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Defect Correction on Non-Uniform Meshes

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Meshes

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Introduction. For uniform discretization meshes theory and applications of defect corrections or iterative improvements for discretization algorithms for ordinary and partial differential equations can be found in Lindberg [1980]. The related technique of iterated deferred correction is described and analyzed for non-uniform meshes in Lentini, Pereyra (1974). A computer code for boundary value problems for systems of ODE's written in the form

$$y' = f(t, y) \qquad t \in (a, b)$$

$$g(y(a), y(b) = 0$$

is described in Lentini, Pereyra (1977).

In this report we will introduce a new idea, the aim of which is to develop the theory for defect correction algorithms for non-uniform, but smoothly varying, meshes and to facilitate efficient computer implementation of defect correction for a wide variety of methods. To present and illustrate the new idea we will study the class of scalar second order two-point boundary value problems

$$F(x, y, y', y'') = 0$$

$$y(a) = \alpha \qquad y(b) = \beta.$$

The same idea can, and will in later reports, be applied to two-point boundary value problems for systems of ordinary differential equations and to partial differential equations such as e.g. the Poisson equation on a rectangular region.

The problem of finding a good non-uniform mesh for a given problem is not studied in this report, but the present work can be viewed as a pre-requisite for such a study which will be reported elsewhere. Some techniques for mesh selection can be found in Russell (1979).

Problem Statement

Consider the two-point boundary value problem

(1) $$F(x, y, y', y'') = 0$$
$$y(a) = \alpha; \qquad y(b) = \beta$$

where $'$ stands for $\frac{d}{dx}$.

Consider a coordinate transformation

$$x = \rho(s) \quad \text{with} \quad \rho(0) = a; \quad \rho(1) = b.$$

If $\rho(s)$ is monotonically increasing the function ρ is a one-to-one function with $\frac{d\rho}{ds} > 0$.

In the new variable s the problem (1) transforms to

(2) $$F(\rho(s), Y, \frac{Y_s}{\rho_s}, \frac{Y_{ss}}{\rho_s^2} - \frac{Y_s \rho_{ss}}{\rho_s^3}) = 0$$
$$Y(0) = \alpha; \quad Y(1) = \beta$$

where $Y(s) = y(\rho(s))$ and index s denotes sifferentiation with respect to s.

The equation (2) follows from

$$\frac{dY}{ds} = \frac{dy}{dx} \cdot \frac{d\rho}{ds}$$

$$\frac{d^2Y}{ds^2} = \frac{d}{ds}\left[\frac{dy}{dx} \cdot \frac{d\rho}{dz}\right] = \frac{d^2y}{dx^2}\left(\frac{d\rho}{ds}\right)^2 + \frac{dy}{dx}\frac{d^2\rho}{dx^2}$$

so

$$y_x = \frac{Y_s}{\rho_s}\ ; \quad y_{xx} = \frac{Y_{ss} - \frac{Y_s\,\rho_{ss}}{\rho_s}}{\rho_s^2}$$

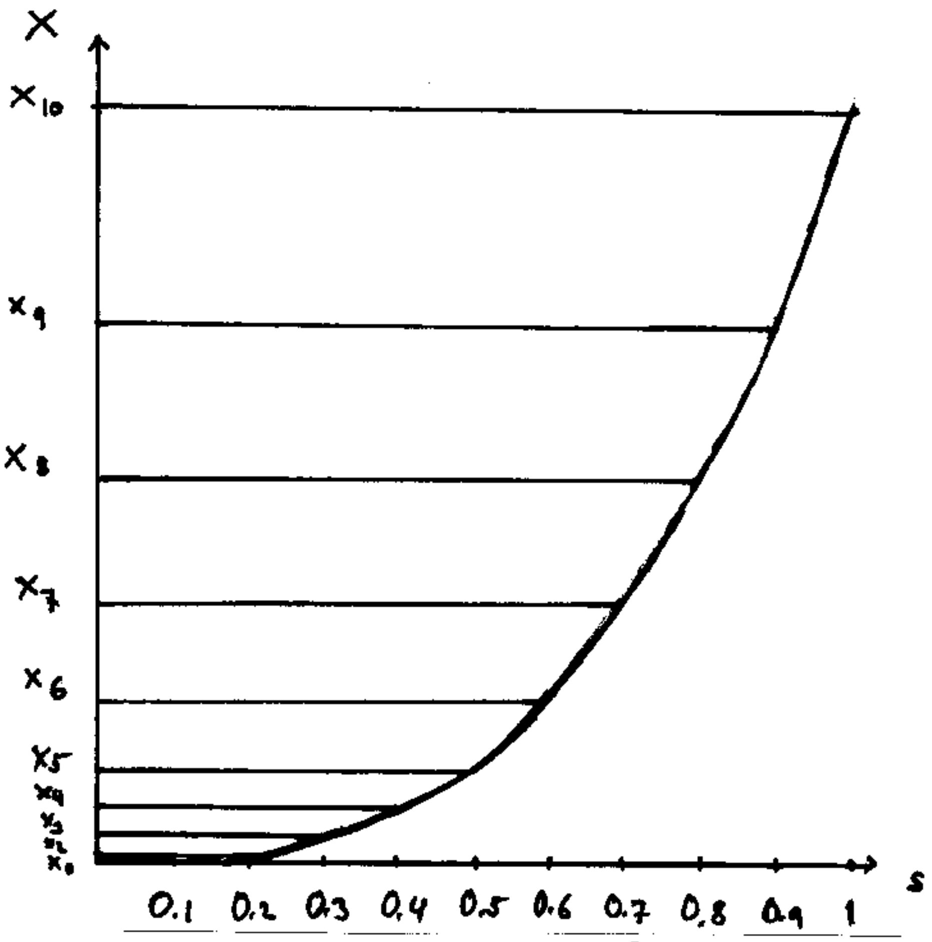
Assume that the function $\rho(s)$ is not explicitly known, but that it is a smooth function for which we can compute values $\rho(s_i)$ for any s_i, then ρ_s and ρ_{ss} at gridpoints s_i may be approximated by finite differences. For these approximations to be good we assume that the function $\rho(s)$ is sufficiently many times differentiable. In this report, we will assume that ρ is a given sufficiently smooth function. In a later report we will address the problem of finding such functions ρ for a given problem.

The coordinate transformation function $\rho(s)$ may be interpreted as a stepsize selection function, viz.,

$$\Delta x_i = x_{i+1} - x_i = \rho(s_{i+1}) - \rho(s_i)$$

See the figure below for a graphical illustration of this interpretation.

A uniform mesh $\{s_i\}_{i=1}^N$, $s_i = i \cdot h$ in the variable s is transformed into a smoothly varying, but non-uniform, mesh $\{x_i\}_{i=0}^N$, $x_i = a + (i \cdot h)^3$ $i = 0, 1, \ldots, N$.



$X = \rho(s)$ where $\rho(s) = a + s^3$

The basic discretization

Discretize according to

$$s_i = i \cdot h, \quad i = 0, 1, \ldots, N; \quad h = 1/N$$

$$Y_i \approx Y(s_i), \quad X_i = \rho(s_i)$$

i.e., choose a uniform mesh in the variable s.

Using second order central difference approximations we get from (2)

$$y_0 = \alpha \qquad y_N = \beta$$

$$F\left(X_i,\ Y_i,\ \frac{\frac{Y_{i+1} - Y_{i-1}}{2h}}{\frac{X_{i+1} - X_{i-1}}{2h}},\ \frac{\frac{Y_{i+1} - 2Y_i + Y_{i-1}}{h^2}}{\left(\frac{X_{i+1} - X_{i-1}}{2h}\right)^2} - \frac{\frac{Y_{i+1} - Y_{i-1}}{2h} \cdot \frac{X_{i+1} - 2X_i + X_{i-1}}{h^2}}{\left(\frac{X_{i+1} - X_{i-1}}{2h}\right)^3}\right) = 0$$

$i=1,2,\ldots, N-1$

Cancelling common factors we get

$$y_0 = \alpha$$

$$(3) \quad F\left(X_i, \frac{Y_{i+1} - Y_{i-1}}{X_{i+1} - X_{i-1}}, 4\frac{Y_{i+1} - 2Y_i + Y_{i-1}}{(X_{i+1} - X_{i-1})^2} - 4\frac{(Y_{i+1} - Y_{i-1})(X_{i+1} - 2X_i + X_{i-1})}{(X_{i+1} - X_{i-1})^3}\right) = 0$$

$$i = 1, 2, \ldots, N-1$$

$$y_N = \beta.$$

Note that in (3) no reference is made to the function $\rho(s)$. Actually we may consider (3) as a finite difference approximation on a non-uniform mesh in the variable X of (1). For our purposes, however, (3) is considered to be a discretization of (2) on a uniform mesh in the variable s.

Define the local discretization error ℓ_i as the residual in (3) when values of the exact solution $Y(s)$ and the coordinate function $\rho(s)$ are substituted for Y_k and X_k respectively. If $Y(s)$ and $\rho(s)$ are sufficiently smooth we get by Taylor expansions

$$\ell_i = c_1(s_i)\, h^2 + c_2(x_i)\, h^4 + \ldots$$

i.e., the method is of second order and has an expansion in even powers of the discretization parameter h.

Defect correction

The basic theorems of Lindberg [1980] do not apply directly to the discretization (3), but they can be modified to allow the discretization of a given function $\rho(s)$.

With this in mind we define the defect operators below. In the notation of Lindberg [1980] the basic discretization operator is

$$\phi(\eta) = \begin{cases} \eta_0 - \alpha \\ F\left(X_i, \eta_i, \dfrac{\eta_{i+1}-\eta_{i-1}}{X_{i+1}-X_{i-1}}, 4\dfrac{\eta_{i+1}-2\eta_i+\eta_{i-1}}{(X_{i+1}-X_{i-1})^2} - 4\dfrac{(\eta_{i+1}-\eta_{i-1})(X_{i+1}-2X_i+X_{i-1})}{(X_{i+1}-X_{i-1})^3}\right) \\ \qquad i = 1, 2, \ldots, N-1 \\ \eta_N - \beta \end{cases}$$

Define a family of defect operators $k = 2, 3, \ldots$

$$\phi_k(\eta) = \begin{cases} \eta_0 - \alpha \\ r_i^{[k]}(\eta) \qquad i = 1, 2, \ldots, N-1 \\ \eta_N - \beta \end{cases}$$

with

$$r^{[k]}(\eta) = F\left(X_i, \eta_i, \frac{A^k[\eta_i]}{A^k[X_i]}, \frac{B^k[\eta_i]}{(A^k[X_i])^2} - \frac{A^k[\eta_i]B^k[X_i]}{(A^k[X_i])^3}\right)$$

where (cf Lindberg [1980]), for equidistant X_n

$$A^k[y(X_n)] = \Big(\sum_{\nu=-k}^{k} \alpha_\nu\, y(X_{n+\nu})\Big)/h \approx y'(X_n)$$

$$B^k[y(X_n)] = \Big(\sum_{\nu=-k}^{k} \beta_\nu\, y(X_{n+\nu})\Big)/h^2 \approx y''(X_n)$$

and the coefficients α_ν, β_ν are chosen such that

$$y'(X_n) - A^k[y(X_n)] = \mathcal{O}(h^{2k})$$

$$y''(X_n) - B^k[y(X_n)] = \mathcal{O}(h^{2k})$$

The coefficients of course depend on k.

Note that these approximation formulas use values of y and x that are outside the interval $[a, b]$. Hence to use them we must extend the solution to the left of $x = a$ and to the right of $x = b$. To do this we use the basic discretization formula but use it in a step-by-step fashion, e.g., to find y_{N+1} we use y_{N-1}, y_N and solve for y_{N+1} from (3). The basic solution is extended as far as we need it for the subsequent calculations. To compute increasingly accurate approximations:

1. Solve for η^1 from $\phi(\eta^1) = 0$

2. Solve for η^k, $k = 2, 3, \ldots$ from
$$\phi(\eta^k) - \phi(\eta^{k-1}) + \phi_k(\eta^{k-1}) = 0.$$

Introducing the notation

$$\Delta_n y = (y(x_0),\ y(x_1),\ \ldots,\ y(x_N))^T$$

we have, cf. Lindberg [1980],

$$\eta^k - \Delta_n y = (h^{2k}) \qquad k = 1, 2, \ldots .$$

Compact defect formulas

Once the basic problem $\phi(\eta) = 0$ has been solved we can find values of $Y(s)$, $Y'(s)$, $Y''(s)$ or approximations to these quantities from the numerical solution η.

$$Y(s_i) \approx \eta_i$$

$$z(s_i) = Y'(s_i) \approx \frac{\eta_{i+1} - \eta_{i-1}}{2h}$$

$$w(s_i) = Y''(s_i) \simeq \frac{\eta_{i+1} - \eta_i + \eta_{i-1}}{h^2} .$$

To define the defect operator for our model problem we need high order approximations to $z(s_i)$, $w(s_i)$ and $\rho'(s_i)$, $\rho''(s_i)$. Rather than using the operators A^k and B^k of the previous section we may derive such approximations in a different way. Cf Lindberg [1982] where compact formulas using $y'(x_i)$ and $y''(x_i)$ are derived. If $y'(x)$ and/or $y''(x)$ can be evaluated directly from the differential equation, e.g. $y'' = f(x, y)$, then these formulas are not equivalent to the formulas for A^k, B^k. If, however, $y'(x_i)$ and $y''(x_i)$ are evaluated numerically the formulas we obtain are essentially the same as the formulas for A^k and B^k.

Define the linear functionals

$$L_1(y) = \Big[\delta^2 y(x_n) - h^2 y''(x_n) + \sum_{k=2} a_k \delta^{2k} y(x_n) + h \sum_{k=2} b_k \mu\delta^{2k-1} y'(x_n) - h^2 \sum_{k=1} c_k \delta^{2k} y''(x_n)\Big] / h^2$$

$$L_2(y) = \Big[\mu\delta y(x_n) - hy'(x_n) + \sum_{k=2} A_k \mu\delta^{2k-1} y(x_n) - h \sum_{k=1} B_k \delta^{2k} y'(x_n) - h^2 \sum_{k=1} C_k \mu\delta^{2k-1} y''(x_n)\Big] / h$$

where δ and μ are difference operators, see Dahlquist, Bjorch (1976).

$$\delta z_{n+1/2} = z_{n+1} - z_n;\ \delta^2 z_n = z_{n+1} - 2z_n + z_{n-1}$$

$$z_{n+1/2} = (z_{n+1} + z_n)/2;\ \mu\delta z_n = (z_{n+1} - z_{n-1}) / 2 .$$

We can determine the coefficients and the upper limits in the sums such that for given j

$$L_1(y) = O(h^{2j}); \quad L_2(y) = O(h^{2j}) .$$

The coefficients will of course depend on k. Coefficients for formulas up to order 10 are given in table 1-2. In Lindberg (1982) coefficients for formulas up to order 16 are tabulated

a_2	b_2	c_1	c_2	order
		1/12		4
54/1080		12/90		6
465/3780		780/3780	23/3780	8
473/420	-79/105	16/35	-1/28	10

Table 1. Coefficients for $L_1(y)$

A_2	B_1	B_2	C_1	order
	1/6			4
1/30	1/5			6
25/210	60/210	3/210		8
-110/2100	480/2100	-1/2100	-240/2100	10

Table 2. Coefficients for $L_2(y)$

From the formula for L, we now solve for $y''(x_n)$ and define

$$A(y, z, w) = [\delta^2 y(x_n) + \sum_{k=2} a_k \delta^{2k} y(x_n)$$

$$+ h \sum_{k=2} b_k \mu \delta^{2k-1} z(x_n)$$

$$- h^2 \sum c_k \delta^{2k} w(x_n)] / h^2$$

Then

$$y''(x_n) - A(y, y', y'') = O(h^{2j})$$

Similarly we get

$$B(y, z, w) = [\mu\delta y(x_n) + \sum_{k=2} A_k \mu\delta^{2k-1} y(x_n)$$

$$- h \sum_{k=1} B_k \delta^{2k} z(x_n) - h^2 \sum_{k=1} C_k \mu\delta^{2k-1} w(x_n)]/h$$

with

$$y'(x_n) - B(y, y', y'') = O(h^{2j})$$

These formulas can now be used to define the defect operator.

Numerical examples

The examples below are studied mainly to convince ourselves that the technique described is feasible and to illustrate how it works on some simple problems. The examples are not intended to demonstrate that the technique is superior to other techniques, nor are they intended as general purpose techniques for the class of problems that we have addressed. In a later paper we will return to the question of how to automatically construct a good coordinate transformation or stepsize selection function $\rho(s)$.

In the two examples below we only make one defect correction using the 4-th order compact defect operators described earlier. To illustrate the order of accuracy of the basic solution and the corrected solution we record the global error at some representative x-values for different stepsizes. For both examples the exact solution is known.

Example 1

$$- y'' + y = 1 \quad Y(0) = 1; \quad y(1) = 2$$

with exact solution

$$y(x) = \frac{e^{x} - e^{-x}}{e^{1} - e^{-1}} + 1$$

This is a trivial example with a very smooth solution that could be solved on a uniform mesh. To illustrate we choose

$$\rho(s) = s^3$$

so the non-uniform mesh for x concentrates most of the meshpoints close to $x = 0$.

At $x = 0.125$ the following errors occur

Stepsize	e_h	e_{2h}/e_h	E_h	E_{2h}/E_h
0.1	$-3.9.10^{-4}$		-4.10^{-5}	
0.005	$-9.9.10^{-5}$	3.9	$-2.2.10^{-6}$	18.2
0.025	$-2.5.10^{-5}$	4.0	$-1.3.10^{-7}$	16.9

e_h = the error in the basic solution (should be $O(h^2)$)

E_h = the error in the improved solution (should be $O(h^4)$)

The theoretical limit values $(h \to 0)$ for $e_{2h}/e_h = 4$ and $E_{2h}/E_h = 16$.

Example 2

$$\varepsilon y'' - y' = 0; \quad y(0) = 1; \quad y(1) = 2$$

with exact solution

$$y(x) = 1 - \frac{\exp(-1/\varepsilon)}{1 - \exp(-1/\varepsilon)} \; (1 - \exp(t/\varepsilon))$$

Near $x = 1$ the solution rises from $y = 1$ to $y = 2$ in a region of width $O(\varepsilon)$. A good mesh for this problem must concentrate most of the gridpoints close to $x = 1$. The coordinate function

$$\rho(s) = \frac{1 - \exp(-s/\sqrt{\varepsilon})}{1 - \exp(-1/\sqrt{\varepsilon})}$$

is used for this example. For $\varepsilon = 0.01$, $h = 0.1$ the figure below gives $\rho(s)$ and the non-uniform mesh in x generated by this function.

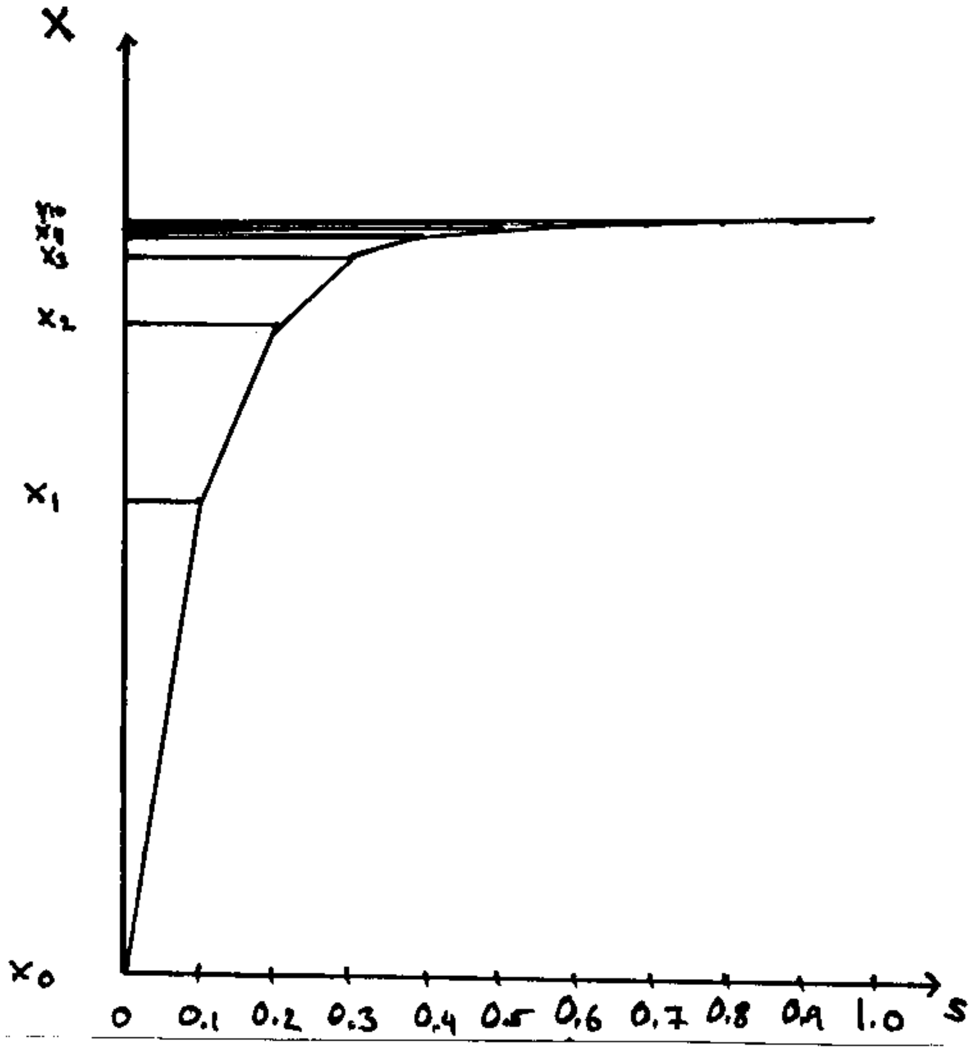
At $x = 0.993307$ we get the following errors for $\varepsilon = 0.01$ (the x-value corresponds to $s = 1/2$, i.e., half the gridpoints are at the right of this value)

Stepsize	e_h	e_{2h}/e_h	E_h	E_{2h}/E_h
0.05	$2.3 \cdot 10^{-2}$		$-4.4 \cdot 10^{-3}$	
0.025	$5.6 \cdot 10^{-3}$	4.1	$-2.5 \cdot 10^{-4}$	17.6
0.0125	$1.4 \cdot 10^{-3}$	4.0	$-1.5 \cdot 10^{-5}$	16.7

e_h = the error in the basic solution (should be $O(h^2)$)

E_h = the error in the improved solution (should be $O(h^4)$)

The theoretical limit values $(h \to 0)$ for $e_{2h}/e_h = 4$ and $E_{2h}/E_h = 16$.


X
x_{10}
x_4
x_3
x_2
x_1
x_0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
s

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