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High Order Finite-Difference Methods for Two-Point Boundary Value Problems with Singular Sources

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This paper is concerned with the numerical approximation by finite differences of the model problem $-u'' + a(x)\,u' + b(x)\,u = \delta(x-y)$, $0 < x < 1$, fixed $y \in (0, 1)$, $u(0) = u(1) = 0$. High-order 3-point schemes are constructed using a general framework of Lynch and Rice (*Math. Comp.* **34** (1980), 333–372) and Doedel (*SIAM J. Numer. Anal.* **15** (1978), 450–465). It is shown that by making modifications on those mesh intervals containing the singular point y one can easily construct difference schemes of arbitrarily high order. The appropriate modifications involve information about the local Green's function, for which a nonstandard perturbation-like series representation is derived. A complete discretization error analysis is given, and numerical experiments exhibiting convergence rates up to and including 6th order (even when the singular-point is not a mesh point) are reported. © 1986 Academic Press, Inc.

1. INTRODUCTION

In the numerical simulation of oil reservoirs, one is led to consider steady state differential equations of the form $Lu = f$, where f can contain a finite number of *point sources* (Dirac delta functions) that model the injection and recovery wells in the field (cf. [6]). Various approaches to handling the numerical difficulties that such singular functions present are discussed in [4, 6, 7, 9, 10]. Typically, one tries to use a weak formulation or subtract the singularity (or both). Even many finite-difference codes change to a finite-element formulation in the neighborhood of the wells to cope with the problem of singular sources.

It is the purpose of this paper to show how to construct compact finite-difference schemes of arbitrarily high order for a model 1-dimensional problem with a single point source. The extension to a finite number of such terms is immediate. We consider the linear 2-point boundary value problem

$$L[u] \equiv -u'' + a(x)\,u' + b(x)\,u = \delta(x-y), \qquad 0 < x < 1, \quad \text{fixed } y \in (0, 1)$$
$$u(0) = u(1) = 0. \tag{1.1}$$

It is assumed that the coefficient functions a and b are sufficiently smooth and such that the problem (1.1) is *well posed*, i.e., $L[u] = 0$ and $u(0) = u(1) = 0$ imply $u = 0$.

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In this case, the solution of (1.1) is the *Green's function* for L, with zero end-point conditions.

The difference schemes are constructed by using a general finite-difference framework of Lynch and Rice [8] and Doedel [2]. Away from those mesh intervals containing the singular point y, high order approximations to $Lu = 0$ are constructed by making the scheme exact on spaces of polynomials. For those (at most 2) subintervals containing y, modifications to the difference scheme must be made. These require information about the *local Green's function* for L. We derive a perturbation-like series in ascending powers of the mesh spacing h for this function; the component functions of this series are higher and higher order piecewise polynomial functions. By forcing the finite-difference scheme to be exact on an appropriate number of these local approximating functions, any desired order of global discretization error can be attained.

In the following sections, the theory and application of this approach are laid out. Low order ($O(h^2)$ and $O(h^4)$) schemes are derived by hand, and an automated approach to constructing high-order schemes is presented and analyzed. In the discretization error analysis, the general stability results of Esser [5] are utilized.

2. The Optimal 3-Point Scheme

There is a 3-point difference equation that the true solution of (1.1) satisfies exactly. This can be derived as follows. For simplicity, we give a uniform partition of the interval $[0, 1]$: $x_i = ih$, $i = 0,..., n$, where $h = 1/n$. Consider a pair of adjacent subintervals (x_{i-1}, x_{i+1}). Suppose that $y \notin (x_{i-1}, x_{i+1})$. Then on this subinterval u satisfies

$$\begin{aligned} &L[u](x) = 0, \qquad x_{i-1} < x < x_{i+1} \\ &u(x_{i-1}) = u_{i-1} \qquad u(x_{i+1}) = u_{i+1}, \end{aligned} \tag{2.1}$$

Now if the coefficient functions a and b are continuous on $[0, 1]$, then all of these subproblems will be well posed for h sufficiently small. Let s_i and t_i be a local basis for the null space of L satisfying

$$\begin{aligned} L[s_i](x) = L[t_i](x) = 0, \qquad & x_{i-1} < x < x_{i+1} \\ s_i(x_{i-1}) = 1 \qquad & t_i(x_{i-1}) = 0 \\ s_i(x_{i+1}) = 0 \qquad & t_i(x_{i+1}) = 1, \end{aligned} \tag{2.2}$$

Then for $x \in (x_{i-1}, x_{i+1})$, the solution u of (2.1) has the representation

$$u(x) = u_{i-1} s_i(x) + u_{i+1} t_i(x).$$

The homogeneous 3-point difference equation satisfied by u is obtained from this by evaluation at $x = x_i$ producing

$$\alpha^*_{i,-1} u_{i-1} + u_i + \alpha^*_{i,1} u_{i+1} = 0,$$

where $\alpha^*_{i,-1} \equiv -s_i(x_i)$ and $\alpha^*_{i,1} \equiv -t_i(x_i)$.

In the case where the subinterval (x_{i-1}, x_{i+1}) contains the singular point y, then u admits the representation

$$u(x) = u_{i-1} s_i(x) + u_{i+1} t_i(x) + g_i(x, y),$$

where g_i is the *local Green's function* for L on (x_{i-1}, x_{i+1}) with zero endpoint conditions, i.e., g_i satisfies

$$\begin{aligned} L_x[g_i] &= \delta(x-y), \qquad x_{i-1} < x,\ y < x_{i+1} \\ g_i(x_{i-1}, y) &= g_i(x_{i+1}, y) = 0. \end{aligned} \tag{2.3}$$

And we get the 3-point difference equation

$$\alpha^*_{i,-1} u_{i-1} + u_i + \alpha^*_{i,1} = g_i(x_i, y).$$

Combining these we have the exact 3-point rule

$$\begin{aligned} \alpha^*_{i,-1} u_{i-1} + u_i + \alpha^*_{i,1} u_{i+1} &= 0, \qquad && y \notin (x_{i-1}, x_{i+1}) \\ &= g_i(x_i, y), && y \in (x_{i-1}, x_{i+1}) \end{aligned} \tag{2.4}$$

satisfied by the true solution of (1.1).

It is not hard to show that the system (2.4) is nonsingular for all h sufficiently small and thus serves to uniquely determine the mesh values of u. We now show that any consistent 3-point discretization of L must be such that these optimal difference coefficients, $\alpha^*_{i,-1}$ and $\alpha^*_{i,1}$, are approached in the limit as $h \to 0$ at a rate proportional to the local truncation error.

Thus we consider, for $i = 1, \ldots, n-1$, a general 3-point discretization of the form

$$L_h[\phi]_i \equiv \alpha_{i,-1} \phi(x_{i-1}) + \alpha_{i,0} \phi(x_i) + \alpha_{i,1} \phi(x_{i+1}) \tag{2.5a}$$

and an associated *identity expansion* of the form

$$I_h[\psi]_i \equiv \beta_{i,1} \psi(\xi_{i,1}) + \cdots + \beta_{i,J} \psi(\xi_{i,J}). \tag{2.5b}$$

Here the weight $\beta_{i,1}, \ldots, \beta_{i,J}$ are assumed to be bounded independent of h and to satisfy $\beta_{i,1} + \cdots + \beta_{i,J} = 1$, and the auxiliary points $\xi_{i,1}, \ldots, \xi_{i,J}$ are assumed to be distinct and satisfy $|\xi_{i,j} - x_i| = O(h)$, $j = 1, \ldots, J$, uniformly in i. For such a scheme we define the local truncation error

$$T_h[\phi]_i \equiv L_h[\phi]_i - I_h[L[\phi]]_i, \qquad i = 1, \ldots, n-1.$$

The difference scheme (L_h, I_h) is said to be *consistent* with L if $\|T_h[\phi]\|_\infty \to 0$ as $h \to 0$ for all smooth functions ϕ; it is said to be *consistent of order p* if $\|T_h[\phi]\|_\infty = O(h^p)$. We have the following.

PROPOSITION 2.1. *Let the difference scheme* (L_h, I_h) *in* (2.5) *and differential operator* L *in* (1.1) *be consistent of order p, some* $p \geqslant 1$. *Then the difference coefficients* $\alpha_{i,-1}$, $\alpha_{i,0}$, *and* $\alpha_{i,1}$ *of* L_h *and the optimal difference coefficients* $\alpha^*_{i,-1}$ *and* $\alpha^*_{i,1}$ *in* (2.4) *satisfy*

$$\max_{i=1,\ldots,n-1} \left| \alpha^*_{i,-1} - \frac{\alpha_{i,-1}}{\alpha_{i,0}} \right|, \qquad \max_{i=1,\ldots,n-1} \left| \alpha^*_{i,1} - \frac{\alpha_{i,1}}{\alpha_{i,0}} \right| = O(h^{p+1}) \qquad \text{as} \quad h \to 0.$$

Proof. First note that

$$\alpha_{i,0} = \frac{2}{h^2}(1 + O(h)) \qquad \text{uniformly in } i.$$

This follows by applying the truncation operator T_h to $\phi(x) \equiv (x - x_{i-1})(x - x_{i+1})$:

$$\begin{aligned} T_h[\phi]_i &= -h^2\alpha_{i,0} - \sum_{j=1}^{J} \beta_{i,j} L[\phi](\xi_{i,j}) \\ &= -h^2\alpha_{i,0} + 2 - \sum_{j=1}^{J} \beta_{i,j}[a(\xi_{i,j})\,\phi'(\xi_{i,j}) + b(\xi_{i,j})\,\phi(\xi_{i,j})] \\ &\Rightarrow \left| \alpha_{i,0} - \frac{2}{h^2} \right| \leqslant \frac{1}{h}\|a\|_\infty + \|b\|_\infty + O(h^{p-2}) = \frac{2}{h^2} \cdot O(h). \end{aligned}$$

Now, let s_i and t_i again denote the null basis elements for L on (x_{i-1}, x_{i+1}) as in (2.2). Then hs_i and ht_i can be bounded together with their derivatives up to any finite order (granted sufficient smoothness) independently of h and i. And we have

$$\begin{aligned} \frac{\alpha_{i,-1}}{\alpha_{i,0}} - \alpha^*_{i,-1} &= \frac{1}{\alpha_{i,0}}(\alpha_{i,-1} + \alpha_{i,0} \cdot (-\alpha^*_{i,-1})) \\ &= \frac{1}{\alpha_{i,0}}(\alpha_{i,-1} s_i(x_{i-1}) + \alpha_{i,0} s_i(x_i) + \alpha_{i,1} s_i(x_{i+1})) \\ &= \frac{1}{\alpha_{i,0}} T_h[s_i]_i = \frac{h^2}{2}(1 + O(h)) \cdot \frac{1}{h} \cdot O(h^p) \\ &= O(h^{p+1}). \end{aligned}$$

The second half of the proposition follows from similar consideration of the basis element t_i. ∎

So we have a characterization (up to normalization) of what are the *optimal* difference coefficients and inhomogeneous term for a discretization of (1.1). It is this discretization, (2.4), that we should strive to emulate. The construction of high-order coefficients $\alpha_{i,-1}$, $\alpha_{i,0}$, and $\alpha_{i,1}$ depends only on the homogeneous equation $Lu=0$ (i.e., on the differential operator) and not on the source function f; it offers no great difficulty. However, we must come up with a compatibly high order approximation to the local Green's function $g_i(x_i, y)$. We take up this issue now.

3. An Expansion for the Local Green's Functions

Let (x_{i-1}, x_{i+1}) be a singular subinterval, i.e., $y \in (x_{i-1}, x_{i+1})$. Let g denote the local Green's function $g_i(x_i, \cdot)$ regarded as a function of its second argument, i.e., $g(x) = g_i(x_i, x)$, $x_{i-1} < x < x_{i+1}$. Then g is uniquely determined by (cf. [11])

$$L^\dagger[g](x) \equiv -g'' - (a(x)\, g)' + b(x)\, g = 0, \qquad x_{i-1} < x < x_i, \quad x_i < x < x_{i+1}$$

$$g(x_{i-1}) = g(x_{i+1}) = 0$$

$$g(x_i^+) - g(x_i^-) = 0$$

$$g'(x_i^+) - g'(x_i^-) = -1.$$

We wish to construct a series for g in ascending powers of the mesh width h. To this end we introduce the stretching transformation $\tilde{x} = (x - x_i)/h$, which produces the problem

$$h^2 \cdot \tilde{L}^\dagger[\tilde{g}] \equiv -\tilde{g}'' - ha(x_i + h\tilde{x})\, \tilde{g}' + h^2(b - a')(x_i + h\tilde{x})\, \tilde{g} = 0,$$

$$-1 < \tilde{x} < 0, \quad 0 < \tilde{x} < 1$$

$$\tilde{g}(-1) = \tilde{g}(1) = 0$$

$$\tilde{g}(0^+) - \tilde{g}(0^-) = 0$$

$$\tilde{g}'(0^+) - \tilde{g}'(0^-) = -h.$$

Seek $\tilde{g}$ in the form

$$\tilde{g} = \tilde{g}_1 h + \tilde{g}_2 h^2 + \cdots.$$

Substituting this expansion into the differential equation above, expanding a and b about $h = 0$, and balancing like powers of h produces the series of problems

$$h: \qquad -\tilde{g}_1'' = 0, \qquad -1 < \tilde{x} < 0, \quad 0 < \tilde{x} < 1$$

$$\tilde{g}_1(-1) = \tilde{g}_1(1) = 0$$

$$\tilde{g}_1(0^+) - \tilde{g}_1(0^-) = 0$$

$$\tilde{g}_1'(0^+) - \tilde{g}_1'(0^-) = -1;$$

$$h^2: \qquad -\tilde{g}_2'' = a(x_i)\,\tilde{g}_1', \qquad -1 < \tilde{x} < 0, \quad 0 < \tilde{x} < 1$$

$$\tilde{g}_2(-1) = \tilde{g}_2(1) = 0$$

$$\tilde{g}_2(0^+) - \tilde{g}_2(0^-) = 0$$

$$\tilde{g}_2'(0^+) - \tilde{g}_2'(0^-) = 0$$

$$\vdots$$

Solving the first two problems gives $\tilde{g}_1(\tilde{x}) \doteq C1\frac{1}{2}(1-|\tilde{x}|)$ and $\tilde{g}_2(\tilde{x}) = \frac{1}{4}a(x_i)\,\tilde{x}(|\tilde{x}|-1)$. Notice that the conditions at $\tilde{x}=0$ are superfluous beyond the first $(O(h))$ problem. Notice also that $\tilde{g}_1$ is an even C^0-linear spline, with knot at $\tilde{x}=0$, that vanishes at $\tilde{x}=\pm 1$ and $\tilde{g}_2$ is an odd C^1-quadratic spline, also with knot at zero and vanishing at ± 1. It can be shown by induction that the function $\tilde{g}_m$ is a C^{m-1} spline of order m with a single knot at $\tilde{x}=0$; it vanishes at $\tilde{x}=\pm 1$ and is an even function (with respect to the point $\tilde{x}=0$) if m is odd and an odd function if m is even.

We thus see that formally the local Green's function $g_i(x_i, \cdot)$ can be expanded in a series of ascending powers in h whose component functions are higher and higher order spline functions with knots at $x = x_i$. In fact, this series is asymptotic (provided a and b are smooth enough). We prove this now.

THEOREM 3.1. *Let the coefficient functions a and b satisfy $a \in C^{p-1}[x_{i-1}, x_{i+1}]$ and $b \in C^{p-2}[x_{i-1}, x_{i+1}]$. Then the asymptotic representation*

$$\tilde{g}(\tilde{x}) = h\tilde{g}_1(\tilde{x}) + \cdots + h^p\tilde{g}_p(\tilde{x}) + \tilde{r}_p(\tilde{x}; h) \tag{3.1}$$

is valid in the sense that $\|\tilde{L}^\dagger[\tilde{r}_p]\|_\infty \leqslant Ch^{p-1}$ and $\|\tilde{r}_p\|_\infty \leqslant Ch^{p+1}$, as $h \to 0$.

Proof. Under the assumptions on a and b, we have from Taylor's formula

$$a(x_i + h\tilde{x}) = a(x_i) + a'(x_i)\,\tilde{x}h + \cdots + a^{(p-2)}(x_i)\frac{\tilde{x}^{p-2}}{(p-2)!}h^{p-2}$$

$$+ a^{(p-1)}(x_i + h\tilde{\xi}_1(\tilde{x}))\frac{\tilde{x}^{p-1}}{(p-1)!}h^{p-1}$$

and

$$(b-a')(s_i + h\tilde{x}) = (b-a')(x_i) + \cdots + (b^{(p-2)} - a^{(p-1)})(x_i + h\tilde{\xi}_2(\tilde{x}))\frac{\tilde{x}^{p-2}}{(p-2)!}h^{p-2}.$$

Using the expansions above for a and $b-a'$ together with the conditions satisfied by $\tilde{g}_1, \ldots, \tilde{g}_p$ we get

$$h^2\,\|\tilde{L}^\dagger[r_p]\|_\infty \leqslant ch^{p+1} \qquad \text{as} \quad h \to 0,$$

and the result follows from the stability of the differential operator $h^2\tilde{L}^\dagger$. ∎

We make note of the fact that a representation similar to the one above but treating the local Green's function g_i as a function of its first argument could just as easily have been constructed. It would consist of higher and higher order splines with knots at the singular point y. It would have the advantage of using the original differential operator L instead of the *adjoint* $L^\dagger$ (and thereby not requiring $a'(x)$), but it would have the disadvantage of losing some of the symmetry of our construction: the alternating oddness and eveness of the spline functions and the location of the knot at a mesh point. The adjoint formulation that we have employed provides a cleaner construction and saves some numerical effort in the automated procedure of Section 5.

4. Low-Order Schemes

We now use the observations of the previous sections to construct explicit $O(h^2)$ and $O(h^4)$ discretizations of (1.1). For the first scheme, we can use standard central differences combined with the leading order term in the local expansion of $g_i(x_i, y)$. Define the difference operator $L_h^{(1)}$ and approximate local Greens function $G_i^{(1)}$ by

$$L_h^{(1)}[U]_i \equiv \alpha_{i,-1}^{(1)} U_{i-1} + \alpha_{i,0}^{(1)} U_i + \alpha_{i,1}^{(1)} U_{i+1},$$

where

$$\alpha_{i,-1}^{(1)} \equiv \frac{-1}{h^2} - \frac{a_i}{2h}$$

$$\alpha_{i,0}^{(1)} \equiv \frac{2}{h^2} + b_i$$

$$\alpha_{i,1}^{(1)} \equiv \frac{-1}{h^2} + \frac{a_i}{2h},$$

and

$$G_i^{(1)}(x_i, y) \equiv \tfrac{1}{2}(h - |y - x_i|).$$

Here $a_i \equiv a(x_i)$, $b_i \equiv b(x_i)$, and so on. Then an $O(h^2)$ discretization of (1.1) is given by

$$\begin{aligned} L_h^{(1)}[U] &= 0, && y \notin (x_{i-1}, x_{i+1}), \\ &= \alpha_{i,0}^{(1)} G_i^{(1)}(x_i, y), && y \in (x_{i-1}, x_{i+1}),\ i = 1, \ldots, n-1, \\ U_0 = U_n &= 0. \end{aligned} \tag{4.1}$$

To construct an $O(h^4)$ approximation to our problem, we first require the finite difference coefficients of an $O(h^4)$ scheme for $Lu=f$ with smooth f. Such a scheme, for uniform mesh spacing, is given by the following, which is due to Chawla [1]:

$$\begin{aligned} L_h^{(2)}[U]_i &\equiv \alpha_{i,-1}^{(2)} U_{i-1} + \alpha_{i,0}^{(2)} U_i + \alpha_{i,1}^{(2)} U_{i+1} \\ &= \beta_{i,-1}^{(2)} f(x_{i-1}) + \beta_{i,0}^{(2)} f(x_i) + \beta_{i,1}^{(2)} f(x_{i+1}) \equiv I_h^{(2)}[f]_i, \end{aligned}$$

where

$$\begin{aligned} \beta_{i,-1}^{(2)} &\equiv \frac{1}{12}\left(1 + \frac{h}{2} a_i\right) \\ \beta_{i,0}^{(2)} &\equiv \frac{10}{12} \\ \beta_{i,1}^{(2)} &\equiv \frac{1}{12}\left(1 - \frac{h}{2} a_i\right) \end{aligned}$$

and

$$\begin{aligned} \alpha_{i,-1}^{(2)} &\equiv \frac{-1}{h^2} + \frac{1}{2h}\left(-3\beta_{i,-1}^{(2)} a_{i-1} - \beta_{i,0}^{(2)} a_i + \beta_{i,1}^{(2)} a_{i+1}\right) + \beta_{i,-1}^{(2)} b_{i-1} \\ \alpha_{i,0}^{(2)} &\equiv \frac{2}{h^2} + \frac{2}{h}\left(\beta_{i,-1}^{(2)} a_{i-1} - \beta_{i,1}^{(2)} a_{i+1}\right) + \beta_{i,0}^{(2)} b_i \\ \alpha_{i,1}^{(2)} &\equiv \frac{-1}{h^2} + \frac{1}{2h}\left(-\beta_{i,-1}^{(2)} a_{i-1} + \beta_{i,0}^{(2)} a_i + 3\beta_{i,1}^{(2)} a_{i+1}\right) + \beta_{i,1}^{(2)} b_{i+1}. \end{aligned}$$

This scheme was derived by seeking a discretization in the assumed form above and then choosing $\alpha_{i,-1}^{(2)}, \ldots, \beta_{i,1}^{(2)}$ to make it locally exact on the collection of polynomials of degree 4 subject to the normalization $\beta_{i,-1}^{(2)} + \beta_{i,0}^{(2)} + \beta_{i,1}^{(2)} = 1$.

We also require a compatibly high-order approximation to the local Green's function; the first 3 terms in our local expansion of the previous section must be used. Thus define

$$\begin{aligned} G_i^{(2)}(x, y) \equiv{}& \tfrac{1}{2}(h - |y - x_i|) + \tfrac{1}{4} a_i(|y - x_i| - h)(y - x_i) \\ &+ \tfrac{1}{24} h(a_i^2 - 2a_i' + 4b_i)((y - x_i)^2 - h^2) \\ &+ \tfrac{1}{12}(-a_i^2 + 2a_i' - b_i)(y - x_i)^2(|y - x_i| - h). \end{aligned}$$

Then an $O(h^4)$ discretization of (1.1) is given by

$$\begin{aligned} L_h^{(2)}[U]_i &= 0, && y \notin (x_{i-1}, x_{i+1}), \\ &= \alpha_{i,0}^{(2)} G_i^{(2)}(x_i, y), && y \in (x_{i-1}, x_{i+1}),\ i = 1, \ldots, n-1, \qquad (4.2) \\ U_0 = U_n &= 0. \end{aligned}$$

These schemes get very complicated very quickly, and the automated approach of the next section is preferred. Also, the discretization error analysis of Section 6 only guarantees that the schemes above are $O(h)$ and $O(h^3)$, respectively. The stated convergence, $O(h^2)$ and $O(h^4)$, is indeed observed, however, as the numerical data below illustrates. The extra order of convergence can be attributed to the oddness of the first omitted term of the local expansion for $g_i(x_i, y)$ in each case and the positivity of the inverses of $L_h^{(1)}$ and $L_h^{(2)}$.

Numerical experiments were performed using the discretizations (4.1) and (4.2). Below are reported results for the test problem

$$-u'' + \frac{2}{x+1}u' + \frac{4}{(x+1)^2}u = \delta(x-y), \qquad 0 < x, y < 1,$$
$$u(0) = u(1) = 0, \tag{4.3}$$

the solution of which is

$$u(x) = \frac{-1}{155}\left[(x+1)^4 - \frac{1}{(x+1)}\right]\left[(y+1)^2 - \frac{32}{(y+1)^3}\right], \qquad 0 < x < y,$$
$$= \frac{-1}{155}\left[(y+1)^2 - \frac{1}{(y+1)^3}\right]\left[(x+1)^4 - \frac{32}{(x+1)}\right], \qquad y < x < 1.$$

The computations were done on a CDC 6600 in single precision arithmetic —equivalent to about 14 decimal digit accuracy. Uniform mesh spacings of $h = \frac{1}{4}$, $\frac{1}{8}, \ldots, \frac{1}{1024}$ were used with the singular point y located at $y = 0.75$ (which is always a mesh point) for one test and $y = \frac{7}{9} = 0.777\ldots$ (which is never a mesh point) for another. The approximate rate of convergence, p, was computed from the formula $p = \log_2(\|e_h\|_\infty / \|e_{h/2}\|_\infty)$ (see Table I).

Notice that the stated convergence rates are more clearly observed in the case where the singular point y is a mesh point. In the test where $y = 0.777\ldots$, the convergence is a bit more erratic. This is due to the fact that the relative position of the singular point in a mesh subinterval changes as the mesh is refined, altering slightly the asymptotic error constants in the local expansion. The high-order convergence is still detectable.

5. High-Order Schemes

Because of the complexity that these explicit discretizations rapidly acquire, we are led to consider simpler techniques for achieving higher order and accuracy. Methods such as deferred corrections or extrapolation suggest themselves. With an eye towards applications in higher dimensions, however, we analyze instead an automated procedure that computes higher order discretizations numerically (rather than evaluating them from explicit closed form expressions for the difference

TABLE I

Maximum Discretization Error and Approximate Rate of Convergence

	Scheme (4.1)				Scheme (4.2)			
	$y=0.75$		$y=0.777...$		$y=0.75$		$y=0.777...$	
h	$\|e_h\|_\infty$	p	$\|e_h\|_\infty$	p	$\|e_h\|_\infty$	p	$\|e_h\|_\infty$	p
1/4	0.66(−2)	2.0	0.87(−2)	1.6	0.29(−3)	4.0	0.44(−3)	3.4
1/8	0.16(−2)	2.0	0.28(−2)	1.7	0.18(−4)	4.0	0.40(−4)	3.5
1/16	0.41(−3)	2.0	0.88(−3)	2.7	0.11(−5)	4.0	0.35(−5)	4.9
1/32	0.10(−3)	2.0	0.14(−3)	1.6	0.71(−7)	4.0	0.12(−6)	3.5
1/64	0.25(−4)	2.0	0.47(−4)	1.7	0.44(−8)	4.0	0.11(−7)	3.6
1/128	0.64(−5)	2.0	0.15(−4)	2.6	0.28(−9)	4.0	0.92(−9)	4.9
1/256	0.16(−5)	2.0	0.23(−5)	1.6	0.17(−10)	4.0	0.30(−10)	3.5
1/512	0.40(−6)	2.0	0.75(−6)	1.7	0.10(−11)	*	0.27(−11)	*
1/1024	0.99(−7)	2.0	0.23(−6)		*		*	

Note. For discretizations (4.1) and (4.2) applied to test problem (4.3) with singular points $y=0.75$ and $y=0.777...$.

coefficients). With this approach it is possible to compute a discrete approximation to the solution of (1.1) of any prescribed order of accuracy.

A general approach to constructing high-order difference approximations to differential equations is analyzed by Lynch and Rice, who refer to the technique as the HODIE method (high order differences via identity expansion) in [8] and by Doedel in [2]. To discretize a regular problem like

$$L[u](x)=f(x)$$

involving a second-order, linear, differential operator L, one seeks (on the ith subinterval) a scheme of the form

$$\begin{aligned} L_h[U]_i &\equiv \alpha_{i,-1} U_{i-1} + \alpha_{i,0} U_i + \alpha_{i,1} U_{i+1} \\ &= \sum_{j=1}^{J} \beta_{i,j} f(\xi_{i,j}) \equiv I_h[f]_i. \end{aligned}$$

Here $\xi_{i,1},..., \xi_{i,J}$ are distinct auxiliary (HODIE) points, some of which may coincide with mesh points, and $\beta_{i,1},..., \beta_{i,J}$ satisfy the normalization

$$\beta_{i,1}+\cdots+\beta_{i,J}=1.$$

The difference coefficients and weights are determined so that the scheme is exact on some suitable collection of local approximating functions (usually polynomials) in the sense that the *truncation error*, given by

$$T_h[\phi]_i \equiv L_h[\phi]_i - I_h[L[\phi]]_i,$$

is zero for all functions ϕ in the specified class.

It is a consequence of the results in [2 and 8], that if one uses J auxiliary evaluation points, then one can construct a scheme exact on polynomials of degree at most $J+1$ and achieve a local truncation error of at least $O(h^J)$. Thus it is possible, given any positive p, to construct the coefficients of a finite-difference scheme (L_h, I_h) that is consistent with the differential operator L of order $O(h^p)$. To complete our discretization of (1.1), we require for those subintervals that contain the singular point y a high-order approximation to the local Green's function $g_i(x_i, y)$. This can be achieved by using this same general approach on a slightly modified local problem (obtained by subtracting the known leading order part of the Green's function). Here it is easier to view this as a local *collocation* procedure, as this whole approach to finite differences can be viewed (cf. [3]).

Let (x_{i-1}, x_{i+1}) be a singular subinterval, so that $y \in (x_{i-1}, x_{i+1})$. Let g denote the local Green's function $g_i(x_i, \cdot)$ regarded as a function of its second variable, so that $g(x) \equiv g_i(x_i, x)$ for all $x \in (x_{i-1}, x_{i+1})$. Then g satisfies

$$\begin{gathered} L^\dagger[g](x) = \delta(x - x_i), \qquad x_{i-1} < x < x_{i+1}, \\ g(x_{i-1}) = g(x_{i+1}) = 0. \end{gathered}$$

Now we know from Section 3 that g admits an expansion of the form

$$g(x) = hg_1(x) + h^2 g_2(x) + \cdots,$$

where $g_1(x) = (h - |x - x_i|)/2h$ and $g_2, g_3, \ldots$ are higher and higher order piecewise polynomials with knots at $x = x_i$.

Define the difference $v \equiv g - hg_1$. Then v satisfies a regular problem of the form

$$\begin{gathered} L^\dagger[v](x) = -hL^\dagger[g_1](x), \qquad x_{i-1} < x < x_i, \quad x_i < x < x_{i+1}, \\ v(x_{i-1}) = v(x_{i+1}) = 0. \end{gathered}$$

Here the right-hand side is a piecewise continuous function with a single (jump) discontinuity at $x = x_i$. Define the local approximating functions p_k and q_k by

$$\begin{aligned} p_k(x) &= \left(\frac{x - x_i}{h}\right)^k, \qquad && x_{i-1} \leqslant x \leqslant x_i, \\ &= 0, && x_i \leqslant x \leqslant x_{i+1}, \end{aligned}$$

and

$$q_k(x) = 0, \qquad x_{i-1} \leqslant x \leqslant x_i,$$
$$= \left(\frac{x - x_i}{h}\right)^k, \qquad x_i \leqslant x \leqslant x_{i+1}.$$

We then seek an approximation to v of the form

$$v_m(x) = c_{-1} \cdot \frac{h - (x - x_i)}{2h} + c_1 \cdot \frac{(x - x_i) + h}{2h} + c_2 p_2(x) + \cdots + c_m p_m(x)$$
$$+ d_2 q_2(x) + \cdots + d_m q_m(x)$$

determined by the collocation conditions

$$\begin{aligned} L^\dagger[v_m](\xi_j) &= -\tfrac{1}{2} L^\dagger[h - |x - x_i|](\xi_j), \qquad j = 1,..., 2m-2 \\ v_m(x_{i-1}) &= v_m(x_{i+1}) = 0. \end{aligned} \tag{5.1}$$

We then accept $hg_1(y) + v_m(y)$ as our approximation to the desired value $g_i(x_i, y)$. If the collocation points $\xi_1,..., \xi_{2m-2}$ satisfy a certain distribution requirement, and if h is sufficiently small, then the system (5.1) uniquely determines v_m and we obtain an $O(h^{m+1})$ approximation to the local Green's function $g_i(x_i, \cdot)$ uniformly on $[x_{i-1}, x_{i+1}]$. We have the following.

THEOREM 5.1. *Let the collocation points $\xi_1,..., \xi_{2m-2}$ in (5.1) be given by $\xi_j = x_i + h\bar{\xi}_j$, $j = 1,..., 2m-2$, where $\bar{\xi}_1,..., \bar{\xi}_{2m-2}$ are independent of h and satisfy*

$$-1 \leqslant \bar{\xi}_1 < \cdots < \bar{\xi}_{m-1} < 0 < \bar{\xi}_m < \cdots < \bar{\xi}_{2m-2} \leqslant 1.$$

Let $X^0_{m,h}$ denote the subspace of $C^1[x_{i-1}, x_{i+1}]$ that consists of piecewise polynomials of degree at most m with single knot at x_i and vanishing at x_{i-1} and x_{i+1}. Then for all h sufficiently small, the local collocation system (5.1) possesses a unique solution and defines a projection, P_m, onto $X^0_{m,h}$ that satisfies

$$\|P_m[v]\|_\infty \leqslant Ch^2 \, \|L^\dagger[v]\|_\infty$$

for all sufficiently smooth v vanishing at x_{i-1} and x_{i+1}.

Proof. If we order and scale the equations of (5.1) according to

$$v_m(x_{i-1}) = 0$$
$$v_m(x_{i+1}) = 0$$
$$h^2 L^\dagger[v_m](\xi_j) = h^2 L^\dagger[-\tfrac{1}{2}(h - |x - x_i|)](\xi_j) \equiv h^2 F(\xi_j), \qquad j = 1,..., 2m-2,$$

then we get a $2m$ by $2m$ system of the form $A_m \mathbf{c} = \mathbf{d}$, where

$$\mathbf{c} \equiv (c_{-1}, c_1 \mid c_2, \ldots, c_m \mid d_2, \ldots, d_m)^{\mathrm{T}},$$

$$\mathbf{d} \equiv (0, 0 \mid h^2 F(\xi_1), \ldots, h^2 F(\xi_{m-1}) \mid h^2 F(\xi_m), \ldots, h^2 F(\xi_{2m-2}))^{\mathrm{T}},$$

and

$$A_m = \left[\begin{array}{c|c|c} I_2 & O(1) & O(1) \\ \hline O(h) & B_{m,1} + O(h) & 0 \\ \hline O(h) & 0 & B_{m,2} + O(h) \end{array}\right]$$

where I_2 is the 2×2 identity and $B_{m,1}$ and $B_{m,2}$ are $(m-1)$ by $(m-1)$ matrices with rows

$$[-2, -3 \cdot 2 \cdot \xi_j, -4 \cdot 3 \cdot \xi_j^2, \ldots, -m(m-1)\, \xi_j^{m-2}]$$

$j = 1, \ldots, m-1$, and $j = m, \ldots, 2m-2$, respectively. These last 2 matrices are nonsingular because they are column equivalent to transposes of Vandermonde matrices. It follows that A_m is nonsingular for all h sufficiently small and that there exists a constant K independent of h such that

$$\|A_m^{-1}\|_\infty \leqslant K \qquad \text{as} \quad h \to 0.$$

We can bound the projection operator P_m pointwise as follows. For sufficiently smooth v we have

$$\begin{aligned} \|P_m[v]\|_\infty &= \max_{x_{i-1} \leqslant x \leqslant x_{i+1}} \left| c_{-1} \cdot \frac{h - (x - x_i)}{2h} + \cdots + d_m q_m(x) \right| \\ &\leqslant \|\mathbf{c}\|_\infty \left\{ \left\| \frac{h - (x - x_i)}{2h} \right\|_\infty + \cdots + \|q_m\|_\infty \right\} \\ &\leqslant 2m\, \|A_m^{-1} \mathbf{d}\|_\infty \\ &\leqslant 2mKh^2\, \|L^\dagger[v]\|_\infty. \quad \blacksquare \end{aligned}$$

We define our approximate local Green's function then as

$$G_{m,i}(x_i, y) \equiv \tfrac{1}{2}(h - |y - x_i|) + v_m(y).$$

THEOREM 5.2. *Let m be an integer greater than* 1, *and let the approximate local Green's function $G_{m,i}$ be defined as above, where v_m is computed by the local collocation scheme* (5.1). *Let g_i denote the true local Green's function as defined in*

(2.3). *Then for sufficiently smooth coefficient functions a and b and for all h sufficiently small, we have*

$$\|g_i(x_i, \cdot) - G_{m,i}(x_i, \cdot)\|_\infty \leqslant Ch^{m+1},$$

where C is a constant that does not depend on h.

Proof. Recall from Theorem 3.1 that for a and b sufficiently smooth, $g_i(x_i, \cdot)$ admits the local expansion (in unstretched coordinates)

$$g_i(x_i, x) = hg_1(x) + \cdots + h^m g_m(x) + r_m(x; h),$$

where $g_2,..., g_m$ are C^1 piecewise polynomials with knots at x_i and r_m satisfies (for h sufficiently small)

$$\|r_m\|_\infty + h^2 \|L^\dagger[r_m]\|_\infty \leqslant Ch^{m+1}.$$

We get that

$$\begin{aligned}
\|g_i(x_i, \cdot) - G_{m,i}(x_i, \cdot)\|_\infty &= \|(I - P_m)\, v\|_\infty \\
&= \|(I - P_m)\, r_m\|_\infty \\
&\leqslant \|r_m\|_\infty + \|P_m[r_m]\|_\infty \\
&\leqslant Ch^{m+1} + (2mK)\, h^2 \|L^\dagger[r_m]\|_\infty \\
&\leqslant C'h^{m+1}. \quad \blacksquare
\end{aligned}$$

Notice that in the case $m = 1$, there is no collocation to do. We just accept as our approximate local Green's function the leading term

$$G_{1,i}(x_i, y) \equiv \tfrac{1}{2}(h - |y - x_i|).$$

This gives us an $O(h^2)$ approximation to $g_i(x_i, \cdot)$, and the conclusion of the theorem remains valid.

Given the coefficients $\alpha_{i,-1}$, $\alpha_{i,0}$, and $\alpha_{i,1}$, $i = 1,..., n-1$, of a finite-difference scheme that is consistent with L, and given a choice for m and the approximate local Green's function computed as above, we define our discretization of (1.1) by

$$\begin{aligned}
\alpha_{i,-1} U_{i-1} + \alpha_{i,0} U_i + \alpha_{i,1} U_{i+1} &= 0, && y \notin (x_{i-1}, x_{i+1}), \\
&= \alpha_{i,0} G_{m,i}(x_i, y), && y \in (x_{i-1}, x_{i+1}).
\end{aligned} \tag{5.2}$$

Below are reported the results of numerical experiments run on the test problem (4.3) exhibiting convergence rates of 5 and 6. The finite-difference coefficients were computed using the regular identity expansion approach discussed at the beginning of this section and analyzed in [2 and 8]. The approximate local Green's function was computed using the collocation procedure analyzed above with $m = 5$ and 6 (see Table II).

TABLE II

Maximum Discretization Error and Approximate Rate of Convergence

	$m=5$				$m=6$			
	$y=0.75$		$y=0.77...$		$y=0.75$		$y=0.77...$	
h	$\|e_h\|_\infty$	p	$\|e_h\|_\infty$	p	$\|e_h\|_\infty$	p	$\|e_h\|_\infty$	p
1/4	0.15(−2)	4.6	0.10(−3)	4.6	0.68(−3)	5.6	0.23(−4)	4.4
1/8	0.61(−4)	4.8	0.41(−5)	2.8	0.14(−4)	5.8	0.11(−5)	3.9
1/16	0.22(−5)	4.9	0.61(−6)	3.5	0.25(−6)	5.9	0.72(−7)	4.5
1/32	0.74(−7)	5.0	0.55(−7)	5.2	0.43(−8)	5.9	0.31(−8)	6.2
1/64	0.24(−8)	5.0	0.15(−8)	5.5	0.70(−10)	5.6	0.44(−10)	5.8
1/128	0.77(−10)	4.1	0.33(−10)	4.0	0.15(−11)		0.78(−12)	
1/256	0.44(−11)		0.20(−11)		*		*	

Note. For discretization (5.2) with $m=5$ and 6 applied to test problem (4.3) with singular points $y=0.75$ and $y=0.777...$.

Notice that the observed discretization error in each case is one order higher than we would initially expect: $\|g_i(x_i, \cdot)-G_{m,i}(x_i, \cdot)\|_\infty = O(h^{m+1})$ and $\alpha_{i,0}=O(h^{-2})$ imply a contribution to the local truncation error of $O(h^{m-1})$, not $O(h^m)$. This higher order is due to the fact that the lower truncation error is contributed at a finite (2 at most) number of points. Convergence of the scheme at the observed rate is rigorously established in the next section.

6. Discretization Error

We can handle the reduced order of the truncation error at a finite number of points if we use a stability result involving a mesh 1-norm, instead of the usual ∞-norm. Thus, let us define the norm $\|\cdot\|_{h,1}$ for mesh functions on our uniform mesh by

$$\|\phi\|_{h,1} \equiv h \sum_{i=1}^{n-1} |\phi(x_i)|.$$

If (L_h, I_h) is a compact finite-difference scheme of the form (2.4) that is consistent with L, then it is a consequence of results in Esser [5, Theorems 3.2 and 3.4] that for all h sufficiently small and for all mesh functions ϕ, we have

$$\|\phi\|_\infty \leqslant C\{\|L_h[\phi]\|_{h,1} + |\phi(0)| + |\phi(1)|\}, \tag{6.1}$$

where C is a constant that does not depend on h. Actually, the notion of consistency used in [5] is the usual one (involving $\|L_h[\phi]-L[\phi]\|_\infty$, but this is implied by the notion used here (which involves $\|L_h[\phi]-I_h[L[\phi]]\|_\infty$), since

$I_h[L[\phi]] = L[\phi] + O(h)$. With the above stability estimate, we can now prove the following.

THEOREM 6.1. *Let m be a given positive integer. Let (L_h, I_h) be a compact finite-difference approximation of the form* (2.4) *that is consistent of order m with the differential operator L of* (1.1). *Let the approximate local Green's functions $G_{m,i}(x_i, \cdot)$ be computed from the local collocation procedure* (5.1). *Then for sufficiently smooth coefficient function a and b and for all mesh spacings h sufficiently small, there is a constant C independent of h such that the discretization error $e_i \equiv u(x_i) - U_i$, $i = 0,\ldots, n$, satisfies*

$$\|e\|_\infty \leqslant Ch^m.$$

Proof. If (x_{i-1}, x_{i+1}) is not a singular subinterval (i.e., if $y \notin (x_{i-1}, x_{i+1})$), then the truncation error τ_i is given by

$$\begin{aligned}\tau_i \equiv L_h[e]_i &= L_h[u]_i - L_h[U]_i\\ &= L_h[u]_i - I_h[L[u]]_i,\end{aligned}$$

and this is $O(h^m)$, uniformly in i, by the assumed order of consistency of the finite-difference scheme. If (x_{i-1}, x_{i+1}) is a singular subinterval, then

$$\begin{aligned}\tau_i &\equiv L_h[e]_i = L_h[u]_i - L_h[U]_i\\ &= \alpha_{i,-1} u(x_{i-1}) + \alpha_{i,0} u(x_i) + \alpha_{i,1} u(x_{i+1}) - \alpha_{i,0} G_{m,i}(x_i, y)\\ &= \alpha_{i,0} \left\{ \left(\frac{\alpha_{i,-1}}{\alpha_{i,0}} - \alpha^*_{i,-1} \right) u_{i-1} + \left(\frac{\alpha_{i,1}}{\alpha_{i,0}} - \alpha^*_{i,1} \right) u_{i+1} \right.\\ &\qquad \left. + g_i(x_i, y) - G_{m,i}(x_i, y) \right\},\end{aligned}$$

where $\alpha^*_{i,-1}$ and $\alpha^*_{i,1}$ are the optimal difference coefficients of (2.3). In this case, we have

$$\begin{aligned}|\tau_i| \leqslant |\alpha_{i,0}| &\left\{ \left| \frac{\alpha_{i,-1}}{\alpha_{i,0}} - \alpha^*_{i,-1} \right| \|u\|_\infty \right.\\ &\left. + \left| \frac{\alpha_{i,1}}{\alpha_{i,0}} - \alpha^*_{i,1} \right| \|u\|_\infty + \|g_i(x_i, \cdot) - G_{m,1}(x_i, \cdot)\|_\infty \right\}.\end{aligned}$$

And it follows from Proposition 2.1 and Theorem 5.2, that τ_i is $O(h^{m-1})$. We therefore have that the discretization error e_i satisfies

$$\begin{aligned}|L_h[e]_i| = |\tau_i| &\leqslant Ch^m, &&y \notin (x_{i-1}, x_{i+1})\\ &\leqslant Ch^{m-1}, &&y \in (x_{i-1}, x_{i+1})\\ e_0 = e_n &= 0.\end{aligned}$$

And we obtain from the stability estimate (6.1) that for h sufficiently small

$$\|e\|_\infty \leqslant Ch^m$$

for some constant C independent of h. ∎

The observed convergence rates are thus proved. In certain special cases, a higher order (usually only 1 order higher) can sometimes be observed due to symmetries or error cancellation effects, as was observed at the end of Section 4.

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