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**NUMERICAL INTEGRATION OF ASYMPTOTIC SOLUTIONS
OF ORDINARY DIFFERENTIAL EQUATIONS**

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INTRODUCTION

Asymptotic analysis was the predominant method for the approximate analysis of shell structures before the advent of the computer. The Geckeler approximation, ref. (1), for the solution of axisymmetric problems for shells of revolution is based on asymptotic analysis, ref. (2). The purpose of this memorandum is to review asymptotic methods of analysis to identify features that can be adapted to numerical solutions for shell problems.

Most of the literature on asymptotic solutions is based on linear shell theory, ref. (3). In linear theory, the coefficients of the differential equations of the theory can be written in closed form for a broad class of problems. The classical asymptotic analysis expands these coefficients in power series. The review of asymptotic methods here focuses on eliminating explicit expansions of the coefficients. Current applications require solutions of nonlinear problems in shell structures. The nonlinear differential equations of shell theory can be solved by Newton's method, which reduces a problem to a sequence of linear differential equations. The linear equations have coefficients that vary with the independent variables and with the current approximate problem solution. For viable numerical solutions, formal series expansions of the coefficients is not feasible.

The development of asymptotic methods in shell analysis paralleled the analysis of the special functions of mathematical physics. Going back to the same starting point, this memorandum is concerned with the derivation of an algorithm for solving second order linear differential equations. The numerical algorithm is applied to several examples for comparison with analytical methods. Bessel's equation is examined as an example of an equation with an irregular singular point at infinity, ref. (4). The results of classical analysis, used in subroutines to compute Bessel functions of large arguments, are compared to the numerical algorithm. The Falkner-Skan equation from boundary layer theory is solved as a nonlinear example using Newton's method, ref. (5), and the numerical algorithm derived in this memorandum.

FIRST ORDER DIFFERENTIAL EQUATIONS

The basic numerical algorithm for second order equations is based on the application of Newton's method to first order nonlinear equations. The first order equation is the simplest example for solving differential equations by Newton's method. Its solution is outlined in general form in this section before applying the algorithm to second order equations in the next section.

Newton's method approximates the solution $y=y(x)$ for the general equation,

$$\frac{dy}{dx} + F(x,y) = 0 \quad (1.1)$$

by solving the following sequence of linear equations:

$$\frac{d\delta y^{(m)}}{dx} + P^{(m-1)}(x) \delta y^{(m)} = -E^{(m-1)}(x) \quad m=1,2,3,\dots \quad (1.2a)$$

$$y^{(m)} = y^{(m-1)} + \delta y^{(m)} \quad (1.2b)$$

$$P^{(m-1)} = F_{,y}(x, y^{(m-1)}) \quad (1.2c)$$

$$E^{(m-1)} = \frac{dy^{(m-1)}}{dx} + F(x, y^{(m-1)}) \quad (1.2d)$$

In equations (1.2), the integer m is an iteration counter. After m iterations, the function $y^{(m)}$ is the approximation to y , the solution of the nonlinear problem, equation (1.1). The function $\delta y^{(m)}$, defined by equation (1.2b) as the correction to the solution after $(m-1)$ iteration cycles, is computed in the m th iteration by solving the linear variational equation, equation (1.2a). The right-hand side of equation (1.2d) identifies $E^{(m-1)}(x)$ as the residual error when the $(m-1)$ st approximation is substituted in the

nonlinear equation. Finally, the subscript comma followed by y on the right-hand side of equation (1.2c) denotes $P^{(m-1)}$ as the partial derivative of $F(x,y)$ with respect to the dependent variable. The partial derivative appears because the linear variational equation results from expanding the nonlinear equation in a Taylor series about the (m-1)st approximate solution for y while holding x constant and from truncating the series after the linear term.

At each iteration step*, the linear variational equation, equation (1.2a), is a first order equation whose general solution can be written

$$\delta y = C e^{-u(x)} + e^{-u(x)} \int^x e^{u(s)} E(s) ds \quad (1.3)$$

where

$$u(x) = \int^x P(t) dt \quad (1.4)$$

For specific problems, the integrals in equation (1.3) can be written in closed form or evaluated by approximate methods. One approximate method for integrals is asymptotic expansions that are closely connected with asymptotic expansions for differential equations. Rather than approximating specific integrals as they arise in Newton's method, the alternative adopted here is to replace the integrals with numerical quadrature formulas.

QUADRATURE FORMULAS

For numerical solutions by integration, accuracy is improved by avoiding numerical computation of the derivative appearing in the residual error, E. Combining equation (1.2a) and equation (1.2b) to eliminate δy gives

$$\frac{dy^{(m)}}{dx} + P^{(m-1)}(x) [y^{(m)} - y^{(m-1)}] = -F(x, y^{(m-1)})$$

*

The superscript (m) for the iteration will be dropped in equations that follow when no confusion arises.

or

$$\frac{dy^{(m)}}{dx} + P^{(m-1)}(x) y^{(m)} = Q^{(m-1)}(x) \quad (1.5)$$

where

$$Q^{(m-1)}(x) = P^{(m-1)}(x) y^{(m-1)} - F(x, y^{(m-1)}) \quad (1.6)$$

It is also useful in numerical solutions to have the capability to integrate both forward and backward. Formulas for integrating forward from $x=b$ and for integrating backward from $x=c$ are:

$$u(x) = \int_b^x P(s) ds \quad x \geq b \quad (1.7a)$$

$$u(x) = - \int_x^c P(s) ds \quad x \leq c \quad (1.7b)$$

$$y(x) = y(b) e^{-u(x)} + I_1(b, x) \quad x \geq b \quad (1.8a)$$

$$I_1(b, x) = \int_b^x e^{-[u(x)-u(t)]} Q(t) dt \quad x \geq b \quad (1.8b)$$

$$y(x) = y(c) e^{-u(x)} - I_2(x, c) \quad x \leq c \quad (1.8c)$$

$$I_2(x, c) = \int_x^c e^{-[u(x)-u(t)]} Q(t) dt \quad x \leq c \quad (1.8d)$$

When $P(x)$ is a smooth function, the integrals for computing $u(x)$, equations (1.7), can use Simpson's rule or other standard quadrature formulas. However, when $P(x)$ is slowly varying but large in absolute value, asymptotic analysis of the convolution integrals I_1 and I_2 in equations

(1.8), ref. (4), suggests using the exponential function, $\exp\{-[u(x)-u(t)]\}$, as a weighting function in the quadrature formula. The exact form of the exponential functions is not known in advance, but recurrence relations for the integrals allow use of approximate weighting functions.

RECURRENCE RELATIONS

The convolution integrals for the particular solutions obey the following recurrence relations between integrals for two consecutive values of x , say $x=x_i$ and $x=x_{i+1}$:

$$I_1(b, x_{i+1}) = I_1(b, x_i) \exp\{-[u(x_{i+1})-u(x_i)]\} + I_1(x_i, x_{i+1}) \quad (1.9a)$$

$$I_2(x_i, c) = I_2(x_{i+1}, c) \exp\{-[u(x_i)-u(x_{i+1})]\} + I_2(x_i, x_{i+1}) \quad (1.9b)$$

For the numerical quadrature formulas, the interval of integration is divided into subintervals determined by a set of stations at $x=x_i$. From the definition of $u(x)$, equation (1.4), and the mean value theorem,

$$u(x) - u(t) = P(\xi) (x-t) \quad t \leq \xi \leq x \quad (1.10)$$

The mean value theorem suggests that a weighting function of an exponential term with a linear argument can be used for each subinterval. Let

$$g(t) = u(x) - u(t) = a(x-t) \quad a=P(x) \quad (1.11)$$

Then, changing the dummy variable reduces the integrals in each subinterval to the standard forms,

$$I_1(x_{i-1}, x_i) = \int_0^{v_i} e^{-as} f_1(s) ds \quad v_i = x_i - x_{i-1} \quad (1.12a)$$

$$I_2(x_i, x_{i+1}) = \int_0^{v_{i+1}} e^{as} f_2(s) ds \quad a = P(x_i) \quad (1.12b)$$

where

$$f_1(s) = \exp [-g(x_i - s) Q(x_i - s)] \quad (1.12c)$$

$$f_2(s) = \exp [-g(x_i + s) Q(x_i + s)] \quad (1.12d)$$

The final steps in deriving quadrature formulas for the integrals in equations (1.12) are to expand the functions $f(s)$ with polynomial interpolation formulas from tabulated values of P , Q , and u and to integrate term by term. A useful formula for summing the integrals is

$$\int e^{-as} s^n ds = \frac{n}{a} \int e^{-as} s^{n-1} ds - \frac{s^n}{a} e^{-as} \quad n=1,2,3,\dots \quad (1.13)$$

SECOND ORDER LINEAR EQUATIONS

The results derived in the preceding section for first order nonlinear differential equations are readily extended to nonlinear second order equations, ref. (5). The linear variational equations of Newton's method at any iteration cycle will have the general form

$$y'' + p(x) y' + q(x) y = - e(x) \quad (2.1)$$

where primes denote differentiation with respect to x . In Newton's method, the dependent variable y is a correction to a current approximation. The concern here is not with the derivation of equation (2.1) for a specific problem, but with its numerical solution. The numerical solution does not operate on equation (2.1) directly, but only a related nonlinear form, suggested by asymptotic theory.

Asymptotic analysis starts by assuming the complementary solution of the second order linear equation in the form

$$y(x) = \exp \left[\int^x \phi(t) dt \right] \quad (2.2)$$

For a solution of the complementary equation, $\phi(x)$, the derivative of the integral at x , must satisfy the Riccati equation, ref. (6),

$$\phi' + \phi^2 + p \phi + q = 0 \quad (2.3)$$

The assumed solution for $y(x)$, equation (2.2), transforms the linear second order equation into a first order nonlinear equation for $\phi(x)$. The first order equation will be solved here by Newton's method as outlined in the section on first order equations. The linear variational equation, equation (1.2a), in an iteration for ϕ is

$$(\delta\phi')^{(m)} + [2\phi^{(m-1)} + p] \delta\phi^{(m)} = - E[\phi(x)]^{(m-1)} \quad (2.4)$$

and equation (1.5) for the Riccati equation is

$$(\phi')^{(m)} + [2\phi^{(m-1)} + p]\phi^{(m)} = [(\phi^2)^{(m-1)} - q] \quad (2.5)$$

The iteration by Newton's method requires a zeroth approximation to start the iteration. For numerical solutions, a boundary condition for ϕ is also required. Insight into stable numerical solutions of the Riccati equation is found in the theory for second order linear equations.

LINEAR INDEPENDENCE OF SOLUTIONS

A fundamental set of solutions for a linear second order differential equation is defined as a pair of linearly independent solutions. Therefore, two solutions, ϕ_1 and ϕ_2 , must be found for the Riccati equation so that a fundamental set of complementary solutions for y can be written in the form

$$y = c_1 y_1(x) + c_2 y_2(x) \quad (2.6)$$

with

$$y_i(x) = \exp [u_i(x)] \quad (2.7)$$

$$u_i = \int^x \phi_i(t) dt \quad i= 1,2$$

To be linearly independent, the Wronskian, W , of the solution must not vanish. The Wronskian of a fundamental set of solutions is

$$W = (y_1 y_2' - y_2 y_1') \quad (2.8)$$

For the fundamental set, equations (2.7), defined by solutions of the Riccati equation, the Wronskian is

$$W(x) = [\phi_2(x) - \phi_1(x)] \exp \left(\int^x [\phi_2(t) + \phi_1(t)] dt \right) \quad (2.9)$$

Since the exponential function never vanishes, the solutions are a fundamental set as long as ϕ_1 and ϕ_2 are distinct solutions of the Riccati equation. Therefore, the choice of zeroth approximation and boundary condition in solving the Riccati equation, equation (2.3), by Newton's method must be influenced by the requirement of finding two solutions that do not intersect in the interval of integration on x , the independent variable.

COMPUTATION OF WRONSKIAN

Solving the linear variational equations by computing convolution integrals numerically has the potential for accurate and numerically stable solutions. The Wronskian is also a measure of the accuracy of the two solutions, ϕ_1 and ϕ_2 . The difference in the two solutions can be checked numerically by a direct integration rather than a convolution integral. The difference can be derived by substituting ϕ_1 and ϕ_2 in the Riccati equation separately and subtracting the two equations. The resulting differential equation for the difference ($\phi_2 - \phi_1$) is

$$(\phi_2 - \phi_1)' + (p + \phi_2 + \phi_1)(\phi_2 - \phi_1) = 0 \quad (2.10)$$

The solution of equation (2.10) can be written as

$$\phi_2(x) - \phi_1(x) = [\phi_2(b) - \phi_1(b)] \exp \left(- \int_b^x [p(t) + \phi_2(t) + \phi_1(t)] dt \right) \quad (2.11)$$

where $x=b$ is any point in the interval of integration. The equation for the difference in the two solutions also follows from substituting Abel's identity for the Wronskian,

$$W(x) = C \exp \left(- \int^x p dt \right) \quad (2.12)$$

into equation (2.9).

ZEROth APPROXIMATION AND BOUNDARY CONDITIONS FOR ϕ

The theory for the second order linear differential equation requires two distinct solutions for the Riccati equation. The solution for the Riccati equation by Newton's method is influenced by the zeroth approximation and by the constant of integration for the linear variational equation in the iteration. When the coefficients p and q in the second order equation are slowly varying functions of x , then classical asymptotic theory suggest two distinct zeroth approximations. First, the theory changes the dependent variable in the Riccati equation to α , where

$$\alpha = \phi + (p/2) \quad (2.13)$$

The change of variable inserted in the Riccati equation, equation (2.3), transforms it to

$$\alpha' + \alpha^2 + \tilde{q} = 0 \quad (2.14)$$

where

$$\tilde{q} = q - (p^2/4) - (p'/2) \quad (2.15)$$

Then, two zeroth approximations to solve the transformed Riccati equation by Newton's method are

$$\alpha_1^{(0)} = (-\tilde{q})^{1/2} \quad (2.16a)$$

$$\alpha_2^{(0)} = -(-\tilde{q})^{1/2} = -\alpha_1^{(0)} \quad (2.16b)$$

When $\tilde{q} = \tilde{q}(x)$ is a real function, the two zeroth approximations for α are both real or both pure imaginary. For the case with complex α , only one iteration sequence is required starting with one of the two zeroth approximations. If α is complex, then by definition, equation (2.13), ϕ is also a complex solution of the Riccati equation, equation (2.3). It follows

by direct substitution that if ϕ_1 is a complex solution, then $\phi_2 = \bar{\phi}_1$, the complex conjugate of ϕ_1 , is another solution.

The second case where $\tilde{q} < 0$ and the two zeroth approximations for α are real requires two iteration sequences in Newton's method starting each sequence with one of the zeroth approximations. If the two converged solutions, α_1 and α_2 , do not vanish in the interval of integration and retain the algebraic signs of the zeroth approximations, their difference, $\alpha_2 - \alpha_1$, will not vanish. By definition, equation (2.13), the difference $(\phi_2 - \phi_1) = (\alpha_2 - \alpha_1)$ will not vanish either. The pair of solutions of the Riccati equation, ϕ_1 and ϕ_2 , when integrated determine two exponential functions that are two linearly independent solutions for y in equation (2.6).

In either case, when the imaginary part of a complex ϕ does not vanish or when two real α of opposite sign are found, the Wronskian will not vanish because of equation (2.9) and the exponential solutions for y will be a fundamental pair of solutions for the linear second order differential equation, equation (2.1).

BESSEL'S EQUATION OF ORDER n

An example problem will clarify the procedure for solving the Riccati equation by Newton's method for two distinct solutions. Consider Bessel's equation of order n for positive values of the real variable x ,

$$y'' + (1/x) y' + (1 - n^2/x^2) y = 0 \quad 0 < x \leq \infty \quad (2.17)$$

For this problem $p = (1/x)$ and

$$\tilde{q} = [1 - (n^2 - 1/4)/x^2] \quad (2.18)$$

For this example, the algebraic sign of \tilde{q} depends on the value of x

$$\bar{q} \geq 0 \quad x \geq \xi = (n^2 - 1/4)^{1/2} \quad (2.19)$$

The point $x = \xi$ is called a turning point or a transition point, because of the change in qualitative behavior in y as the exponential solutions, equation (2.6), pass from real to imaginary as x passes through the point. The classical literature seeks a uniform asymptotic expansion valid on both sides of the turning point. For numerical solutions, the additional analysis is not necessary since linearly independent solutions on either side of the turning point can be matched by a direct computation to determine constants of integration. Therefore, solutions to the left and right of the turning point for Bessel's equation are computed separately here.

Consider first, solutions of the Riccati equation for Bessel's equation in the interval $b \leq x \leq \xi$ where $b > 0$ to exclude the regular singular point at $x = 0$. The zeroth approximation

$$\alpha_1^{(0)} = (\xi^2/x^2 - 1)^{1/2}$$

for $n=1$ is shown in figure 1 along with the approximation after one iteration cycle of Newton's method, $\alpha_1^{(1)}$, and the converged solution, $\alpha_1^{(4)}$. The first approximation lies above the zeroth approximation and is positive at the turning point of the zeroth approximation.

The first approximation for α remaining positive when the zeroth approximation is positive is a general result. Because the zeroth approximation satisfies equation (2.16a), the residual error in the linear variational equation for the first iteration is minus the derivative of the zeroth approximation

$$\delta\alpha_1' + 2\alpha_1 \delta\alpha_1 = -\alpha_1' \quad (2.20)$$

where superscripts denoting the first iteration have been dropped. Integrating the variational equation between limits gives

$$\delta\alpha_1(x) = \int_b^x e^{-[u(x)-u(t)]} (-\alpha_1') dt \quad (2.21)$$

Since

$$u(x)-u(t) = \int_t^x 2\alpha_1(s) ds \geq 0 \quad (2.22)$$

the exponential function in the integral in equation (2.21) is less than unity,

$$0 \leq e^{-[u(x)-u(t)]} \leq 1 \quad (2.23)$$

For cases where $\alpha_1' \leq 0$ in the interval of integration, as is true for the zeroth approximation in figure 1, the properties of the integral in equation (2.21) shows that the first correction to α_1 is always positive,

$$0 \leq \delta\alpha_1(x) \leq \int_b^x (-\alpha_1') dt = \alpha_1(b) - \alpha_1(x) \geq 0 \quad (2.24)$$

or writing the result of the first iteration with superscripts,

$$\alpha_1^{(1)} = \delta\alpha_1^{(1)} + \alpha_1^{(0)} \geq \alpha_1^{(0)} \geq 0 \quad (2.25)$$

When the slope of the zeroth approximation is positive in the interval of integration rather than negative, the particular solution for the first correction will give the same result as equation (2.24) by interchanging the end points to integrate from x to b.

It also follows by a similar proof that the second correction in Newton's method is negative. The converged solution for α_1 in figure 1 lies between the first approximation and the zeroth approximation, but the proof that this is true is problem dependent and not examined here. Also, the

numerical solution does not use the linear variational equation directly to solve for the correction $\delta\alpha$ because the derivative of the zeroth approximation does not exist at the turning point ξ . The form corresponding to the general equation (1.5) is used for the numerical solution for α .

Once the positive solution, α_1 , of the transformed Riccati equation, equation (2.14), for Bessel's equation is computed, a second iteration sequence of Newton's method is required to compute a second solution, α_2 . The result of this iteration, starting with a negative zeroth approximation, is shown in figure 2. The integration direction in the particular solutions for this case is backward from the turning point, $x=\xi$. The backward integration makes the first correction lie between the x-axis and the zeroth approximation. The converged solution for α_2 is less than or equal to zero, α_1 is always greater than zero. In the interval $0 < x \leq \xi$, Newton's method gives two real α of opposite sign and two linearly independent solutions of Bessel's equation follow from computing two solutions of the original Riccati equation,

$$\phi_i = (-1/2x) + \alpha_i \quad i=1,2 \quad (2.26)$$

The solution of Bessel's equation is then written in the form

$$y = C_1 \exp[u_1(x)] + C_2 \exp[u_2(x)] \quad 0 \leq x \leq \xi \quad (2.27)$$

where

$$u_1(x) = - \int_x^\xi \phi_1(t) dt \leq 0$$

$$u_2(x) = \int_b^x \phi_2(t) dt \leq 0$$

The directions of integration to compute the integrals $u_i(x)$ are chosen to normalize the exponential solutions of Bessel's equation to less than or equal to unity.

COMPLEX EXPONENTIAL SOLUTIONS OF BESSEL'S EQUATION

For solutions of Bessel's equation to the right of the turning point, $x \geq \xi$, the two zeroth approximations for α in equation (2.16) are pure imaginary complex conjugates. In this case, only one solution of the transformed Riccati equation is required for α as long as the imaginary part of the complex solution does not vanish. Since complex algebra is required in the numerical solution, the amount of computation is approximately the same for one complex solution for α as for two real solutions. The quadrature formulas derived for first order linear real equations are identical for complex equations so that computer subroutines in real variables are readily converted to complex subroutines.

The derivative of the zeroth approximation for α approaches zero as x goes to infinity so that the residual error in the linear variational equation, equation (2.20), is small for large values of x . Setting the correction equal to zero at a finite x and integrating backward in the quadrature formulas gives rapid convergence for Newton's method to compute a complex solution α of the transformed Riccati equation. Real and imaginary components of α_1 for the case of order $n=1$ are shown in figure 3.

With $\alpha_2 = \bar{\alpha}_1$, a complex solution for Bessel's equation follows from equation (2.26) and equation (2.27), or the final result for y can be written in real form since $C_2 = \bar{C}_1$. The numerical results for y from Newton's method compare favorably with tabulated values for Bessel functions of the first and second kinds, $J_n(x)$ and $Y_n(x)$. The quadrature formulas for the interval of integration in figure 3 used 41 stations. The numerical solution for $J_1(x)$ and $Y_1(x)$ is accurate to six digits. The solutions for the Bessel functions are less accurate to the left of the turning point reflecting the rapid variation in α caused by the regular singular point at $x=0$.

IMPROVED ANALYTICAL RESULTS FOR BESSEL FUNCTIONS

The numerical results for the complex solution of the transformed Riccati equation, equation (2.14), for Bessel's equation suggest an analytical improvement in the zeroth approximation for α in the general case. The real component of α in figure 3 is small compared to the imaginary component. A look at the first iteration in Newton's method suggests that a small real part for a complex α can be expected when \tilde{q} is positive, large, and slowly varying.

Dropping the superscript zero in equation (2.16a),

$$\alpha = i (\tilde{q})^{1/2}$$

Also, differentiating $\alpha^2 = -\tilde{q}$ gives the expression for the derivative,

$$\alpha' = -\tilde{q}'/2\alpha \tag{2.28}$$

The derivative is the residual error appearing in the first iteration of Newton's method for the correction $\delta\alpha$,

$$\delta\alpha' + 2\alpha \delta\alpha = -\alpha' \tag{2.29}$$

When α' is small in absolute value compared to α and slowly varying, an approximate particular solution of equation (2.29) is obtained by neglecting the derivative on the left-hand side and substituting for α' from equation (2.28),

$$\delta\alpha \approx -\tilde{q}'/4\alpha^2 = \tilde{q}'/4\tilde{q} \tag{2.30}$$

Therefore, adding the approximate correction to the zeroth approximation gives a first approximation,

$$\alpha^{(1)} = (\tilde{q}'/4\tilde{q}) + i \tilde{q}^{1/2} \tag{2.31}$$

The corresponding approximation to the solution of the Riccati equation is

$$\phi = -p/2 + \alpha^{(1)}$$

The approximate complex solution for y is

$$y = (\tilde{q})^{-1/4} \exp \left[-\int (p/2) dx + i \int \tilde{q}^{1/2} dx \right] \quad (2.32)$$

For Bessel's equation, the approximate solution for y can be written in closed form. By selecting a complex constant of integration that makes the approximate complex solution agree with the Hankel function of the first kind as x goes to infinity, the real and imaginary parts of y approximate the real Bessel functions of the first and second kinds:

$$J_n(x) \approx (2/\pi X)^{1/2} \cos [X + \xi \tan^{-1}(\xi/X) - n\pi/2 - \pi/4] \quad (2.33a)$$

$$Y_n(x) \approx (2/\pi X)^{1/2} \sin [X + \xi \tan^{-1}(\xi/X) - n\pi/2 - \pi/4] \quad (2.33b)$$

where

$$X^2 = x^2 - \xi^2 \quad \text{and} \quad \xi^2 = n^2 - 1/4$$

The corresponding result from the pure imaginary zeroth approximation, $\alpha = iX/x$, is

$$J_n(x) \approx (2/\pi x)^{1/2} \cos [X + \xi \tan^{-1}(\xi/X) - n\pi/2 - \pi/4] \quad (2.34a)$$

$$Y_n(x) \approx (2/\pi x)^{1/2} \sin [X + \xi \tan^{-1}(\xi/X) - n\pi/2 - \pi/4] \quad (2.34b)$$

The approximation from Newton's method for the two solutions of Bessel's equation can be compared to the leading term from the classical asymptotic expansion,

$$J_n(x) \sim (2/\pi x)^{1/2} \cos(x - n\pi/2 - \pi/4) \quad (2.35a)$$

$$Y_n(x) \sim (2/\pi x)^{1/2} \sin(x - n\pi/2 - \pi/4) \quad (2.35b)$$

or the first approximation from perturbation theory, ref. (7),

$$J_n(x) \sim (2/\pi x)^{1/2} [\cos(x - n\pi/2 - \pi/4) - (\xi^2/2x) \sin(x - n\pi/2 - \pi/4)] \quad (2.36a)$$

$$Y_n(x) \sim (2/\pi x)^{1/2} [\sin(x - n\pi/2 - \pi/4) + (\xi^2/2x) \cos(x - n\pi/2 - \pi/4)] \quad (2.36b)$$

Numerical results from the various approximations for $J_6(x)$ are compared to exact values in Table 1. The approximation in equation (2.33a) derived from the approximate first iteration for α , equation (2.31), in Newton's method is the most accurate of the approximations in the interval $\xi \leq x \leq \infty$ except near $x=\xi$. The approximation breaks down at the turning point ξ since the derivative on the left-hand side of the linear variational equation, equation (2.29), cannot be neglected near the turning point.

The general case will give results similar to those for Bessel's equation. Whenever \tilde{q} is large, positive and varies slowly with x , equation (2.32) is a good approximation for a complex solution of the second order linear equation (2.1)

INTEGRAL REPRESENTATION OF THE PARTICULAR SOLUTION

The general solution of a second-order linear differential equation requires a particular solution in addition to two solutions of the

homogeneous equation. Variation of parameters is a general method for determining particular solutions by integration. The integrals that appear in the particular solution are of the same form as those for the solution of first order linear equations when the solutions, equations (2.7), of the homogeneous equations have the exponential form derived from the solutions of the Riccati equation. The general expression for the particular solution of the inhomogeneous equation, equation (2.1), is

$$y_p(x) = y_1(x) \int^x [y_2(t) e(t)/W] dt - y_2(x) \int^x [y_1(t)e(t)/W] dt \quad (2.37)$$

where W is the Wronskian of the two solutions, $y_1(t)$ and $y_2(t)$. When y_1 and y_2 are of the exponential form in equation (2.7) and the Wronskian is also exponential, equation (2.9), the particular solution is

$$y_p(x) = y_{p1}(x) + y_{p2}(x) \quad (2.38)$$

where

$$y_{p1}(x) = \int^x \exp [u_1(x) - u_1(t)] \{e(t)/[\phi_2(t) - \phi_1(t)]\} dt$$

$$y_{p2}(x) = - \int^x \exp [u_2(x) - u_2(t)] \{e(t)/[\phi_2(t) - \phi_1(t)]\} dt$$

The integrals in the particular solution are of the same type as the convolution integrals, equations (1.8), representing the solution of first order linear differential equations. The numerical quadrature formulas derived for an exponential weighting function, equations (1.12), apply to the particular solution with the ϕ_i functions in the role of the weighting function, $P(x)$.

The properties of the method of variation of parameters make the derivative of the particular solution simple to compute from the expression,

$$y'_p(x) = \phi_1(x) y_{p1}(x) + \phi_2(x) y_{p2}(x) \quad (2.39)$$

ASYMPTOTIC INTEGRATION APPLIED TO THE FALKNER-SKAN EQUATION

The numerical analysis of the previous section is applied here to the Falkner-Skan equation.

$$f''' + f f'' + \beta [1 - (f')^2] = 0 \quad (3.1)$$

with boundary conditions,

$$f(0) = 0 \quad (3.2a)$$

$$f'(0) = 0 \quad (3.2b)$$

$$f'(\infty) = 1. \quad (3.2c)$$

The Falkner-Skan equation is a third-order nonlinear ordinary differential equation derived from Prandtl's partial differential equations for fluid flow in laminar boundary layers, ref. (8). In order to test the method of the previous section, the third-order system is solved here by a modified form of Newton's method. The modification reduces each iteration cycle to solving a linear second order equation and integrating a simple first-order equation.

The modified form of Newton's method converges rapidly for positive values of the parameter β and more slowly for negative values. The convergence is somewhat surprising since recent literature conveys the impression that Newton's method is unstable for the Falkner-Skan equation, ref. (9). The analysis in this section shows that the instability is in shooting methods, ref. (10) and ref. (11), that use forward integration. The numerical instability is not in Newton's method per se.

The convergence properties arise naturally as part of the iteration cycle. Two zeroth approximations that start the iteration and the resulting first approximations provide insight into the qualitative behavior of the final solutions. The qualitative behavior has been studied by Hartree, ref. (12) and by Smith, ref. (13), but they overlooked the approach of combining

asymptotic analysis and numerical analysis through Newton's method that is used here.

THE TRANSFORMED NONLINEAR PROBLEM

The zeroth approximations suggest a change in the dependent variable. The derivation of the iteration cycle begins with rewriting the problem in terms of w where

$$f = x + w \tag{3.3}$$

The transformed nonlinear problem in w is

$$w'''' + (x+w) w'' - \beta(2+w') w' = 0 \tag{3.4}$$

$$w(0) = 0 \tag{3.5a}$$

$$w'(0) = -1 \tag{3.5b}$$

$$w'(\infty) = 0 \tag{3.5c}$$

MODIFIED NEWTON'S METHOD

The linear form of Newton's method for the m th iteration cycle in operator notation is

$$L(\delta w^{(m)}) = -e(w^{(m-1)}) \text{ and } w^{(m)} = w^{(m-1)} + \delta w^{(m)} \tag{3.6a}$$

$$L(w^{(m)}) = L(w^{(m-1)}) - e(w^{(m-1)}) \tag{3.6b}$$

The modified form of Newton's method does not update the coefficients in the linear operator $L(\)$ with the current approximation for w but retains an earlier approximation $w = w_0$.

Omitting details of the derivation, the modified form of Newton's method for solving equation (3.4) for w used here is

$$y'' + py' + qy = -e \quad (3.7a)$$

where

$$y = w' \quad (3.7b)$$

$$p = (x + w_0) \quad (3.7c)$$

$$q = -2\beta(1 + w_0') \quad (3.7d)$$

$$e = (w - w_0)w'' - \beta(w' - 2w_0')w' \quad (3.7e)$$

The system of equations (3.7) is solved iteratively by substituting the $(m-1)$ st approximation for w into the expression for the residual e , equation (3.7e), and solving the linear system, equation (3.7a) and equation (3.7b), for the m th approximation for w that satisfies the boundary conditions, equations (3.5). The iteration procedure is started by letting the zeroth approximation for w be equal to w_0 . The term e is not the usual residual error in Newton's method because of the $L(w)$ term in its definition, which corresponds to the right-hand side of equation (3.6). However, when $L(w) = 0$, then e is the usual residual error and will be referred to as the residual error below.

ZEROth APPROXIMATION AND FIRST ITERATION

If $w_0 = 0$, the first iteration cycle solves the linear equations

$$y'' + xy' - 2\beta y = 0 \quad (3.8a)$$

$$w' = y \quad (3.8b)$$

The solution w gives a first approximation for the solution of the nonlinear problem in w , equations (3.3) and equations (3.4), and also a good approximation for $f=x+w$ with the error in f equal to the error in w . Assuming the solution of the form,

$$w' = y = \exp \int^x \phi dt \quad (3.9)$$

leads to the Riccati equation for equation (3.8a)

$$\phi' + \phi^2 + x \phi - 2\beta = 0 \quad (3.10)$$

As x goes to infinity, two distinct solutions of the Riccati equation can be identified, $\phi_1 \sim -x$ and $\phi_2 \sim 2\beta/x$. The solution for equation (3.8a) can be written as

$$w' = c_1 \exp \left[\int_0^x \phi_1 dt \right] + c_2 \exp \left[\int_0^x \phi_2 dt \right] \quad (3.11)$$

where c_1 and c_2 are constants of integration. For large values of x , an asymptotic expression for the solution is

$$w' \sim c_1 \exp(-x^2/2) + c_2 x^{2\beta} \quad (3.12)$$

When β is positive, the constant of integration c_2 must be zero in order to satisfy the boundary condition on w' at infinity, equation (3.5c). When β is negative, w' vanishes at infinity for any real, finite choice of the constants of integration. Hartree, ref. (12), derived the equivalent of equations (3.8) and argued on physical grounds that the constant c_2 should also be set to zero for negative values of β . When $1 < 2\beta < 0$, it seems that a stronger argument could be made by noting that the integral of w' does not have a finite limit at infinity. The nondimensional stream function $f=x+w$ appears in the dimensional expression for the transverse component of the flow velocity, ref. (13), and the physics of the problem suggest requiring

that w be finite at infinity. In any case, the constant c_2 is suppressed in the numerical results reported here.

Smith, ref. (13), observed that, when 2β is zero or a positive integer, an exact solution of equations (3.8) can be written in terms of integrals of the error function. These integrals are computed for large values of the argument by asymptotic expansions. However, Smith did not pursue asymptotic expansions as a method of computation. Instead he used a power series solution for solving the nonlinear problem starting the solution at $x=0$ and using trial-and-error to establish the value of $f''(0)$ necessary to start the forward integration.

The form of the asymptotic solutions for the first correction suggests the opposite approach of integrating backward from infinity. The Riccati equation can be solved numerically for two distinct solutions, $\phi_1 \sim -x$ and $\phi_2 \sim 2\beta/x$ by integrating backward. For each iteration cycle, the numerical solution of equation (3.7a) finds the solution by the method of the previous section with the solutions of the associated Riccati equation computed by backward integration. This procedure identifies a constant of integration corresponding to c_2 that is explicitly set to zero for every iteration cycle. Before examining the numerical solution for the first approximation and for succeeding iterations for f , another choice for w_0 , the zeroth approximation for w , is introduced here. The second choice is $w_0 = -c$, where c is a constant. For this choice, the first iteration solves

$$y'' + (x-c)y' - 2\beta y = 0 \quad (3.13a)$$

$$w' = y \quad (3.13b)$$

instead of equations (3.8), which becomes the special case of $c=0$. The choice of c is arbitrary. It is an input parameter that can be used to make the solution of equations (3.13) a better approximation to the solution of the nonlinear problem in w , equation (3.4) and equations (3.5). The residual e

computed by substituting the solution of equations (3.13) into equation (3.7e) is a true residual error since equations (3.13) are homogeneous.

$$e = (w+c) w'' - \beta (w')^2 \quad (3.14)$$

For positive values of β , there is a real constant c that speeds the rate of decay of e as x goes to infinity. This choice is

$$c = - \int_0^{\infty} w'(t) dt \quad (3.15)$$

The reason for the improved rate of decay is clearer for the special case of $\beta=n/2$ where n is zero or a positive integer. For this case, the solution of equations (3.14) can be written in terms of functions with known asymptotic expansions.

CHOICE OF c WHEN 2β IS AN INTEGER

The solution of equations (3.13) for the first approximation for w can be written in terms of integrals of the error function when

$$2\beta = n \quad n= 0,1,2, \dots$$

For brevity, the usual notation, ref. (14), is abbreviated here. Let

$$z = d (x-c) \quad d^2 = 1/2 \quad (3.16)$$

$$i^n(z) = \int_z^{\infty} i^{(n-1)}(t) dt \quad n= 0,1,2,3,\dots \quad (3.17)$$

where

$$i^{-1}(z) = (2/\pi)^{1/2} \exp(-z^2)$$

and

$$i^0(z) = (2/\pi)^{1/2} \int_z^{\infty} \exp(-t^2) dt$$

The solution of equations (3.13) that satisfies the boundary conditions, equations (3.5), when $2\beta=n$ is

$$w' = -i^n(z)/i^n(-dc) \quad (3.18a)$$

$$w = [i^{n+1}(z) - i^{n+1}(-dc)]/[di^n(-dc)] \quad (3.18b)$$

For this case the constant c in equation (3.15) is defined as

$$c = [i^{n+1}(-dc)]/[di^n(-dc)] \quad d^2=1/2 \quad (3.19)$$

making

$$w+c = i^{n+1}(z)/i^n(-dc) \sim A \exp(-z^2)/z^{n+1} \quad (3.20)$$

where A is a constant. The asymptotic behavior of $w+c$ shows that the order of the residual error, e , equation (3.14), is quadratic in w' .

The actual computation of e requires a numerical value for the constant c . The equation that defines the constant c for $2\beta=n$ is transcendental, but an exact solution is not necessary since the first approximation for w is corrected later in the iteration. Graphical solutions, equating both sides of equation (3.19), are shown in figure 4 for different values of n . Interpolating the tabulated values used in plotting the curves in the figure gives the values for c for integer values of n that are listed in Table 2. A cross-plot for interpolating c when 2β is not an integer is shown in figure 5.

Given c for each n , the residual error e can be computed using w and its derivatives from equations (3.18). The residual error is plotted as a function of x for integer values of $n=2\beta$ in figure 6. There is no finite solution for c when $n=0$ in equation (3.19) and the residual error for $n=0$ is

from the error function with $c=0$. Even though the term in β is zero, the error for this case is larger for values of x away from the origin than the error for positive values of n associated with a finite value of c .

NUMERICAL RESULTS FROM THE MODIFIED NEWTON'S METHOD

The numerical solution of the Riccati equations for equations (3.13) has been programmed on a microcomputer for any input value of β and c . The solutions for $\beta = n/2$ in terms of repeated integrals of the error function provide a check of the accuracy of the numerical solution. The next step in the general case, after solving equations (3.13), is to compute the residual e from equation (3.14) and start the iterative solution of equations (3.7). The inhomogeneous second-order differential equation, equation (3.7a), provides a test case for computing particular solutions from the integrals in equation (2.38).

The first approximation for w from equations (3.13) is a special case of the first iteration of the general form of the modified Newton iteration, equations (3.7) where $w_0 = -c$ and $e=0$. A second program was also written that updates w_0 with the current approximation for w from the first program that uses $w_0 = -c$.

Numerical results from the two programs are summarized in Table 3. All the numerical results were computed using 41 equally spaced stations for x . The numerical solutions for the special cases of repeated integrals of the error function are accurate to five or six digits. Based on published values for $f''(0)$, the particular solutions computed from the integrals of equations (2.38) retain the same accuracy.

The modified Newton's method gives good convergence for positive values of β . The first program with $w_0 = -c$ in the linear operator gives fair results for $f''(0)$ after a few iterations. The behavior at infinity is numerically stable so that the numerical solution follows the form of equation (3.12) plus a particular solution at each iteration step. The

constant $c_2=0$ for a finite solution at infinity and the constant $c_1=-1$ to satisfy the condition on w' at $x=0$.

If the iteration of equations (3.7) is carried out using shooting methods with forward integration, suppressing the solution multiplied by the constant c_2 by adjusting $f''(0)$ requires a good approximation for $f''(0)$. The asymptotic analysis shows that a more stable shooting method would be to integrate backward with $w(\infty)$ as the initial condition to be determined.

The modified Newton's method has poor convergence for negative values of β ; the linear form of Newton's method also has slow convergence for this case, ref. (15). The slow convergence is a consequence of the lack of uniqueness of solutions of the nonlinear problem when β negative. Stewartson, ref. (16), showed the existence of solutions with negative values of $f''(0)$ for certain values of β . Since the nonlinear problem is autonomous, it should be possible to alter the iteration along the lines of ref. (17) while retaining the numerical asymptotic integration to solve the linear variational equations. That approach requires more analysis and additional programming and is not explored further here.

CONCLUDING REMARKS

An investigation was conducted to study numerical analysis of asymptotic expansions that arise in shell theory. The study showed that it is feasible to achieve the linear independence of the asymptotic theory for general cases while avoiding algebraic manipulations for each special case. Second-order nonlinear ordinary equations were examined in detail in this study. The results have desirable mathematical properties that can be extended to higher-order equations that appear in shell theory.

The analysis of the Riccati equation derived from Bessel's equation produced a closed-form exponential approximation for Bessel functions of large argument that is more accurate than the leading terms of the usual expansion in negative powers of x . The result is general and applies to other problems whose solutions are nearly periodic over some range of the independent variable.

Numerical quadrature formulas were derived to compute the convolution integrals that are part of the asymptotic analysis. The formulas use an exponential weighting function to produce a better fit of the integrand than a standard polynomial fit.

The Falkner-Skan equation was examined as an example of a nonlinear problem treated by asymptotic methods. The analysis using linearly independent solutions at infinity allowed accurate computations of the solutions in the boundary layer and suggested that shooting methods applied to the problem should integrate backward from infinity rather than starting the solution at the origin.

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Table 1. Asymptotic Approximations for $J_6(x)$, Bessel Function of First Kind and Order 6 for Large x .

x	Exact value	Newton's Method		Perturbation Method	
		Approximation		Approximation	
		First Eq. (2.33a)	Zereth Eq. (2.34a)	Zereth Eq. (2.35a)	First Eq. (2.36a)
5.98	.243406659478	0.00000000	0.00000000	-.15106856	-1.01572984
6.00	.245836863364	.77225975	.22293219	-.15679786	-1.00738895
6.20	.268597150751	.44343614	.22807271	-.20697376	-.91224979
6.40	.289958360953	.39840139	.23792512	-.24748793	-.79352271
6.60	.309275672516	.38345790	.24952179	-.27709881	-.65697857
6.80	.325899479373	.37851419	.26122912	-.29500488	-.50844102
7.00	.339196604983	.37695478	.27182801	-.30086304	-.35363680
7.20	.348572602373	.37556888	.28032534	-.29479002	-.19805436
7.40	.353494359028	.37245303	.28589146	-.27734706	-.04681405
7.60	.353512167554	.36635530	.28783970	-.24950883	.09544723
7.80	.348280396189	.35642320	.28562343	-.21261767	.22467440
8.00	.337575900114	.34209466	.27884054	-.16832536	.33747340
8.20	.321313356102	.32304740	.26724063	-.11852458	.43116997
8.40	.299556779154	.29917343	.25073178	-.06527280	.50384658
8.60	.272526588542	.27056419	.22938517	-.01071154	.55435761
8.80	.240601729158	.23749901	.20343630	.04301599	.58232254
9.00	.204316517680	.20043323	.17328187	.09384575	.58809821
9.20	.164352066323	.15998377	.13947200	.13986925	.57273137
9.40	.121522333286	.11691131	.10269746	.17940273	.53789346
9.60	.076755051090	.07209854	.06377198	.21104660	.48579985
9.80	.031067984231	.02652454	.02361001	.23373316	.41911637
10.00	-.014458842085	-.01876427	-.01679964	.24676089	.34085607
10.20	-.058714127480	-.06268601	-.05642347	.24981441	.25426955
10.40	-.100588533517	-.10415719	-.09421547	.24296933	.16273215
10.60	-.139009092875	-.14212759	-.12915072	.22668229	.06963152
10.80	-.172973630937	-.17561498	-.16025935	.20176666	-.02174126
11.00	-.201584000874	-.20373856	-.18665967	.16935504	-.10829367
11.20	-.224076937511	-.22574999	-.20758919	.13085024	-.18722411
11.40	-.239851384024	-.24106084	-.22243262	.08786670	-.25610192
11.60	-.248491238197	-.24926544	-.23074553	.04216483	-.31293313
11.80	-.249782599151	-.25015826	-.23227284	-.00441932	-.35621012
12.00	-.243724767229	-.24374494	-.22696138	-.05004610	-.38494417
12.20	-.230534453434	-.23024670	-.21496589	-.09294334	-.39868021
12.40	-.210642883654	-.21009751	-.19664810	-.13147387	-.39749390
12.60	-.184685728838	-.18393416	-.17256878	-.16419667	-.38197150
12.80	-.153486046509	-.15257939	-.14347284	-.18991972	-.35317358
13.00	-.118030672130	-.11701838	-.11026792	-.20774240	-.31258420
13.20	-.079440741520	-.07836949	-.07399710	-.21708612	-.26204745
13.40	-.038937248376	-.03785000	-.03580641	-.21771198	-.20369389
13.60	.002197264605	.00326205	.00309151	-.20972517	-.13985934
13.80	.042659624317	.04366858	.04145673	-.19356595	-.07299893
14.00	.081168183426	.08209341	.07806274	-.16998779	-.00559950
14.20	.116504774373	.11732408	.11173727	-.14002372	.05990705
14.40	.147555004998	.14825196	.14140177	-.10494224	.12122613
14.60	.173345475655	.17390930	.16610813	-.06619474	.17627638

Table 1. Continued.

x	Newton's Method			Perturbation Method	
	Exact value	Approximation		Approximation	
		First Eq. (2.33a)	Zeroth Eq. (2.34a)	Zeroth Eq. (2.35a)	First Eq. (2.36a)
14.80	.193076585993	.19350189	.18507128	-.02535643	.22325627
15.00	.206149737480	.20643617	.19769657	.01593665	.26069971
15.20	.212187920995	.21233968	.20360074	.05605233	.28751874
15.40	.211048901297	.21107417	.20262591	.09342595	.30303224
15.60	.202830464206	.20274078	.19484573	.12662057	.30697995
15.80	.187867468976	.18767707	.18056363	.15438157	.29952153
16.00	.166720737703	.16644584	.16030311	.17568339	.28122115
17.00	.000715333443	.00028441	.00027517	.16920613	.07047137
18.00	-.155956234195	-.15618751	-.15168840	.01205744	-.17431553
19.00	-.178767171544	-.17870512	-.17410631	-.14737116	-.24951527
20.00	-.055086049564	-.05487232	-.05360289	-.16665635	-.10973177

TABLE 2. Solution of Equation (3.19) $c = [i^{n+1}(-dc)]/[d i^n(-dc)]$ where $i^n(z)$ is the n th Repeated Integral of the Error Function and $d^2 = 1/2$.

n	β	c
5	2.5	.427
4	2.0	.473
3	1.5	.537
2	1.0	.639
1	0.5	.840
0	0.0	∞

Table 3. Summary of Numerical Results for the Falkner-Skan Equation from the modified Newton iteration

β	c	$w(\infty)$	$f''(0)$ $-w''(0)$	$f''(0)$ Published	Ref. No.	Number of Iterations	w_0
2.4	.495	-.4614	1.8384	1.837	12	7	$w_0 = -c$
2.4	.495	-.45985	1.8378	1.837	12	1	$w_0 = w^{(7)}$
2.0	.473	-.497	1.6873	1.687218	13	7	$w_0 = -c$
1.5	.54	-.558	1.4772	7	$w_0 = -c$
1.0	.64	-.648	1.232	1.232588	13	7	$w_0 = -c$
0.5	.84	-.8046	.92762	.92768	10	7	$w_0 = -c$
0.0	0.	-1.2162	.4694	.469603	10	7	$w_0 = -c$
-0.1	0.	-1.4365	.3197	.319278	10	7	$w_0 = w^{(7)}$
-0.19	0.	-1.874	.1099	.085702	10	7	$w_0 = -c$
-0.19	1.875	-2.87	-.0897	7	$w_0 = -c$
-0.19	...	-2.003	-.0864	20	$w_0 = w^{(7)}$

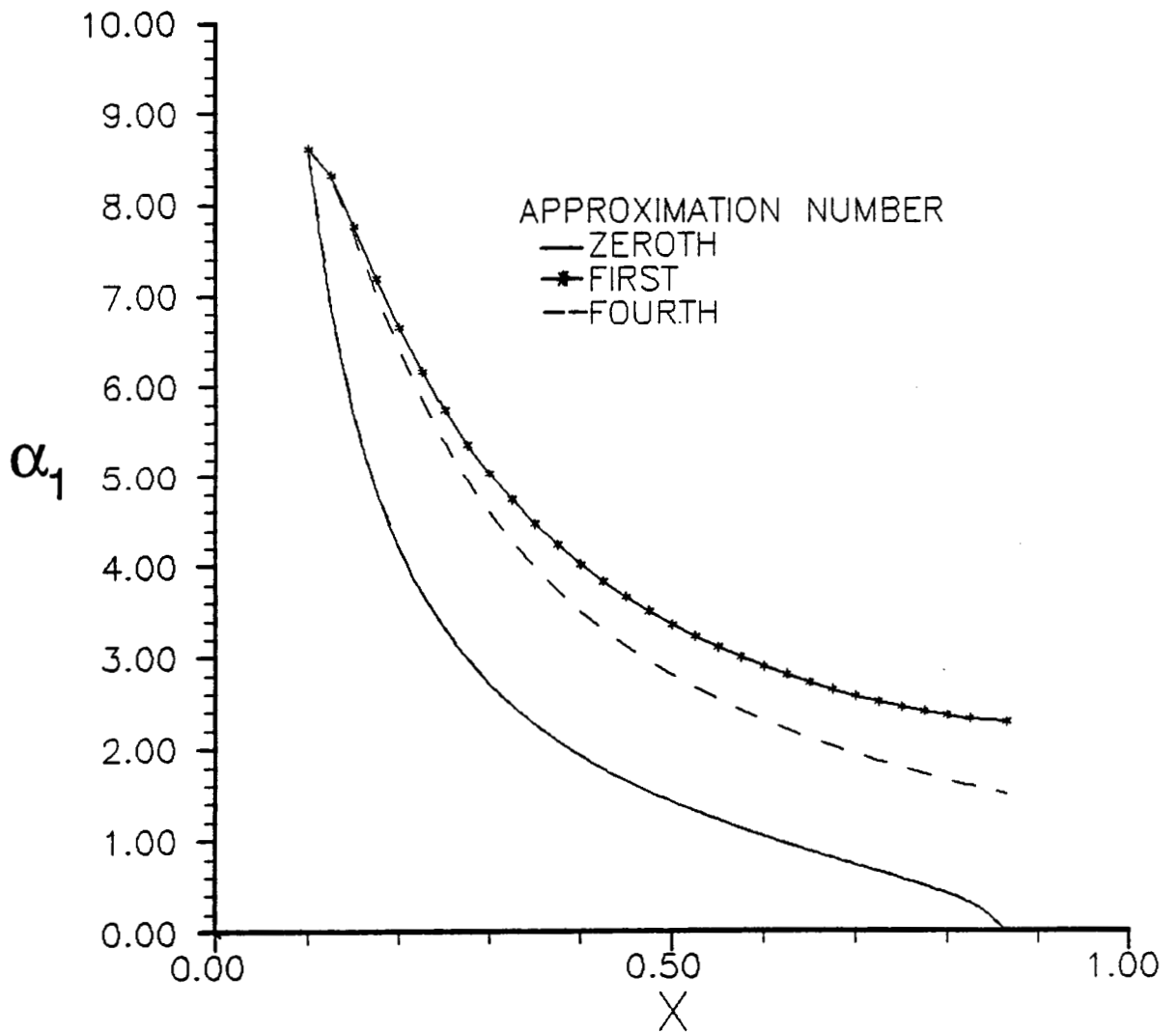


Fig. 1. Positive, real solution α_1 of Riccati equation derived from Bessel's equation. The fourth approximation is the converged solution.

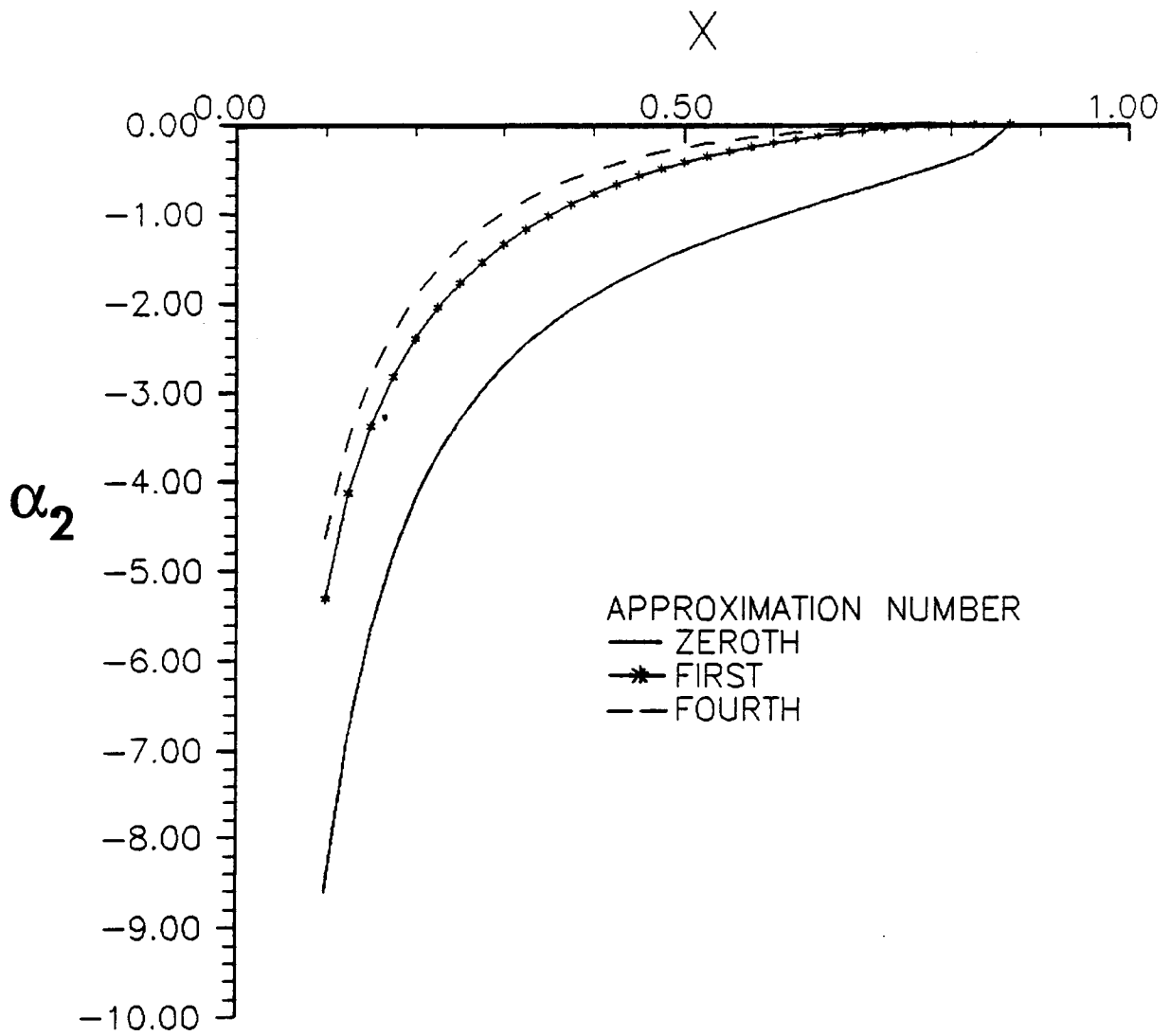


Fig. 2. Negative, real solution α_2 of Riccati equation derived from Bessel's equation. The fourth approximation is the converged solution.

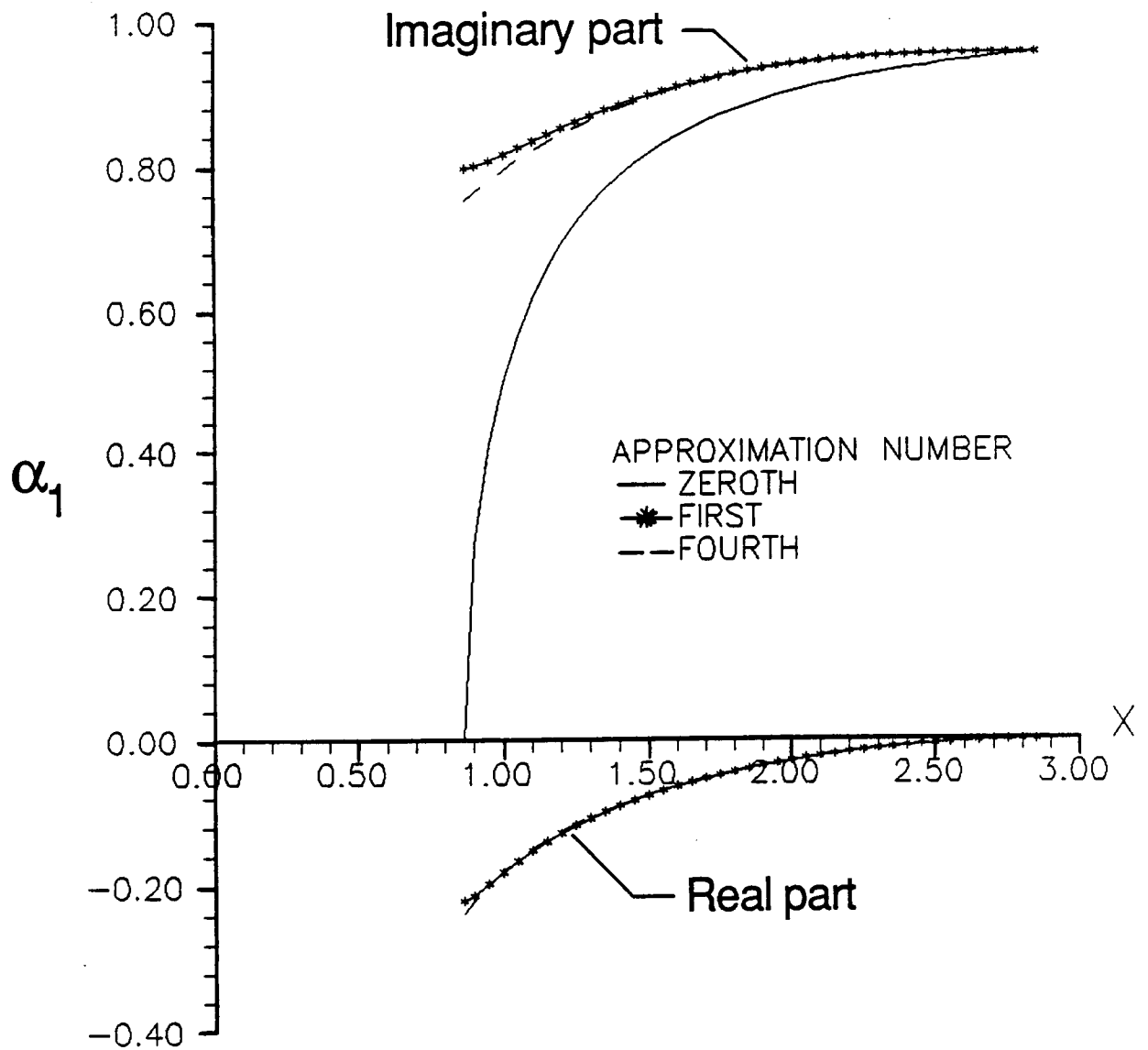


Fig. 3. Real and imaginary parts of solution α_1 of Riccati equation derived from Bessel's equation. The fourth approximation is the converged solution.

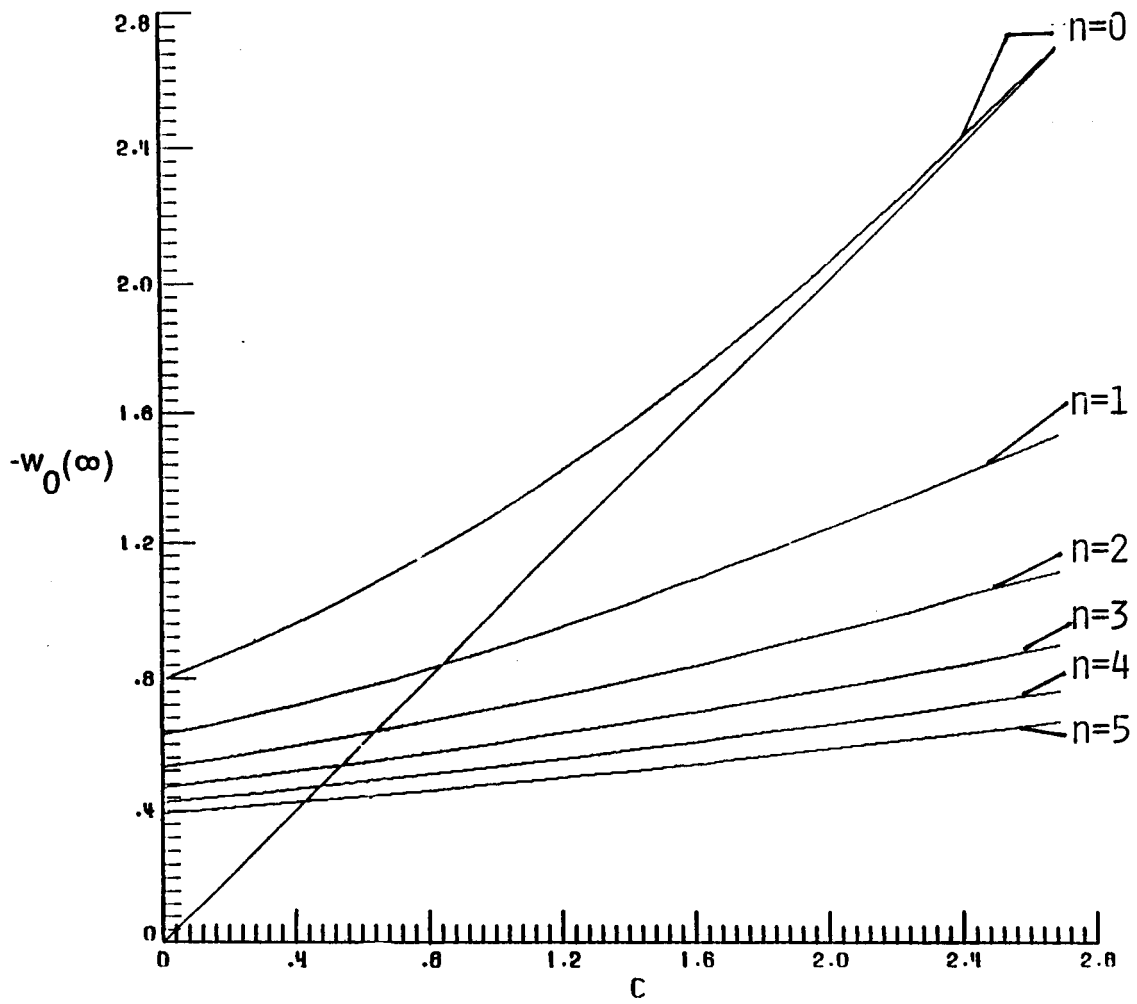


Fig. 4. Graphical solution of $-w_0(\infty)=c$ for integer values of $2\beta=n$ in solution of the Falkner-Skan equation.

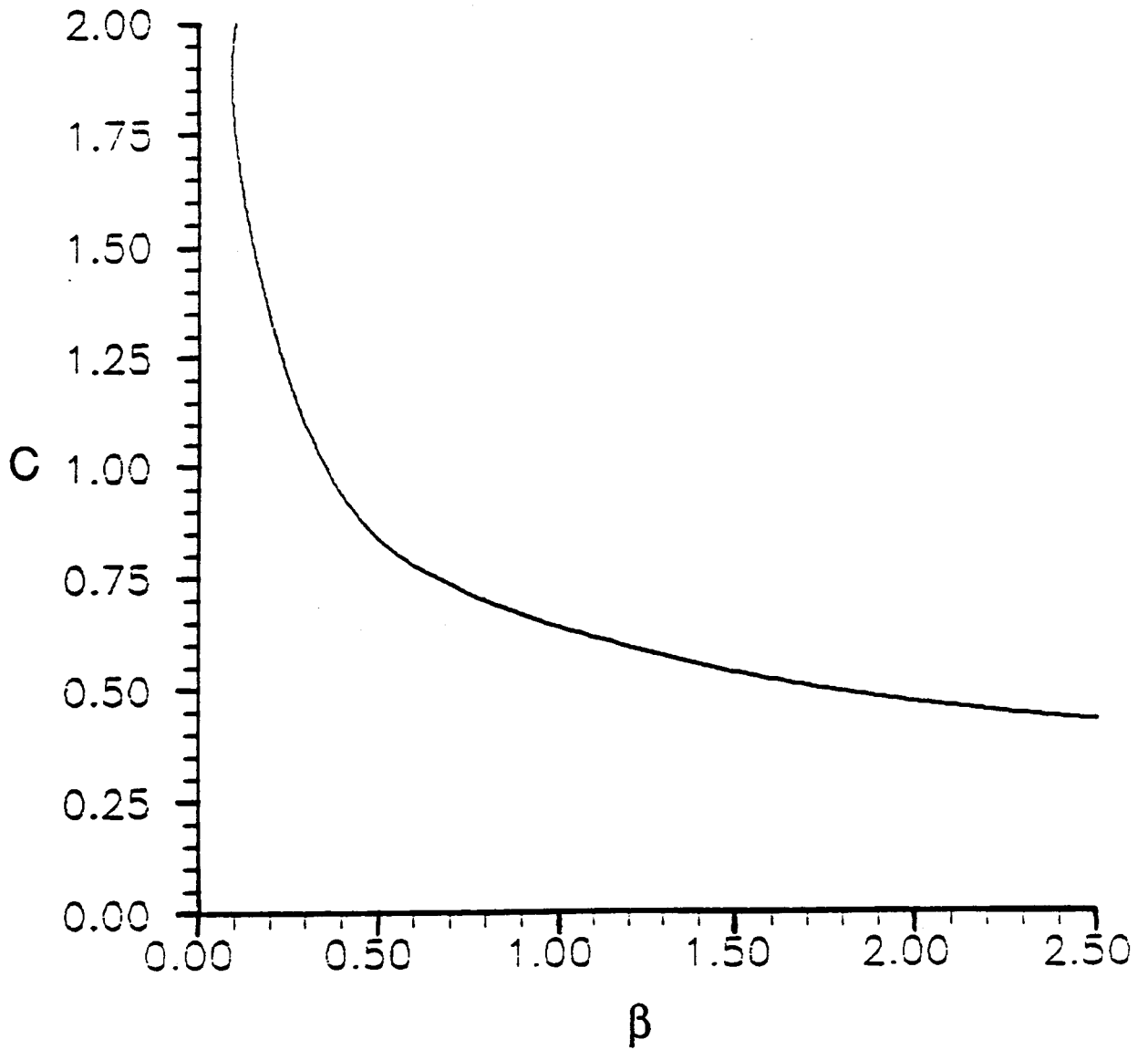


Fig. 5. Cross-plot for approximate values of c when $\beta \neq n/2$ in solution of the Falkner-Skan equation. Values of c for the zeroth approximation to $-w$ at infinity.

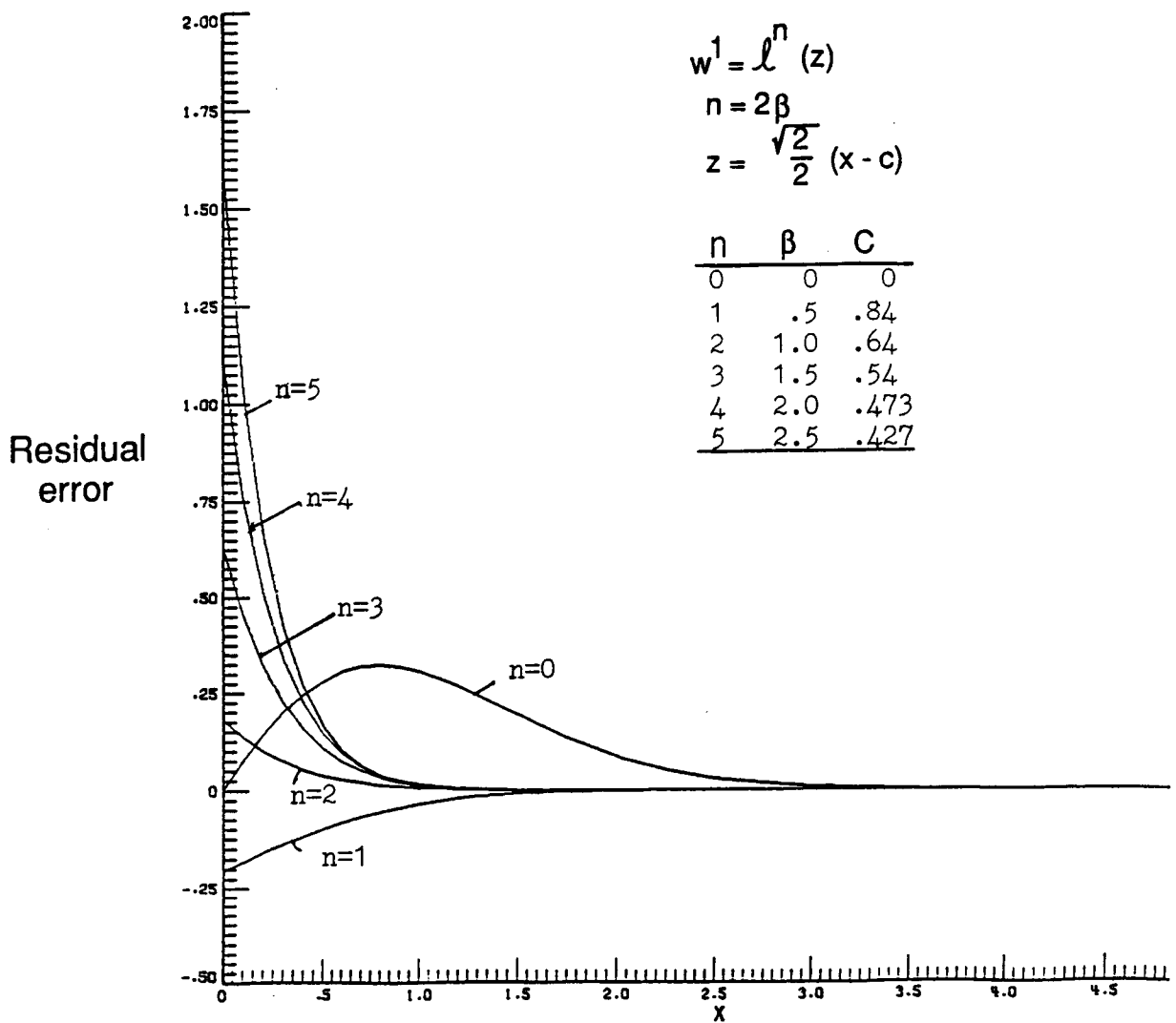


Fig. 6. Residual error confined to region of origin by proper choice of c in solution of the Falkner-Skan equation.



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