CONTROL THEORY AND THE NUMERICAL SOLUTION OF ODES[*]

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Abstract. The goal of this paper is to study the entire class of linear second order multi-point methods. We characterize, as a three parameter family, those methods with good numerical properties. We will examine the error analysis of the class of second order methods and will study in some detail the statistics of switching between two methods. We characterize the average value obtained by switching and construct the covariance matrix. Two examples are done in some detail.

1. Introduction. In 1969 David Evans graduated from MIT. His dissertation, [4], done under the direction of Roger Brockett, was the first time that the connection between numerical methods for the solution of ordinary differential equations and modern control theory was noted. Part of the dissertation was published in the SIAM Journal of Applied Mathematics, [5]. In this paper we extend the applications, that were pioneered by Evans and Brockett, of control theoretic methods to the problem of obtaining numerical solutions of ODEs. This continues a line of investigation that Martin and students have been pursuing, [6, 7, 10, 11, 12]. Our goal is to study the entire class of linear second order multi-point methods. We characterize, as a three parameter family, those methods with good numerical properties, i.e., consistency, convergence, numerical stability, etc. We will examine the error analysis of the class of second order methods and will study in some detail the statistics of the error obtained by switching between two methods. We characterize the average value obtained by switching and construct the covariance matrix. We will use as primary examples a scalar Riccati equation and a time varying second order linear system. As is usual in the numerical literature the theory will be built using a first order linear system. We will accomplish two major goals in this paper. The first is a serious study of the effect of randomly switching between two numerical procedures and the second is to tailor a method for the solution of a fixed differential equation. This second goal is not the usual numerical procedure. Normally a method is derived that has good general properties, such as Adams-Bashforth, but here we are asking to find a method that is "optimal" for a specific differential equation.

There are a few papers in the numerical literature that are relevant. The work of Dahlquist, [1, 2], are important in the classification of linear multi-point methods and for describing the limits to accuracy for specific methods, Dahlquist's first and second

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barriers. The book of Lambert, [14], is written in a very control theoretic manner and was the inspiration for much of this work. Henrici, [8, 9] studies the statistical nature of the error for first order methods and we extend part of his results to second order methods.

The object of study is the difference equation

(1.1) $$y_{n+2} + \alpha_1 y_{n+1} + \alpha_0 y_n = h(\beta_2 f_{n+2} + \beta_1 f_{n+1} + \beta_0 f_n)$$

and its relation to the differential equation

$$\dot{y} = f(t, y), \quad y(0) = y_0.$$

This difference equation come from considering

$$\int_t^{t+h} \dot{y} dt = \int_t^{t+h} f(y(t), t) dt$$

and approximating both sides using various techniques. The reader should consult a good book such as Lambert's, [14], for more details.

Using standard material we must have

$$1 + \alpha_1 + \alpha_0 = 0$$

and

$$2 + \alpha_1 = \beta_2 + \beta_1 + \beta_0$$

in order to have consistency and convergence, again see [14] for details. Thus we can write the difference equation as

(1.2) $$y_{n+2} - (1 + \alpha_0) y_{n+1} + \alpha_0 y_n = h(\beta_2 f_{n+2} + \beta_1 f_{n+1} + (1 - \alpha_0 - \beta_1 - \beta_2) f_n).$$

We will be particulary interested in the case that $\beta_2 = 0$, the explicit case as opposed to the implicit case when $\beta_2 \neq 0$. Using Dahlquist's second barrier, [14] we will reduce this to a one parameter family of systems. One of the main objectives of this paper is to optimize with respect to that single parameter. This is done in Section 4.

There is a corresponding control system namely

(1.3) $$y_{n+2} - (1 + \alpha_0) y_{n+1} + \alpha_0 y_n = \beta_2 u_{n+2} + \beta_1 u_{n+1} + (1 - \alpha_0 - \beta_1 - \beta_2) u_n.$$

Note that the transfer function is

$$\frac{\beta_2 s^2 + \beta_1 s + (1 - \alpha_0 - \beta_1 - \beta_2)}{s^2 - (1 + \alpha_0) s + \alpha_0}.$$

It is never explicitly stated in the numerical literature that the transfer function should be proper but it is implicitly assumed. This has a realization of the form

$$x_{n+1} = Ax_n + bu_n, \quad y_n = cx_n + u_n$$

and the explicit case of course has a realization of the form

$$x_{n+1} = Ax_n + bu_n, \quad y_n = cx_n.$$

Applying a nonlinear feedback

$$u_n = hf_n + v_n,$$

we recover the original system when $v_n = 0$. However the goal of the feedback is not to produce a system that is asymptotically correct but one that is close to exact for the first few values of n. This approach has been recently exploited in a masterful paper by Kashima and Yamamoto, [13]. An approach using optimal control has been studied in some detail in [10, 12]. There the control v_n plays an essential role.

2. Error Analysis. The error that occurs when solving an ODE is basically of two types. There is error inherent in the method and there is accumulated roundoff error. We will characterize the inherent error in this section for linear differential equations. The error that is due to roundoff is random in nature and can be captured using time series. However, not much is known about the statistical properties of this error. Time series analysis is very much related to modern control theory. We begin by considering two first order methods, Euler explicit and the so called theta method. We will then consider the general form of the error for second order methods.

2.1. Euler Methods. We begin with the two methods

(2.1) $y_{n+1} = y_n + hf_n$ *Euler explicit*

and

(2.2) $y_{n+1} = y_n + h(\theta f_n + (1 - \theta)f_{n+1})$ *Theta method.*

We will apply these two methods to the differential equation

$$\dot{x} = \lambda x, \quad x(0) = 1.$$

2.1.1. Euler explicit. Now the error inherent in either method is given by

$$e_n = y_n - e^{\lambda h n}$$

and hence by substituting we have

$$e_{n+1} = e_n + h\lambda e_n - e^{\lambda h(n+1)} + e^{\lambda h n} + h\lambda e^{\lambda h n}$$
$$= (1 + h\lambda)e_n + (1 + h - e^{\lambda h})e^{\lambda h n}.$$

Now $e_0 = 0$ and so we have the error given neatly as a convolution.

$$e_n = \sum_{i=0}^{n-1}(1 + \lambda h - e^{\lambda h})e^{\lambda ih}(1 + \lambda h)^{n-1-i}$$

$$= (1 + \lambda h - e^{\lambda h})\sum_{i=0}^{n-1} e^{\lambda ih}(1 + \lambda h)^{n-1-i}$$

$$= (1 + \lambda h - e^{\lambda h})(1 + \lambda h)^{n-1}\sum_{i=0}^{n-1}\left(\frac{e^{\lambda h}}{1 + \lambda h}\right)^i$$

$$= (1 + \lambda h - e^{\lambda h})(1 + \lambda h)^{n-1}\frac{1 - \left(\frac{e^{\lambda h}}{1+\lambda h}\right)^n}{1 - \left(\frac{e^{\lambda h}}{1+\lambda h}\right)}$$

$$= (1 + \lambda h)^n - e^{\lambda hn}.$$

This is the accumulated error that is inherent in the Euler method. It is independent of machine error. If λ is negative then e_n tends to 0 but if λ is positive then the error approaches minus infinity since $e^{\lambda h} > 1 + \lambda h$. However the percentage error is of order nh^2.

2.1.2. Theta method. For the theta method we have

$$y_{n+1} = y_n + h\lambda(\theta y_n + (1 - \theta)y_{n+1})$$

and solving we have

$$y_{n+1} = \left(\frac{1 + \theta\lambda h}{1 - \lambda h(1 - \theta)}\right)y_n = \Lambda y_n.$$

Calculating the error we have as for Euler explicit

$$e_{n+1} = \Lambda e_n + (\Lambda - e^{\lambda h})e^{nh\lambda}\}$$

and

$$e_n = (\Lambda - e^{\lambda h})\sum_{i=0}^{n-1} e^{i\lambda h}\Lambda^{(n-1)-i}$$

$$= (\Lambda - e^{\lambda h})\Lambda^{n-1}\sum_{i=0}^{n-1}\left(\frac{e^{\lambda h}}{\Lambda}\right)^i$$

$$= (\Lambda - e^{\lambda h})\Lambda^{n-1}\frac{1 - \left(\frac{e^{\lambda h}}{\Lambda}\right)^n}{1 - \left(\frac{e^{\lambda h}}{\Lambda}\right)}$$

$$= \Lambda^n - e^{n\lambda h}.$$

This raises the possibility of choosing θ to minimize the error. We can ask for example that the error be zero. To determine if there is such a θ we simply have to solve

$$\Lambda = e^{\lambda h}.$$

TABLE 1

Optimal choices for θ

λ	-10	-5	-2	-1	1	2	5	10
θ	0.491	0.495	0.498	0.499	0.501	0.502	0.504	0.508

In Table 1 a few values are calculated using $h = .01$. These methods then closely approximate the classical trapezoid rule.

2.2. Two Step Methods. We consider the general two step method.

$$(2.3) \quad y_{n+2} - (1 + \alpha_0)y_{n+1} + \alpha_0 y_n = h(\beta_2 f_{n+2} + \beta_1 f_{n+1} + (1 - \alpha_0 - \beta_1 - \beta_2)f_n).$$

For simplicity we will assume that $\beta_2 = 0$ and we will let $1 - \alpha_0 - \beta_1 - \beta_2 = \gamma$. So we have

$$y_{n+2} - (1 + \alpha_0)y_{n+1} + \alpha_0 y_n = h(\beta_1 f_{n+1} + \gamma f_n).$$

We apply this to the differential equation $\dot{x} = \lambda x$. We then have the recurrence

$$y_{n+2} = (1 + \alpha_0 + h\lambda\beta_1)y_{n+1} + (h\lambda\gamma - \alpha_0)y_n.$$

As before we let

$$e_n = y_n - e^{\lambda h n}$$

and we then have the forced recurrence

$$(2.4) \qquad e_{n+2} = (1 + \alpha_0 + h\lambda\beta_1)e_{n+1} + (h\lambda\gamma - \alpha_0)e_n$$
$$+(-e^{2\lambda h} + (1 + \alpha_0 + h\lambda\beta_1)e^{\lambda h} + (h\lambda\gamma - \alpha_0))e^{n\lambda h}.$$

Examining the forcing term we see that we reach Dahlquist's second barrier, [14], by expanding the expression in a Taylor series and setting the first three coefficients to zero. This gives $\alpha_0 = 3 - 2\beta_1$ or as we will use later

$$(2.5) \qquad\qquad\qquad \beta_1 = \frac{1}{2}(3 - \alpha_0).$$

This gives the error as

$$e_{n+2} = (1 + \frac{3h\lambda}{2} + (1 - \frac{h\lambda}{2})\alpha_0)e_{n+1} - (\frac{h\lambda}{2} + (\frac{h\lambda}{2} + 1)\alpha_0)e_n +$$
$$\left[-e^{2\lambda h} + (1 + \frac{3h\lambda}{2} + (1 - \frac{h\lambda}{2})\alpha_0)e^{\lambda h} - (\frac{h\lambda}{2} + (\frac{h\lambda}{2} + 1)\alpha_0) \right] e^{n\lambda h}.$$

Evaluating this at $h = .01$ and $\lambda = 1$ we have

$$e_{n+2} = (1.015 - 8.375E - 08\alpha_0)e_{n+1} - (.005 + 1.005\alpha_0)e_n + (-.005 - 8.375E - 08\alpha_0)e^{.01n}.$$

This is numerically equivalent to

$$e_{n+2} = (1.015)e_{n+1} - (.005 + 1.005\alpha_0)e_n - .005e^{.01n}.$$

Writing this in matrix form we have

$$\begin{pmatrix} e_{n+1} \\ e_{n+2} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -.005 - 1.005\alpha_0 & 1.015 \end{pmatrix} \begin{pmatrix} e_n \\ e_{n+1} \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (-.005e^{.01n})$$

$$(2.6) \qquad = A\hat{e}_n + bu_n$$

and the eigenvalues of the matrix are

$$\frac{1}{2}(1.015 \pm \sqrt{.830225 - 4.02\alpha_0}).$$

At $\alpha_0 = -1$ we have eigenvalues of 1.6 and $-.59$ and so we lose stability. At $\alpha_0 = .034$ stability is regained and the system is stable for $\alpha_0 \in (.034, 1)$. Interestingly though, the eigenvalues are complex for part of this range. This is somewhat dual to the stability analysis in most of the numerical theory. There the parameter α_0 is specified and the analysis is done in terms of which values of $h\lambda$ produce stable systems, see for example [14].

The complete analysis of the second order methods is exactly the same as for first order methods. The only difference is that we have to consider the effect of mismatched initial conditions. The initial error $e_0 = 0$ but usually we have to calculate e_1. Thus there is a certain amount of error propagated via $A^n(0, e_1)^{\perp}$.

3. Switching. Consider two simple first order methods, Euler explicit and implicit, for solving $\dot{x} = x$, $x(0) = 1$. After a minimal amount of effort we have from the explicit method

$$x_n = (1 + h)^n$$

and from the implicit method

$$x_n = (1 - h)^{-n}.$$

The true solution is of course $x(t) = e^t$ and the two methods should both approximate e^{nh}. Now

$$e^{nh} = 1 + nh + \frac{1}{2}n^2h^2 + \frac{1}{6}n^3h^3 + \cdots.$$

Expanding the explicit solution we have,

$$x_n = 1 + nh + \frac{n(n-1)}{2}n^2h^2 + \cdots$$

and expanding the implicit solution we have,

$$x_n = 1 + nh + \frac{n(n+1)}{2}n^2h^2 + \cdots.$$

Comparing these solutions to e^{nh} we have

$$1 + nh + \frac{n(n-1)}{2}n^2h^2 + \cdots < e^{nh} < 1 + nh + \frac{n(n+1)}{2}n^2h^2 + \cdots .$$

so for this differential equation the explicit solution always under estimates the true solution and the implicit solution always over estimates the true solution. This suggests that by using the two methods in some alternating model we should be able to find a very accurate method. The problem with this in general is that we have no way of knowing, expect for a few very special differential equations, when we should switch between the two methods. A natural alternative is to construct all possible switching schemes and average of over all such schemes.

3.1. Euler Methods. The idea is to flip a coin at each step and use explicit if heads and implicit if tails. Because the process is scaler we have at the nth step

$$x_n = (1+h)^i(1-h)^{-(n-i)}.$$

Let $C_{n,i} = \frac{n!}{i!(n-i)!}$ the combinatorial symbol. There were $C_{n,i}$ different ways we could have arrived at this x_n. Then averaging over all possible switching patterns we have

$$
\begin{align}
(3.1) \qquad x_n^{avg} &= \frac{1}{2^n}\sum_{i=0}^{n} C_{n,i}(1+h)^i(1-h)^{-(n-i)} \\
(3.2) \qquad &= \frac{1}{2^n}(1 + h + (1-h)^{-1})^n \\
(3.3) \qquad &= \left(\frac{(1+h) + (1-h)^{-1}}{2}\right)^n \\
(3.4) \qquad &= \left(\frac{2 - h^2}{2(1-h)}\right)^n .
\end{align}
$$

Expanding this as a Taylor series we have

$$x_n^{avg} = 1 + nh + \frac{1}{2}n^2h^2 + \cdots .$$

From this we see that $e^{nh} - x_n^{avg} = O(h^3)$ as compared to order h^2 approximation for both the explicit and implicit methods. So the average is a much better approximation than either the implicit or the explicit.

It is worth while to calculate more than the average value for we would like to know how much spread we can expect if we calculate several but not all switching

Method	h	Eigenvalue	Approx. to e
Euler-explicit	.1	1.1	-0.124539368
	.01	1.01	-0.013467999
	.001	1.001	-0.001357896
Euler-implicit	.1	1.111111	0.149690162
	.01	1.01010101	0.013717198
	.001	1.001001001	0.001360388
Switched	.1	1.105555556	0.009475386
	.01	1.010050505	9.09562E-05
	.001	1.001000501	9.06434E-07

patterns and average numerically. The variance of course is a good measure of spread.

$$
\begin{aligned}
x_n^{var} &= \frac{1}{2^n} \sum_{i=0}^{n} C_{n,i} (1+h)^{2i} (1-h)^{-2(n-i)} - (x_n^{avg})^2 \\
&= \frac{1}{2^n} \left((1+h)^2 + (1-h)^{-2} \right)^n - (x_n^{avg})^2 \\
&= \left(\frac{(1+h)^2 + (1-h)^{-2}}{2} \right)^n - \left(\frac{(1+h) + (1-h)^{-1}}{2} \right)^{2n} \\
&= (1 + 2h + 2h^2 + 2h^3 + 5h^4 + \cdots)^n - (1 + 2h + 2h^2 + 2h^3 + \frac{5}{4}h^4 + \cdots)^n
\end{aligned}
$$

$$
(3.5) \quad = O(h^4).
$$

It is interesting that this is independent of n. The variance is very small so this suggests that it is feasible to numerically calculate several different switching regimes and average them as a good approximation of the average of all of the means. Of course the central limit theorem guarantees the convergence but it says very little directly about the spread. In Table 2 we show the level of approximation obtained by each method. Note that the switching method is two orders of magnitude better than either the Euler implicit or explicit.

These calculations were done with the differential equation $\dot{x} = x$ but the conclusions would have been the same for $\dot{x} = \lambda x$. In the formulas we would have replaced h with λh.

3.2. Higher order methods. We consider here the problem of switching between two higher order methods. Part of the first order method material generalizes quite nicely. As we saw in the introduction we can write a linear method applied to a first order linear differential equation in the form $x_{n+1} = Ax_n$. Now suppose we have two methods of the same order, the second being $x_{n+1} = Bx_n$. We have initial value

x_0. The switching system can be written in the form

$$x_{n+1} = (\delta_n A + (1 - \delta_n)B)x_n$$

where $\delta_n \in \{0, 1\}$. Thus we have

$$x_n = (\delta_{n-1}B + (1 - \delta_{n-1})A) \cdots (\delta_0 B + (1 - \delta_0)A)x_0.$$

Let

$$S_\delta^n = (\delta_{n-1}B + (1 - \delta_{n-1})A) \cdots (\delta_0 B + (1 - \delta_0)A).$$

Now let

$$S^n = \frac{1}{2^n} \sum_{\delta \in 2^n} S_\delta^n.$$

We use the notation $\delta \in 2^n$ to indicate that δ is a mapping from $\{i : i = 0, \cdots, n-1\}$ to $2 = \{0, 1\}$. S^n is the average taken over all possible switching patterns.

Now we can write the following.

(3.6) $$\{S_\delta^n : \delta \in 2^n\} = \{AS_\delta^{n-1} : \delta \in 2^{n-1}\} \cup \{BS_\delta^{n-1} : \delta \in 2^{n-1}\}.$$

From this we have

$$S^n = \frac{1}{2^n} \sum_{\delta \in 2^n} S_\delta^n$$

$$= \frac{1}{2} \left(\frac{1}{2^{n-1}} \sum_{\delta \in 2^{n-1}} AS_\delta^{n-1} + \frac{1}{2^{n-1}} \sum_{\delta \in 2^{n-1}} BS_\delta^{n-1} \right)$$

(3.7) $$= \frac{1}{2}(A + B)S^{n-1},$$

the next theorem then follows immediately.

THEOREM 3.1. *Let* $x_{n+1} = (\delta_n A + (1 - \delta_n)B)x_n$, $x_n^\delta = (\delta_{n-1}B + (1 - \delta_{n-1})A) \cdots$ $(\delta_0 B + (1 - \delta_0)A)x_0$ *and let*

$$x_n^{avg} = \frac{1}{2^n} \sum_{\delta \in 2^n} x_n^\delta.$$

Then $x_n^{avg} x_0$ *is the solution of the equation*

$$x_{n+1} = \frac{A + B}{2} x_n, \quad x_0 \text{ given.}$$

Using these techniques we can also calculate the covariance of the x_n^δ. We have

$$\text{covariance}(x_n^\delta) = \frac{1}{2^n} \sum_{\delta \in 2^n} (x_n^\delta - x_n^{avg})^\perp (x_n^\delta - x_n^a vg)$$

$$= \frac{1}{2^n} \sum_{\delta \in 2^n} (x_n^\delta)^\perp x_n^\delta - (x_n^{avg})^\perp x_n^{avg}.$$

We now concentrate on the sum. Here C_n is the covariance of the erro at time step n.

$$\begin{aligned}
x_0^{\perp} C_n x_0 &= \frac{1}{2^n} \sum_{\delta \in 2^n} (x_n^{\delta})^{\perp} x_n^{\delta} \\
&= \frac{1}{2^n} \sum_{\delta \in 2^n} (S_n^{\delta} x_0)^{\perp} S_n^{\delta} x_0 \\
&= \frac{1}{2} x_0^{\perp} \left(\frac{1}{2^{n-1}} \sum_{\delta \in 2^{n-1}} A^{\perp} (S_{n-1}^{\delta})^{\perp} S_{n-1}^{\delta} A + \right. \\
&\qquad \left. \frac{1}{2^{n-1}} \sum_{\delta \in 2^{n-1}} B^{\perp} (S_{n-1}^{\delta})^{\perp} S_{n-1}^{\delta} B \right) x_0
\end{aligned}$$

(3.8)
$$= x_0^{\perp} \frac{1}{2} \left(A^{\perp} C_{n-1} A + B^{\perp} C_{n-1} B \right) x_0.$$

Thus both the average and the covariance are generated by linear difference equations.

3.3. An example.   We consider here two standard 2nd order methods–the Adams-Bashforth and the Adams-Moulton methods.

(3.9)
$$y_{n+1} - y_n = \frac{h}{2}(3f_n - f_{n-1}) \quad Adams - Bashforth,$$

(3.10)
$$y_{n+1} - y_n = \frac{h}{12}(5f_{n+1} + 8f_n - f_{n-1}) \quad Adams - Moulton.$$

Following the first order example we will solve $\dot{y} = y \quad y(0) = 1$. Thus we have

$$y_{n+1} - y_n = \frac{h}{2}(3y_n - y_{n-1})$$

and

$$y_{n+1} - y_n = \frac{h}{12}(5y_{n+1} + 8y_n - y_{n-1}).$$

Rewriting these in matrix form we have

(3.11)
$$\begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{h}{2} & \frac{2+3h}{2} \end{pmatrix} \begin{pmatrix} y_n \\ y_{n+1} \end{pmatrix},$$

(3.12)
$$\begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{h}{12-5h} & \frac{12+8h}{12-5h} \end{pmatrix} \begin{pmatrix} y_n \\ y_{n+1} \end{pmatrix}.$$

For the average we have

(3.13)
$$\begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \frac{5h^2-14h}{48-20h} & \frac{-15h^2+42h+48}{48-20h} \end{pmatrix} \begin{pmatrix} y_n \\ y_{n+1} \end{pmatrix}.$$

Evaluating at various values of h we get Table 3. We now consider the covariance.

TABLE 3
Values for Adams Methods

Method	h	Max. eigenvalue	Min. eigenvalue	Approx. to e
Adams-Bashforth	.1	1.104740503	0.045259497	-0.01056798
	.01	1.010049749	0.004950251	-0.000112573
	.001	1.0010005	0.0004995	-1.13194E-06
Adams-Moulton	.1	1.105175358	0.00786812	0.000109217
	.01	1.010050168	0.000828494	1.12847E-07
	.001	1.0010005	8.32847E-05	1.13618E-10
Switched	.1	1.1049617	0.026560039	-0.005141555
	.01	1.010049959	0.002889372	-5.61153E-05
	.001	1.0010005	0.000291392	-5.65794E-07

We calculate the properties of the linear operator defined by

$$L(X) = A^{\perp}XA + B^{\perp}XB$$

where X is a symmetric 2×2 matrix and A and B are in companion form. We begin by calculating

$$\begin{pmatrix} 0 & a \\ 1 & b \end{pmatrix} \begin{pmatrix} x & y \\ y & z \end{pmatrix} \begin{pmatrix} 0 & 1 \\ a & b \end{pmatrix} = \begin{pmatrix} 0 & a \\ 1 & b \end{pmatrix} \begin{pmatrix} ay & x+yb \\ az & y+zb \end{pmatrix}$$

$$= \begin{pmatrix} a^2z & ay+abz \\ ay+abz & x+2by+b^2z \end{pmatrix}.$$

Vectorizing this we have

$$L(X) = \begin{pmatrix} a^2 & 0 & 0 \\ ab & a & 0 \\ b^2 & 2b & 1 \end{pmatrix} \begin{pmatrix} z \\ y \\ x \end{pmatrix}$$

and thus for Adam-Bashforth we have

$$AB(X) = \begin{pmatrix} (\frac{h}{2})^2 & 0 & 0 \\ -\frac{2h+3h^2}{4} & -\frac{h}{2} & 0 \\ (\frac{2+3h}{2})^2 & \frac{4+6h}{2} & 1 \end{pmatrix} \begin{pmatrix} z \\ y \\ x \end{pmatrix}$$

and for Adams-Moulton we have

$$AM(X) = \begin{pmatrix} (\frac{h}{12-5h})^2 & 0 & 0 \\ -\frac{12h+8h^2}{(12-5h)^2} & -\frac{h}{12-5h} & 0 \\ (\frac{12+8h}{12-5h})^2 & \frac{24+16h}{12-5h} & 1 \end{pmatrix} \begin{pmatrix} z \\ y \\ x \end{pmatrix}.$$

We then have the sum

$$\frac{1}{2}(AM + AB)(X) = \begin{pmatrix} \frac{1}{2}(\frac{h}{2})^2 + \frac{1}{2}(\frac{h}{12-5h})^2 & 0 & 0 \\ -\frac{1}{2}\frac{2h+3h^2}{4} - \frac{1}{2}\frac{12h+8h^2}{(12-5h)^2} & -\frac{1}{2}\frac{h}{2} - \frac{1}{2}\frac{h}{12-5h} & 0 \\ \frac{1}{2}(\frac{2+3h}{2})^2 + \frac{1}{2}(\frac{12+8h}{12-5h})^2 & \frac{1}{2}\frac{4+6h}{2} + \frac{1}{2}\frac{24+16h}{12-5h} & 1 \end{pmatrix} \begin{pmatrix} z \\ y \\ x \end{pmatrix}.$$

Switching systems play an important role in modern system theory. there is a large literature on the stability of switching systems, [3], but this set of literature is not particulary relevant to the development of this paper. In systems theory stability is an asymptotic phenomena and for ODEs we are only interested in the first few values of n. There is a literature concerned with the controllability of switched systems and this theory will probably eventually be relevant. However both the theory of switched systems from control theory and from ODEs need refinement before they can be merged. The theory of random products of matrices seems to be quite relevant. The paper of Wang and Martin, [15], is developing the theory in this direction.

4. Two Major Examples. We consider two major examples. The first is a second order time varying differential equation. The theory of second order time varying differential equation is vastly complex. It contains the bulk of the theory of special functions. See for example Watson's *A Treatise on the Theory of Bessel Functions* , [16]. The second example is the scalar Riccati equation. Riccati equations are also closely related to second order linear differential equations. We exploit the theory of second order equations to study the numerical solutions of this equation.

4.1. A Second Order Differential Equation. The differential equation, $(x - a)^2(x - b)^2y'' = cy$, is very interesting due to several factors. The first things that can be noticed are the singularities in the independent variable, x. This gives rise to challenges in finding a numerical solution as well as in computing the exact solution. The nonlinearity and symmetry of the differential equation is another interesting feature. Still, except at the discontinuities at $x = a$ and $x = b$, the system is fairly well behaved. It is possible to notice that the equation, when written as a system, is Lipschitz in any finite interval which does not include the singularities.

Further more, depending on the parameters a, b and c, the solution of the equation can take different forms. The exact solutions are found via substitutions given in [17], for $a \neq b$, and in [18], for $a = b$.

4.2. The Exact Solution.

4.2.1. For $a \neq b$. The given equation: $(x - a)^2(x - b)^2y'' = cy$, can be exactly solved following the variable transformations given in [17], for $a \neq b$. The transformation prescribed is:

$$\xi = \ln\left|\frac{x - a}{x - b}\right|, \quad y = (x - b)\eta.$$

Above transformation will convert the original differential equation to a second order constant coefficient differential equation of the following form:

$$(a-b)^2 \left(\frac{d^2\eta}{d\xi^2} - \frac{d\eta}{d\xi} \right) = c\eta.$$

We may now write this as $(a-b)^2\eta''_{\xi\xi} - (a-b)^2\eta'_\xi - c\eta = 0$. This is nothing more than a second order differential equation with constant coefficients. For this we can write the auxiliary equation: $(a-b)^2 m^2 - (a-b)^2 m - c = 0$. Such m will produce the solution to the above equation.

On solving for m:

$$m = \frac{(a-b)^2 \pm \sqrt{(a-b)^4 + 4c(a-b)^2}}{2(a-b)^2}.$$

Set $\lambda^2 = 1 + \frac{4c}{(a-b)^2}$, then,

$$m = \frac{1 \pm \lambda}{2}.$$

With this, we can identify three classes of solutions for $\lambda^2 > 0$, $\lambda^2 = 0$ and $\lambda^2 < 0$.

4.2.2. When $\lambda^2 > 0$ or $\lambda^2 < 0$ (i.e. $\lambda^2 \neq 0$). After considerable calculation
When $\lambda^2 > 0$:

$$y = \sqrt{|(x-a)(x-b)|} \left(C_1 \left| \frac{x-a}{x-b} \right|^{\lambda/2} + C_2 \left| \frac{x-b}{x-a} \right|^{\lambda/2} \right).$$

When $\lambda^2 < 0$:

$$y = \sqrt{|(x-a)(x-b)|} \left(C_c \cos \left(\frac{\Im(\lambda)}{2} \ln \left| \frac{x-a}{x-b} \right| \right) + C_s \sin \left(\frac{\Im(\lambda)}{2} \ln \left| \frac{x-a}{x-b} \right| \right) \right)$$

where $C_s = C_1 + C_2$, $C_s = i(C_1 - C_2)$ and $\Im(\lambda)$ is the imaginary part of λ. Since λ is purely imaginary, it should be noted that $\lambda = i\Im(\lambda)$.

4.2.3. When $\lambda^2 = 0$.

$$y = \sqrt{|(x-a)(x-b)|} \left(C_1 + C_2 \ln \left| \frac{x-a}{x-b} \right| \right).$$

4.2.4. For $a = b$. When $a = b$ the equation becomes $(x-a)^4 y'' = cy$ and the above technique will fail. Instead, the following substitutions can be used as in [18]:

$$\xi = \frac{1}{(x-a)}, \quad \eta = \frac{y}{x-a} = y\xi.$$

This means after significant computation,

$$\frac{d^2\eta}{d\xi^2} = cy\xi = c\eta.$$

We can write this equation as $\eta''_{\xi\xi} - c\eta = 0$.

Here again we can analyze different cases depending on the value of c.

4.2.5. When $c = 0$.

$$y = C_1(x - a) + C_2.$$

4.2.6. When $c > 0$. Then we get $\eta = C_1 \cosh(\xi) + C_2 \sinh(\xi)$. Therefore, we get the solution

$$y = (x - a) \left(C_1 \cosh \left(\frac{1}{(x - a)} \right) + C_2 \sinh \left(\frac{1}{(x - a)} \right) \right).$$

4.2.7. When $c < 0$. Then we get $\eta = C_1 \cos(\xi) + C_2 \sin(\xi)$ Therefore, we get the solution

$$y = (x - a) \left(C_1 \cos \left(\frac{1}{(x - a)} \right) + C_2 \sin \left(\frac{1}{(x - a)} \right) \right).$$

4.3. Association of Initial Conditions. In general, solving for the exact solution, incorporating the initial conditions in x and y, into the above solutions does not give a very clean result. It is quite messy and does not end up with a nice answer for most cases. Therefore, we shall employ an indirect method of incorporating the initial conditions by assuming a "nice" choice for x.

$x = a$ or for that matter, $x = b$ "seems" to be "nice" for initial conditions, but those are the exact locations where the discontinuities occur. Therefore, those locations have to be ruled out. The next "good" initial point is $x = 0$. We will try to solve the initial value problem, IVP, for initial conditions specified at this point in terms of x and y, transform them to the initial conditions in terms of ξ and η, solve the IVP, for ξ and η, re-transform to the IVP of $x = 0$ and y and finally generalize the result to an arbitrary initial conditions of x and y, in particular to any arbitrary x.

We pick $x = 0$, $y(x)|_{x=0} = y_0$ and $y'(x)|_{x=0} = y_0'$. Then we have, for $a \neq b$:

$$\xi_0 = \xi|_{x=0} = \ln \left| \frac{a}{b} \right|, \quad \text{and} \quad \eta_0 = \eta|_{x=0} = -\frac{y_0}{b}.$$

Furthermore

$$\frac{dy}{dx} \bigg|_{x=0} = \frac{(a - b)}{(0 - a)} \frac{d\eta}{d\xi} \bigg|_{x=0} + \eta_0,$$

$$\frac{d\eta}{d\xi} \bigg|_{x=0} = \frac{-a}{(a - b)} \left(\frac{y_0}{b} + y_0' \right) = \eta_0'.$$

For $a = b$, similarly for $x = 0$ we see that, $\xi_0 = -1/a$, $\eta_0 = -y_0/a$, and $\eta_0' = a \left(\frac{y_0}{a} + y_0' \right)$.

Now we shall analyze how this is done for each case.

For $\lambda^2 = 1 + \frac{4c}{(a-b)^2} \neq 0$, we had

$$\eta = C_1 e^{\xi(1+\lambda)/2} + C_2 e^{\xi(1-\lambda)/2}.$$

On matching the initial conditions at $\xi = \xi_0$, $\eta(\xi_0) = \eta_0$ and $\eta'(\xi_0) = \eta'_0$,

$$\eta_0 = C_1 e^{\xi_0(1+\lambda)/2} + C_2 e^{\xi_0(1-\lambda)/2},$$

$$\eta'_0 = C_1 \frac{(1+\lambda)}{2} e^{\xi_0(1+\lambda)/2} + C_2 \frac{(1-\lambda)}{2} e^{\xi_0(1-\lambda)/2}.$$

By setting $D_1 = C_1 e^{\xi_0/2}$ and $D_2 = C_2 e^{\xi_0/2}$ they become

$$\eta_0 = D_1 e^{\xi_0\lambda/2} + D_2 e^{-\xi_0\lambda/2},$$

$$\eta'_0 = D_1 \frac{(1+\lambda)}{2} e^{\xi_0\lambda/2} + D_2 \frac{(1-\lambda)}{2} e^{-\xi_0\lambda/2}.$$

Look at the last of the above two equations:

$$\eta'_0 = D_1 \frac{(1+\lambda)}{2} e^{\xi_0\lambda/2} + D_2 \frac{(1-\lambda)}{2} e^{-\xi_0\lambda/2},$$

$$2\eta'_0 = D_1(1+\lambda)e^{\xi_0\lambda/2} + D_2(1-\lambda)e^{-\xi_0\lambda/2}$$

$$= \left(D_1 e^{\xi_0\lambda/2} + D_2 e^{-\xi_0\lambda/2} \right) + \lambda \left(D_1 + e^{\xi_0\lambda/2} - D_2 e^{-\xi_0\lambda/2} \right)$$

$$= \eta_0 + \lambda \left(D_1 + e^{\xi_0\lambda/2} - D_2 e^{-\xi_0\lambda/2} \right).$$

Eventually, we have to solve the two equations:

$$\eta_0 = D_1 e^{\xi_0\lambda/2} + D_2 e^{-\xi_0\lambda/2},$$

$$\frac{2\eta'_0 - \eta_0}{\lambda} = D_1 e^{\xi_0\lambda/2} - D_2 e^{-\xi_0\lambda/2}.$$

This yields,

$$D_1 = \frac{2\eta'_0 - (1-\lambda)\eta_0}{2\lambda} e^{-\xi_0\lambda/2},$$

$$D_2 = \frac{-2\eta'_0 + (1+\lambda)\eta_0}{2\lambda} e^{\xi_0\lambda/2}.$$

Hence for the required C_1 and C_2

$$C_1 = \frac{2\eta'_0 - (1-\lambda)\eta_0}{2\lambda} e^{-\xi_0(\lambda+1)/2},$$

$$C_2 = \frac{-2\eta'_0 + (1+\lambda)\eta_0}{2\lambda} e^{-\xi_0(1-\lambda)/2}.$$

The initial conditions can be associated to the other cases in a similar manner, but to write them down for all the cases is quite tedious and hence will be omitted.

4.4. Nature of Solutions and Other Considerations. As it was explained in the previous sections, the solution to the differential equation can have one of six possible different solutions. To complicate the matters further, the initial conditions associate to the solutions in quite an obscure manner, making the initial value problem non-trivial to solve. Furthermore, there could be two second order (when $a \neq b$) or one fourth order (when $a = b$) singularities on the x-axis. Therefore, it is very interesting to see how the solutions of the IVP behaves under different parameter values as well as initial conditions.

This could be done by means of a phase diagram, with y and y' defined as the states. Let $y_1 = y(x)$ and $y_2 = y(x)'$. Then we have the following system.

$$y_1' = y_2,$$
$$y_2' = \frac{cy_1}{(x-a)^2(x-b)^2}.$$

Since there is a multitude of cases to analyze, a computational software tool can be used to develop a good intuition of the system, despite the fact that numerical software tools only provide an approximation. For this paper, MATLAB was used to find the numerical solutions. It should be understood that MATLAB, as any other numerical method, can solve only within an interval which does not include a singularity. Therefore, the time interval on which the simulation should be run, has to selected so that no singularities are included.

4.5. Optimization Problem.

4.5.1. A Complete Parameterization of Two Step Methods. The two step method in 2.3, can be completely parameterized for the optimization problem for an explicit method by setting $\beta_2 = 0$ and 2.5. Hence we can completely characterize all the second order two step methods by a single parameter, α_0.

For the implicit methods we can use the same Taylor Series method used to find 2.5 using 2.3. But this time it is easier to work on 1.1, and parameterize the entire class of implicit second order two step methods by the parameters α_0 and β_0 as follows.

$$(4.1) \qquad\qquad\qquad a_1 = -1 - a_0,$$

$$(4.2) \qquad\qquad\qquad b_1 = (1 - 3a_0 - 4b_0)/2,$$

$$(4.3) \qquad\qquad\qquad b_2 = (1 + a_0 + 2b_0)/2.$$

The implicit method has to be implemented as a predictor-corrector pair. In this implementation, we can use a explicit two-step second-order method method as the predictor. Hence we end up with a three parameter family for the implementation. The additional parameter is inherited due to the 'α_0' of the predictor. To reduce the burden on computation time, we may use the same $alpha_0$ for both and simplify the optimization problem to a two parameter problem.

To inspect the stability, look at the left hand side of the difference equation: $y_{j+2} + a_1 y_{j+1} + a_0 y_j$. We need the auxiliary equation $z^2 + a_1 z + a_0 = 0$ to have solutions $|z| \leq 1$ if the solutions for z are distinct, if not, we need $|z| < 1$.

By substituting the values of a_1 we see that the auxiliary equation becomes, $z^2 - (1 + a_0)z + a_0 = 0$. This gives

$$z = \frac{(1 + a_0) \pm \sqrt{(1 + a_0)^2 - 4a_0}}{2},$$

$$z = \frac{(1 + a_0) \pm (1 - a_0)}{2},$$

$$z = 1, \quad \text{or} \quad a_0.$$

Hence, for stability we need, $|a_0| \leq 1$ but $a_0 \neq 1$.

These steps completes the parameterization of the numerical methods of interest using a least number of parameters and gives their applicable ranges. The two-step second-order explicit methods were parameterized with a single a_0, $|a_0| \leq 1, a_0 \neq 1$ parameter and all such implicit methods were parameterized with two parameters, a_0 and b_0, $|a_0| \leq 1, a_0 \neq 1$ no restrictions had been yet set on b_0.

4.5.2. Minimizing Error. One of the main goals of this paper is to develop, or to be more precise, "tailor", a numerical method to solve the given differential equation.

A heuristic approach is employed for the optimization process. The error is quantified using the $L^2 - norm$ and the $\infty - norm$ of the difference between the computed solution and the exact solution. A specific case with parameter values, $a = 12$, $b = 14$, and $c = -100$ was picked and it was numerically solved in the interval $[0, 10]$ with initial conditions $y(0) = 1$ and $y'(0) = 1$.

For the above choice of equation, with $a_0 \approx .333766$ the explicit method gives the minimum error in the $L^2 - norm$. Figure 1 shows the actual variation of the error with α_0 for it and Figure 2 shows the numerical solution in relation to the exact solution. Figure 3 shows the variation of the error for the 2-parameter implicit method.

4.6. The Riccati Equation. Here we consider the Riccati equation $\dot{y} = 1 + y^2$, $y(0) = 0$. Simple integration shows that the solution of the equation is $y(x) = \tan x$. The Riccati equation is intimately related to the linear initial value problem

$$\begin{pmatrix} \dot{z} \\ \dot{w} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} z \\ w \end{pmatrix} \quad \begin{pmatrix} z(0) \\ w(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Interestingly this correspondence is almost as old as the calculus. The relationship was discussed in correspondence between Leibnitz and Bernoulli in 1697 and the reduction to a linear equation was accomplished in 1702, [16].

The solution of the linear equation is bounded and it would be desirable for the numerical solution to likewise be bounded. We first consider the Theta method.
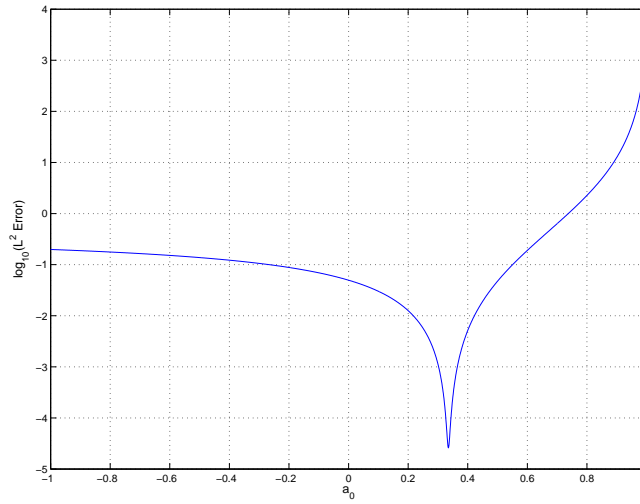
FIG. 1. *Logarihtmetic error pattern for* $(x-12)^2(x-14)^2 y'' = -100y$ *with variation at* α_0.
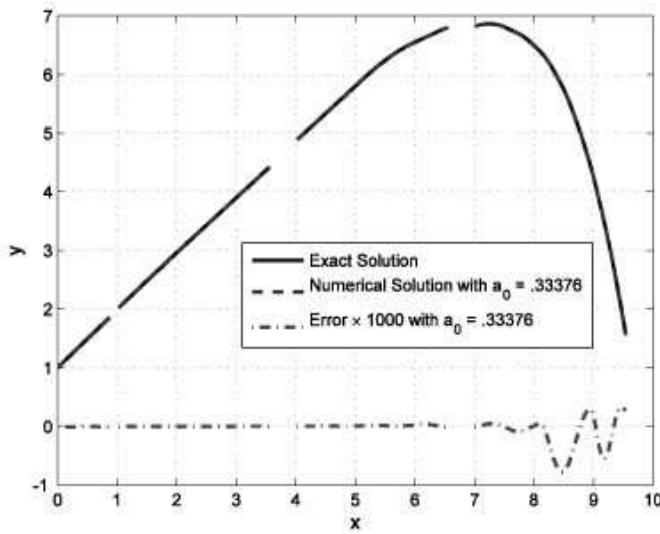

FIG. 2. *Solution and error pattern for* $(x-12)^2(x-14)^2 y'' = -100y$.

Applying the Theta method we obtain after a few calculations

$$
(4.4) \qquad \begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = \begin{pmatrix} \frac{1-\theta(1-\theta)h^2}{1+(1-\theta)^2 h^2} & \frac{h}{1+(1-\theta)^2 h^2} \\ \frac{-h}{1+(1-\theta)^2 h^2} & \frac{1-\theta(1-\theta)h^2}{1+(1-\theta)^2 h^2} \end{pmatrix} \begin{pmatrix} y_n \\ y_{n+1} \end{pmatrix}.
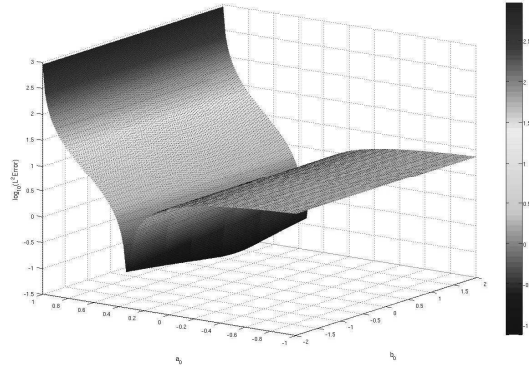$$

FIG. 3. *Logarihtmetic error pattern for* $(x-12)^2(x-14)^2 y'' = -100y$

The eigenvalues of the matrix are

$$\frac{1 - \theta(1-\theta)h^2}{1 + (1-\theta)^2 h^2} \pm \frac{hi}{1 + (1-\theta)^2 h^2}$$

and for the iteration to be bounded we must have

$$\left(\frac{1 - \theta(1-\theta)h^2}{1 + (1-\theta)^2 h^2}\right)^2 + \left(\frac{h}{1 + (1-\theta)^2 h^2}\right)^2 \le 1.$$

For $\theta = 0$ the inequality is satisfied and for $\theta = 1/2$ the expression is equal to 1 and so for $\theta \in [0, 1/2)$ the numerical solution is bounded. This give hope that second order methods may give good results.

On varying the parameter a_0, which determines all the constants of the method, between -1 and 1, we find that the error, defined as (exact solution - numerical solution) does not change sign (i.e. it is always positive). This can be clearly seen from figures 4 and 5. The solution with the least error was observed when $a_0 = -1$. This is actually the mid point method:

$$y_{j+2} = y_j + 2hf(x_{j+1}, y_{j+1}).$$

In order to find two methods that gives similar positive and negative error, the second order constraint had to be sacrificed. Meaning that, in order to find two such methods, it was necessary to employ two first order methods instead of second order methods.
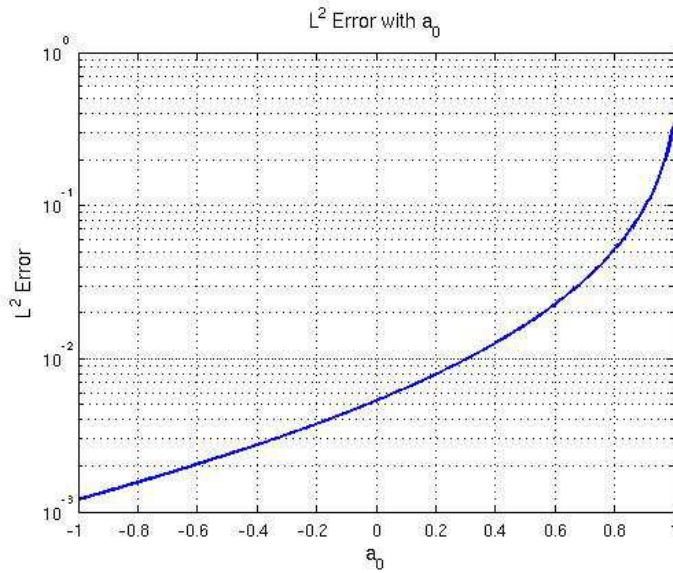
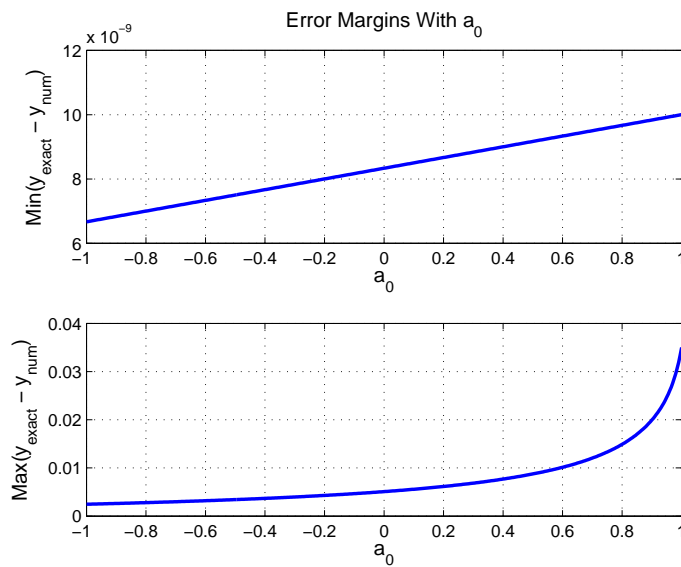FIG. 4. L^2 error for the Riccati equation $\dot{y} = 1 = y^2$ with variation at α_0.

FIG. 5. Error pattern for the Riccati equation $\dot{y} = 1 + y^2$ with variation at α_0

First order methods were found by relaxing the condition on b_0. In other words, the first order methods were constructed as to be $b_0 \neq -(1 + a_0)/2$. As such, for both methods $a_0 = -1$ was used with $b_0 = -.3$ for the first method $b_0 = .3$ for the second. The equation was solved by randomly switching between the two methods each step. By repeating this several times, it was observed that the distribution of

error was approximately normal.

Since there were no applicable explicit two step second order methods, two step implicit methods were considered. Referring to the general two step method, the following relations can be found in order to satisfy the consistency and order with an analysis identical to the case of explicit method.

On further analysis, two second order implicit two step methods were found which gives positive and negative error. Rather surprisingly, it was observed that the two methods had extremely close error values in absolute value. The method with $a_0 = -1$ and $b_0 = -1$ gives the positive error where as the method with $a_0 = .3$ and $b_0 = .28$ gives the negative error.

That is, for positive error, the pair:

$$y_{j+2} = y_j + 2hf(x_{j+1}, y_{j+1}) \quad : \quad Predictor$$
$$y_{j+2} = y_j + 2h(-f(x_{j+2}, y_{j+2}) + 4f(x_{j+1}, y_{j+1}) - f(x_j, y_j)) \quad : \quad Corrector$$

For the negative error, the pair:

$$y_{j+2} = -.3y_j + 1.3y_{j+1} + h(1.35f(x_{j+1}, y_{j+1}) - .65f(x_j, y_j)) \quad : \quad Predictor$$
$$y_{j+2} = -.3y_j + 1.3y_{j+1} + h(.93f(x_{j+2}, y_{j+2}) - 1.02f(x_{j+1}, y_{j+1}) + .28f(x_j, y_j))$$
$$Corrector$$

5. Conclusion. This paper provides a broad discussion on the entire class of linear second order multi-point methods. We characterize, as a three parameter family, those methods with good numerical properties. We also examine the error analysis of the class of second order methods and discuss in some detail the statistics of switching between two methods. We provide a closed form expression for the average value obtained by switching and construct the covariance matrix. Two examples are done in some detail, to emphasize the notion of 'tailoring' numerical methods to solve differential equations.

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