x) = x^5$ could be more easily explored by dividing Σ_2 by h^4, and so consider instead the hypothesis that

$$\sigma(\xi_1, \ldots, \xi_{n+1}) := \sum_{i=1}^{n} \xi_i \xi_{i+1} (\xi_{i+1}^2 - \xi_i^2), \quad \text{all } \xi_j \text{ in } [0,1], \text{ some } \xi_j = 1,$$

could be bounded independent of ξ in $[0,1]^{n+1}$ and of n. Tests of this were easily generated by fixing n, randomly generating a few thousand ξ's, and then examining log-log plots of the maximum magnitude of this sum versus n. And such experiments suggested there was no bound to be found—in fact, the maximum magnitude often grew at a rate like $n^{1/2}$. The periodic counterexample, subsequently found, also evolved into a succinct solution of the following related problem (Faber and White [1985], or Appendix 2 below): Given $m > 0$, find a condition on a bounded function $F(\eta_0, \ldots, \eta_m)$ that is both necessary and sufficient for $\sum_{i=1}^{n} F(\xi_i, \ldots, \xi_{i+m})$ to be uniformly bounded in ξ and n.

Appendix 1: Stability. For completeness, we append a proof that the compact difference operators

$$(MU)_{i+k} := \left[(\Delta^k + \hat{L})U\right]_{i+k/2}, \qquad i \geqslant 0,$$

which we have considered, are stable for the initial-difference quotient problem. For this, we shall continue to assume—with a shift of index—that $(MU)_i$ consists of the kth-order difference quotient Δ^k, based on the stencil ending with x_i, plus a uniformly bounded linear combination $\hat{L}$ of those pth-order difference quotients $(p < k)$ whose stencils $x_{j-p}, \ldots, x_j$ are subsets of $x_{i-k}, \ldots, x_i$.

The proof will generalize the proof for the case in which $\hat{L}$ involves only Δ^{k-1}, i.e., when

$$(MU)_i = (\Delta^k U)_{i-k/2} + a_i(\Delta^{k-1}U)_{i-(k-1)/2} + b_i(\Delta^{k-1}U)_{i-1-(k-1)/2}.$$

For this simple case, and with U in hand, set $v_i := (\Delta^{k-1}U)_{i-(k-1)/2}$. Then the relation between Δ^k and Δ^{k-1} means that

$$(1 + \bar{h}_i a_i)v_i = (1 - \bar{h}_i b_i)v_{i-1} + \bar{h}_i(MU)_i, \qquad \bar{h}_i := (x_i - x_{i-k})/k.$$

Using, say, $(1 + s)/(1 - s) \leqslant \exp(3s)$ for $0 \leqslant s \leqslant 1/2$, it follows that

$$|v_j| \leqslant \exp(3a\bar{h}_j)|v_{j-1}| + 2\bar{h}_i|(MU)_j|, \qquad k \leqslant j \leqslant i,$$

if $a \max_{j \leqslant i} \bar{h}_j < 1/2$, where $a := \max_j(|a_j|, |b_j|)$. Recurring from i back to the initial data, we have

$$|v_i| \leqslant \exp(3ax_i)\left[|v_{k-1}| + 2x_i \max_{k \leqslant j \leqslant i} |(MU)_j|\right],$$

since $\sum_{j=k}^{i} \bar{h}_j < \sum_{j=0}^{i-1} h_j = x_i$. Invoking, finally, the recursions for the lower-order difference quotients, we have the desired stability result:

$$\max_{p<k} \|\Delta^p U\|_\infty \leqslant \text{const}\left[\max_{p<k} |(\Delta^p U)_{p/2}| + \|MU\|_\infty\right],$$

independent of U and the mesh, if only $a \max_i \bar{h}_i < 1/2$ and $\sum h_i$ is bounded.

Given a vector U, now, for the general case, let $v_i^{(j)}$ be the jth difference quotient of $U_{i-j}, \ldots, U_i$ based on $x_{i-j}, \ldots, x_i$. We append, to the $k - 1$ relations between the $k - 1$ lower-order difference quotients, i.e., to

$$v_i^{(p-1)} - (x_i - x_{i-p})v_i^{(p)}/p = v_{i-1}^{(p-1)} \qquad (1 \leqslant p < k),$$

the full-difference equation written with only $v_i^{(0)}, \ldots, v_i^{(k-1)}$ on the left-hand side. We thereby obtain a recursive system

$$\begin{aligned}(I + \bar{h}_i A_i^k)v_i = (I - \bar{h}_i A_i^{k-1})v_{i-1} - \bar{h}_i A_i^{k-2}v_{i-2} - \cdots - \bar{h}_i A_i^0 v_{i-k} \\ + \bar{h}_i(MU)_i(0, \ldots, 0, 1)^T,\end{aligned}$$

for the vectors $v_j := (v_j^{(0)}, \ldots, v_j^{(k-1)})^T$. In this recursion, the entries of all k by k matrices A_j^p are uniformly bounded because of our assumption above concerning $\hat{L}$, and (in each lower Hessenberg matrix A_i^k) also because $(x_i - x_{i-p})/(p\bar{h}_i) \leqslant k/p$. Hence, with $w_i := \max_{j \leqslant i} \max_{p<k} |v_j^{(p)}|$, it follows that

$$w_i \leqslant (1 + a\bar{h}_i)w_{i-1}/(1 - a\bar{h}_i) + \bar{h}_i|(MU)_i|/(1 - a\bar{h}_i)$$

for $a := k \sup_{j,p} \|A_j^p\|_\infty$ and all small $\bar{h}_i$. Noting that w_{k-1} is uniformly bounded in terms of the k initial-difference quotients using the difference quotient recursions, we conclude the desired stability result as before.

Appendix 2: Periodic Sums and Supra-Convergent Functions, with V. Faber (December, 1984). For $k \geqslant 2$, let F map Ξ^k into a group $(\mathscr{G}, +, 0)$; here Ξ is some arbitrary set. We begin by characterizing those functions F which possess the

following additional property: The sum of the values of F, as one translates over one period of arbitrary periodic sequences made up from elements of Ξ, vanishes identically. More specifically, and for some $p \geqslant 1$, by a *periodic sum of period* p we mean

$$\sigma_p(\xi) := \sum_{i=1}^{p} F(\xi_i, \ldots, \xi_{i+k-1}), \qquad \xi \text{ in } \Xi_p; \text{ we take } \xi_{p+j} := \xi_j \text{ as required.}$$

And we shall say that *F sums to zero over the periods of arbitrary periodic sequences* if $\sigma_p = 0$ on Ξ^p for all $p \geqslant 1$. The prettiest result is the following:

THEOREM 1. (a) *F sums to zero over the periods of arbitrary periodic sequences if and only if*

(b) *there exists a function f of $k-1$ variables such that*

$$F(\xi_1, \ldots, \xi_k) \equiv f(\xi_1, \ldots, \xi_{k-1}) - f(\xi_2, \ldots, \xi_k).$$

Proof. (b) implies (a). For (b) means that σ_p is a collapsing sum:

$$\begin{aligned}\sigma_p(\xi) &= [f(\xi_1, \ldots, \xi_{k-1}) - f(\xi_2, \ldots, \xi_k)] \\ &\quad + \cdots + [f(\xi_p, \xi_1, \ldots, \xi_{k-2}) - f(\xi_1, \ldots, \xi_{k-1})] \\ &= f(\xi_1, \ldots, \xi_{k-1}) - f(\xi_1, \ldots, \xi_{k-1}) = 0, \qquad \xi \text{ in } \Xi^p.\end{aligned}$$

(a) implies (b). First, form the $(2k-1)$-periodic sequence

$$s_{2k-1} := (\ldots, \eta, \ldots, \eta, \xi_1, \ldots, \xi_k, \ldots)$$

(there are $k-1$ η's here); then, as a particular instance of (a),

$$\begin{aligned}0 &\equiv \sigma_{2k-1}(s_{2k-1}) \\ &\equiv [F(\eta, \ldots, \eta, \xi_1) + \cdots + F(\eta, \xi_1, \ldots, \xi_{k-1})] + F(\xi_1, \ldots, \xi_k) \\ &\quad + [F(\xi_2, \ldots, \xi_k, \eta) + \cdots + F(\xi_k, \eta, \ldots, \eta)] \\ &=: A(\xi_1, \ldots, \xi_{k-1}, \eta) + F(\xi_1, \ldots, \xi_k) \\ &\quad + g(\xi_2, \ldots, \xi_k, \eta).\end{aligned}$$

Next, form the $(2k-2)$-periodic sequence

$$s_{2k} := (\ldots, \eta, \ldots, \eta, \xi_1, \ldots, \xi_{k-1}, \ldots)$$

(there are $k-1$ η's here, also); then, as another instance of (a),

$$\begin{aligned}0 &\equiv \sigma_{2k-2}(s_{2k-2}) \\ &\equiv [F(\eta, \ldots, \eta, \xi_1) + \cdots + F(\eta, \xi_1, \ldots, \xi_{k-1})] \\ &\quad + [F(\xi_1, \ldots, \xi_{k-1}, \eta) + \cdots + F(\xi_{k-1}, \eta, \ldots, \eta)] \\ &\equiv A(\xi_1, \ldots, \xi_{k-1}, \eta) + g(\xi_1, \ldots, \xi_{k-1}, \eta).\end{aligned}$$

We do not need "+" to be commutative to conclude that

$$F(\xi_1, \ldots, \xi_k) \equiv g(\xi_1, \ldots, \xi_{k-1}, \eta) - g(\xi_2, \ldots, \xi_k, \eta). \tag{1}$$

For (b), now, let $\eta_c(\cdot)$ be any constant map of Ξ^{k-1} onto c in Ξ; and set

$$f(\xi_1, \ldots, \xi_{k-1}) := g(\xi_1, \ldots, \xi_{k-1}, \eta_c(\xi_1, \ldots, \xi_{k-1})).$$

A third equivalent statement is that periodic sums of periods $2k-2$ and $2k-1$ vanish identically (for that is all we used in the second half of the proof).

The final appendix uses the following rather unsymmetric

COROLLARY 1.1. *F sums to zero over the periods of arbitrary periodic sequences if and only if, for some c in Ξ, $F(c,\dots,c)=0$, and the function*

$$G_c(\xi_1,\dots,\xi_k) := F(\xi_1,\dots,\xi_k) + F(\xi_2,\dots,\xi_k,c) + \cdots + F(\xi_k,c,\dots,c)$$

is independent of ξ_k.

Proof. From the definitions of G_c and g, we have

$$G_c(\xi_1,\dots,\xi_k) \equiv F(\xi_1,\dots,\xi_k) + g(\xi_2,\dots,\xi_k,c),$$

and (as we have seen) this is $g(\xi_1,\dots,\xi_{k-1},c)$ if we assume (a) of Theorem 1; moreover, that assumption implies $F(c,\dots,c)=0$. On the other hand, if G_c is independent of ξ_k, then

$$\begin{aligned} F(\xi_1,\dots,\xi_k) + g(\xi_2,\dots,\xi_k,c) &\equiv G_c(\xi_1,\dots,\xi_{k-1},\xi_k) \equiv G_c(\xi_1,\dots,\xi_{k-1},c) \\ &\equiv g(\xi_1,\dots,\xi_{k-1},c) + F(c,\dots,c), \end{aligned}$$

the last from the definitions of G_c and g. Thus, (1) holds with $\eta = c$ if also $F(c,\dots,c)=0$ for some c in Ξ; (b) of Theorem 1 then follows as before, and therefore, (a).

It was results like these that inspired Faber and White's graph-theoretic approach to our problem [1985], while the final section of that paper motivated Appendix 3 here to follow.

P. Lax has observed that Theorem 1 has a known continuous analog. For this, recall that a p-periodic sequence ξ is a p-periodic function on the integers into Ξ. Let δ be the forward-difference operator, so that, e.g., $(\delta\xi)(i) := \xi(i+1) - \xi(i)$ is also p-periodic. We presume Ξ is such that the map (taking Ξ^k into Ξ^k) given by

$$(\xi(1),\xi(2),\dots,\xi(k)) \to (\xi(1),\delta\xi(1),\dots,\delta^{k-1}\xi(1))$$

is 1-1 and onto (as it would be if Ξ were the reals—by solving the initial value problem for δ^{k-1} on $1,\dots,k$). Then, associated with each F on Ξ^k is a unique function R, also on Ξ^k, satisfying

$$F(\xi(1),\xi(2),\dots,\xi(k)) = R(\xi(1),\delta\xi(1),\dots,\delta^{k-1}\xi(1)),$$

and vice versa. With this, Theorem 1 may be restated as

COROLLARY 1.2. *Let R take Ξ^k into a group. Then,*

$$\sum_{i=1}^{p} R(\xi,\delta\xi,\dots,\delta^{k-1}\xi)(i) = 0$$

for arbitrary p-periodic functions ξ (on the integers into Ξ) and for arbitrary p, if and only if there exists a function r on Ξ^{k-1} so that

$$R(\xi,\delta\xi,\dots,\delta^{k-1}\xi) = -\delta\left[r(\xi,\delta\xi,\dots,\delta^{k-2}\xi)\right].$$

(Here, $r(\xi(1),\dots,\delta^{k-2}\xi(1)) = f(\xi(1),\dots,\xi(k-1))$.) This corollary is a discrete

analog of the following result (Lax [1975, Lemma 5.8], there stated for polynomials R):

"CALCULUS LEMMA" (LAX). *Let R be a function of k variables. With $(D\eta)(x) := (d\eta/dt)(x)$, suppose*

$$\int_0^p R(\xi, D\xi, \ldots, D^{k-1}\xi)(x)\, dx = 0$$

for every sufficiently differentiable p-periodic function $\xi(x)$. Then, there exists a function r of $k-1$ variables, so that

$$R(\xi, D\xi, \ldots, D^{k-1}\xi) = -D\left[r(\xi, D\xi, \ldots, D^{k-2}\xi)\right].$$

Recall, now, that we have associated the phrase "supra-convergent difference scheme" with difference schemes possessing truncation errors whose sums were unexpectedly small. We are thereby led to the following definition. We shall say that *the function F is supra-convergent* if the average of its values, as one translates over arbitrary finite sequences, goes to zero as the length of those sequences increases; i.e.,

$$\sum_{i=1}^{n} F(\xi_i, \ldots, \xi_{i+k-1}) = o(n), \qquad n \to \infty, \text{ pointwise on } \Xi^\infty.$$

With this, we have the following

THEOREM 2. *Suppose the range of F lies in a normed linear space, and suppose F is bounded on its domain. Then, F is supra-convergent if and only if F sums to zero over the periods of arbitrary periodic sequences.*

Proof. Necessity is clear, since a p-periodic sequence ξ_p is also an np-periodic sequence for any n, whence $\sigma_{np}(\xi_p, \ldots, \xi_p) = n\sigma_p(\xi_p) \neq o(np)$ unless $\sigma_p(\xi_p) = 0$.

On the other hand, suppose $\sigma_p = 0$ on Ξ^p for all $p \geqslant 1$. Associate with the finite sequence $\xi_1, \ldots, \xi_m$ its m-periodic extension $\hat{\xi}_m := \ldots, \xi_1, \ldots, \xi_m, \ldots$. We have

$$\begin{aligned} 0 = \sigma_m(\hat{\xi}_m) = F(\xi_1, \ldots, \xi_k) + \cdots + F(\xi_{m-k+1}, \ldots, \xi_m) \\ + F(\xi_{m-k+2}, \ldots, \xi_m, \xi_1) + \cdots + F(\xi_m, \xi_1, \ldots, \xi_{k-1}); \end{aligned}$$

but each of the last $k-1$ terms is uniformly bounded since F is. Hence, the first part of the sum is *uniformly* bounded; and its bound yields the following

COROLLARY 2. *Suppose F bounded by B on Ξ^k, and that F is supra-convergent. Then the average of the n values of F, as one translates over an arbitrary finite sequence with $n+k-1$ elements, is uniformly bounded by $(k-1)B/n$.*

That is to say, not just the pointwise, $o(1)$ value required by the definition.

Appendix 3. Fixed Weights Allowable to Supra-Convergent Compact Difference Schemes. (December, 1984). Among the compact difference schemes one can consider for approximating the simple kth-order differential equation $y^{(k)} = f$ are those schemes utilizing the kth difference quotient as follows:

$$(1) \qquad k![x_i, \ldots, x_{i+k}]Y =: \Delta^k Y_{i+k/2} = \sum_{j=0}^{k} w_j y_{i+j}^{(k)}, \qquad y_m^{(k)} := y^{(k)}(x_m),$$

where $[z_0, \ldots, z_k]W$ is the kth-order divided difference of W based on $z_0, \ldots, z_k$. This may be reexpressed in terms of $h_j := x_j - x_{j-1}$ as

$$S(Y; h_{i+1}, \ldots, h_{i+k})$$
$$:= (h_{i+1} + \cdots + h_{i+k})\left\{ \sum_{j=0}^{k} w_j y_{i+j}^{(k)}/k! - [x_i, \ldots, x_{i+k}]Y \right\} = 0$$

(S, here, is for "scheme"). Subtraction of $S(y)$ from $S(Y)$ yields a recursion for the $(k-1)$st divided difference of the error e:

$$[x_{i+1}, \ldots, x_{i+k}]e = [x_i, \ldots, x_{i+k-1}]e + S(y);$$

and this is why one is concerned with the possibility that S be supra-convergent. Note that $S(y)$, for a general function $y(x)$, will depend on more than the indicated arguments $h_{i+1}, \ldots, h_{i+k}$; but there are two cases, namely $y(x) = x^k$ or x^{k+1}, when it often depends only on these arguments, as we shall see. (The weights could also depend on i, as they do in Numerov's scheme, or in those of Osborne, Swartz, Lynch, and Rice or Doedel).

Now, we showed at the end of Section 1, that if the weights $(w_j)_0^k$ not only were independent of i (and, hence, of the mesh spacings) but also represented a *symmetric average*; i.e.

$$\sum_{j=0}^{k} w_j f_j = \sum_{j=0}^{\lfloor k/2 \rfloor} \theta_j \left[(f_j + f_{k-j})/2 \right]; \qquad \sum_{j=0}^{\lfloor k/2 \rfloor} \theta_j = 1,$$

$$\lfloor k/2 \rfloor := \text{the greatest integer in } k/2;$$

then the corresponding difference schemes were supra-convergent; in particular, $S(x^k)$ and $S(x^{k+1})$ were then necessarily supra-convergent functions. Our goal here is to apply Appendix 2 to show that, if the weights are independent of i, then they *must* form a symmetric average if the difference scheme is to be supra-convergent. So, we assume them independent of i henceforth.

If (1) yields supra-convergence in general, then it must, in particular, for x^k and x^{k+1}. That is to say, $S(x^k)$ and $S(x^{k+1})$, if dependent only on $h_{i+1}, \ldots, h_{i+k}$, must be supra-convergent functions. Consider first x^k: Since $[x_i, \ldots, x_{i+k}]x^k = 1$ while $(x^k)^{(k)} = k!$, we conclude

$$S(x^k) = (h_{i+1} + \cdots + h_{i+k})\left(\sum_{j=0}^{k} w_j - 1 \right).$$

With S, associate the function F, given by

$$F(\xi_1, \ldots, \xi_k) := S(x^k; h_1, \ldots, h_k)/h, \qquad h_i = h\xi_i,\ \xi \text{ in } [0,1]^k;$$

recall h is the maximum mesh size. (Although it makes sense to ask if S is a supra-convergent function, the effect of bounds on $\sum S$ for, say, $h < 1/3$, is less interesting than the effect of bounds on $\sum F$ for $\|\xi\|_\infty \leqslant 1$. Offhand, F depends also on h. However, since S is homogeneous of order 1, we see that $F(\xi) \equiv S(\xi)$). Now, F supra-convergent implies

$$\sum_{j=0}^{k} w_j = 1, \tag{2}$$

which follows from the requirement (Theorem 2) that $F(1,\dots,1)=0$. This is equivalent to requiring that the scheme be exact for polynomials of degree k as well as degree $k-1$; and we assume it hereafter.

Henceforth, we examine what is necessary for $S(x^{k+1})$ to be supra-convergent as well; in particular, we would like to show that, then, each $w_{k-j}-w_j$ is necessarily zero. Since the scheme is exact for polynomials of degree k, we may consider $(x-x_i)^{k+1}$ instead of x^{k+1}; and, indeed, may concentrate only on the generic case $x_0=0$. For this we recall, from the beginning of Section 1, that

$$[x_0,\dots,x_k]x^{k+1}=x_0+\cdots+x_k=h_1+(h_1+h_2)+\cdots+(h_1+\cdots+h_k),$$

while

$$(x^{k+1})^{(k)}(x_j)=(k+1)!x_j=(k+1)!(h_1+\cdots+h_j),\qquad j>0.$$

Consequently, we find that $S(x^{k+1})$ is given generically by

$$S(x^{k+1};h_1,\dots,h_k):=(h_1+\cdots+h_k)\left\{(k+1)\sum_{j=0}^{k}(h_1+\cdots+h_j)w_j\right.$$
$$\left.-[kh_1+(k-1)h_2+\cdots+h_k]\right\}.$$

With $S(x^{k+1})$ associate

$$F(\xi_1,\dots,\xi_k):=S(x^{k+1};h_1,\dots,h_k)/h^2,\qquad h_i=h\xi_i,\ \xi \text{ in } [0,1]^k$$

(again, $F=S$ since S is homogeneous of order 2). We take $c=0$ and construct G_0 from F as in Corollary 1.1. Since the weights are mesh-independent, F is a homogeneous quadratic form; since $c=0$, so is G_0. Theorem 2 and Corollary 1.1 insist that G_0 must be independent of ξ_k for F to be supra-convergent. Thus, the coefficient of each term $\xi_i\xi_k$ in G_0 must vanish. But, G_0 is linear in $(w_j)_0^k$, so the weights must satisfy k corresponding linear (but inhomogeneous) equations.

These k equations, when all divided by $k+1$ (and the last then doubled), constitute the system $Aw=b$, where, for $1\leqslant i\leqslant k$ and $0\leqslant j\leqslant k$,

$$A_{ij}:=\min(i,j)+(i+j-k)_+,\quad (z)_+:=\text{the nonnegative part of } z;\quad \text{and } b_i:=i.$$

To show this implies that all $w_{k-j}-w_j$ must vanish, we begin with a slight detour.

Note that for two-vectors $u=(u_0,u_1)$,

$$u\cdot v=(\Sigma u\Sigma v-\Delta u\Delta v)/2,\quad \text{where } \Delta u:=u_1-u_0,\ \Sigma u:=u_1+u_0.$$

We may extend this to row-vectors and to matrices $(M_{ij})_1^n{}_0^k$ by differencing or summing columns, working from the outside in, as follows: Define matrices

$$(\Delta M)_{ij}:=M_{i,k-j}-M_{ij},\qquad 0\leqslant j\leqslant \lfloor (k-1)/2\rfloor,$$

and

$$(\Sigma M)_{ij}:=M_{i,k-j}+M_{ij},\qquad 0\leqslant j\leqslant \lfloor k/2\rfloor.$$

Then, for $(k+1)$-vectors u, v,

$$u\cdot v=(\Sigma u\cdot\Sigma v-\Delta u\cdot\Delta v)/2,$$

in particular (using (2)),

$$1=\sum_{j=0}^{k}1\cdot w_j=\left[\sum_{j=0}^{\lfloor k/2\rfloor}2(\Sigma w)_j\right]/2; \tag{3a}$$

while

$$\text{(3b)} \qquad Aw = b \quad \text{iff } \Sigma A\, \Sigma w - \Delta A\, \Delta w = 2b.$$

But for our matrix A, $(\Sigma A)_{ij} = 2i$ independent of j; so, given the form of b,

$$\Sigma A = 2\,\mathrm{diag}(b)J, \quad \text{the matrix } J \text{ consisting entirely of 1's.}$$

Hence, from (3b) and (3a),

$$0 = \Sigma A\, \Sigma w - 2b - \Delta A\, \Delta w = -\Delta A\, \Delta w.$$

So, we will have proved what we seek, namely, $w_j = w_{k-j}$ for all j, if ΔA has full rank $\lfloor (k-1)/2 \rfloor + 1 =: m$. But, for $1 \leqslant i \leqslant k$ and $0 \leqslant j < m$,

$$(\Delta A)_{ij} = 2[(i-j)_+ - (i+j-k)_+].$$

In particular, the upper m by m half of ΔA is lower triangular with 2's on its main diagonal.

And we have proved that $\Delta w = 0$, so that the symmetric averages which we considered at the end of Section 1 are the *only* averages one can use which are both independent of the mesh and yield supra-convergence. These last two appendixes have also provided an alternative to Section 1 for proof that its difference schemes, using symmetrically averaged source terms, are supra-convergent with $O(h^2)$ error—at least for polynomial solutions $y(x)$ of degree $k+1$.

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