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Integrating ODE's in the Complex Plane–Pole Vaulting

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Abstract. Most existing algorithms for solving initial value problems in ordinary differential equations implicitly assume that all variables are real. If the real-valued assumption is removed, the solution can be extended by analytic continuation along a path of integration in the complex plane of the independent variable. This path is chosen to avoid singularities which can make the solution difficult or impossible for standard methods. We restrict our attention to Taylor series methods, although other methods can be suitably modified. Numerical examples are given for (a) singularities on the real axis, (b) singularities in derivatives higher than those involved in the differential equation, and (c) singularities near the real axis. These examples show that the pole vaulting method merits further study for some special problems for which it is competitive with standard methods.

1. Introduction. Nearly all existing numerical methods for solving initial value problems in ordinary differential equations implicitly assume that all variables are real. Normally the ability to integrate along a path in the complex plane is only of academic interest because most problems are known to have real solutions. When complex-valued solutions are needed, the real and imaginary parts are usually computed separately. In many problems, though, the computation of the solution is hampered by the presence of singularities

(a) on the real axis, e.g. (Painlevé equation)

$$y'' = 6y^2 + x, \quad y(0) = 1, \quad y'(0) = 0;$$

(b) in derivatives higher than those which appear in the differential equation, e.g.

$$y' = (5/3)y/x, \quad y(-1) = -1, \quad y(x) = x^{5/3}; \qquad \text{or}$$

(c) near the real axis, e.g.

$$y' = -2xy^2, \quad y(-10) = 1/101, \quad y(x) = 1/(1 + x^2).$$

The technique of "pole vaulting" extends the solution to the ordinary differential equation by analytic continuation into the complex plane along a path which avoids the troublesome singularity as shown in Figure 1. The classical theory of ordinary differential equations can be given in the context of complex variables [4].

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We consider the ordinary differential equation (or system)

$$y' = f(x, y), \quad y(x_0) = y_0,$$

where both x and y may be complex. We give some of the possible applications of the pole vaulting approach and indicate its promise.

2. Analytic Continuation of Solutions to ODE's. The technique of analytic continuation is well known in complex analysis. An analytic function is uniquely determined by its values on any set with a limit point interior to the domain of analyticity, but the problem of determining a function f in a region from its values in a subset of the region is an ill-posed problem. Miller [6] shows that an arbitrarily small error in the data can introduce an arbitrarily large error in f at other points.

Analytic continuation is usually done by expanding f in a Taylor series about a point interior to the domain of analyticity and rearranging the series. Henrici [5, p. 170] shows that using this approach for numerical analytical continuation, by using a truncated Taylor series, is a divergent process unless the series is shortened at each stage by a fixed reduction factor. However, if an expression for computing successive derivatives can be found, the divergence discussed by Henrici is no longer present. This is precisely the setting for the numerical solution to initial value problems in ordinary differential equations. Standard methods are constructed to agree with the first few terms of the Taylor series for the solution, so they can be viewed as using derivatives computed (usually indirectly) from the differential equation to analytically continue the solution away from the initial point. The problems considered in [5] and [6] then appear as the familiar problems of convergence and stability which have been well studied.

This view of numerical ODE solvers as methods for analytic continuation adds nothing to our understanding as long as the independent variable x is real. If x is complex, this view helps to account for the behavior of the solution observed near poles, branch points, and essential singularities. For example, if the path of integration circles a branch point, the computed solution may appear on a different sheet of the Riemann surface from the desired solution.

The technique of pole vaulting may be implemented using any standard numerical method. Taylor series or Runge-Kutta type methods require no essential modifications to be able to step in any direction in the complex plane, although some changes may be necessary in coding and fine tuning. Multistep methods are more difficult to convert because the direction, if not the size, of the step must be changed constantly.

An implementation based on long Taylor series [1], [7] was chosen for the examples in this paper because of the ease and accuracy with which an optimal stepsize could be determined. Chang's Automatic Taylor Series (ATS) translator [1] was used to produce a FORTRAN code for generating the first 30 terms of the Taylor series for the solution. This code was converted into a complex implementation which used the three-term test [2] to determine the location and order of the singularity closest to the point of expansion at each step. The length of each step of the analytic continuation along a prescribed path was taken as large as possible consistent with error control demands. Thus much smaller steps were taken near a singularity. Computations were done on a Xerox Sigma 9 computer in single-precision complex arithmetic.

The three-term test was developed to estimate the location and order of a single primary singularity by comparing the series for the solution to the series for the model problem

$$v(z;\, a,\, s) = (a - z)^{-s}, \qquad s \neq 0, -1, \ldots .$$

THEOREM [2]. *Let $\Sigma_{i=1}^{\infty} a_i$ be a nonzero series such that*

$$\lim_{i\to\infty}\left[i\,\frac{a_{i+1}}{a_i} - (i-1)\,\frac{a_i}{a_{i-1}}\right]$$

exists and equals L. Then

(i) *if $|L| < 1$, Σa_i is absolutely convergent,*

(ii) *if $|L| = 1$, the test fails, and*

(iii) *if $|L| > 1$, Σa_i diverges.*

Let g be an analytic function, $a_{i+1} := g^{(i)}(x_0)h^i/i!$ (where $h := x - x_0$), and $R_i := ia_{i+1}/a_i$. Then we can estimate the radius of convergence from

$$h/R_c \approx R_i - R_{i-1}, \tag{1}$$

and the order of the primary singularity by

$$s \approx R_i/(R_i - R_{i-1}) - i + 1. \tag{2}$$

Several estimates from (1) are then compared to estimate the error in the estimate for h/R_c. [2] shows that the three-term test is superior to several other well-known methods for estimating the radius of convergence of a series for many examples.

Pole vaulting is an interesting application of this theorem. It can be viewed as a natural generalization of the usual paths of integration. As implemented with the Taylor series method, the solution is available not only at discrete points but also at any point in some region of the complex plane containing the desired path. This technique promises improved speed and accuracy for some types of problems. The remainder of this paper considers several numerical examples showing how to apply the pole vaulting technique to problems with singularities on the real axis, with singularities in derivatives higher than those appearing in the differential equation, and with conjugate pairs of singularities near the real axis.

3. Poles on the Real Axis. The problem of extending the solution of the first Painlevé equation,

$$y'' = 6y^2 + x, \quad y(0) = 1, \quad y'(0) = 0, \tag{3}$$

beyond its first singular points (poles of order 2) on the real axis was considered by Davis [3, p. 245]. He outlined two methods by which this can be done. The first method of pole vaulting is specific to this equation, but the second method extended the solution by analytic continuation around the path shown in Figure 1. We will follow the latter approach. Davis' two approaches gave $y(1.5) = 11.63$ and $y'(1.5) = -79.46$, or $y(1.5) = 11.78 + 0.11\,i$ and $y'(1.5) = -79.50 + 0.59\,i$, respectively. One measure of the error is the imaginary components of these estimates, both of which should be 0.

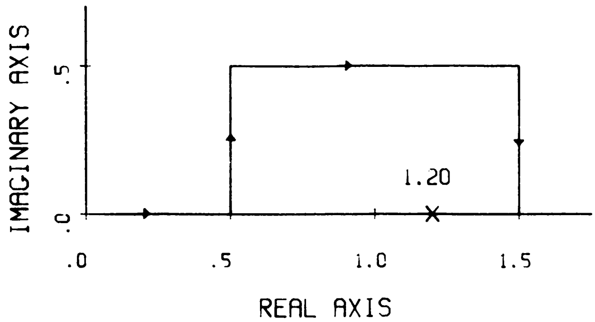

FIGURE 1
Pole vaulting for the Painlevé equation

We solved the Painlevé equation using 30 terms and a variable stepsize instead of 5 terms and constant steps of 0.01 used by Davis. The results are summarized in Table I. Since the exact value of $y(1.5)$ is not known, the error in these computations may be estimated by the magnitude of the imaginary part of the computed solution at 1.5.

TABLE I
Pole vaulting for the Painlevé equation

Step	Number Steps	$y(0.5 + 0.5i)$ $y'(0.5 + 0.5i)$	$y(1.5)$ $y'(1.5)$
$0.6R_c$	9	$0.3462 + 1.2075\,i$	$11.6160 + 5E\text{–}4\,i$
		$-0.7405 + 3.4193\,i$	$-79.4260 - 7E\text{–}3\,i$
$0.2R_c$	24	$0.3462 + 1.2075\,i$	$11.6136 - 1E\text{–}4\,i$
		$-0.7408 + 3.4200\,i$	$-79.4025 + 9E\text{–}4\,i$
0.01*	250	$0.3289 + 1.2119\,i$	$11.7796 + 0.1152\,i$
		$-0.7011 + 3.4670\,i$	$-79.5588 + 0.5880\,i$

*Davis' results using a 5 term-series.

The pole vaulting approach can also be used in conjunction with the three-term test to accurately locate a sequence of poles. In Figure 2, the first six poles of (3) on the negative real axis are found in 33 steps using a stepsize of $0.6R_c$. As a test of the accuracy of the solution, which was being analytically continued past a sequence of poles, these values were also computed:

After passing 3 poles,

$$y(6) = 2.16 + 2.6\text{E}{-4}\, i, \quad y'(6) = -0.53 - 2.0\text{E}{-3}\, i.$$

After passing 6 poles,

$$y(10.5) = 5.59 + 2.5\text{E}{-3}\, i, \quad y'(10.5) = 23.50 + 1.8\text{E}{-2}\, i,$$

where the true values must have imaginary part 0. The computed location of the sixth pole was $-10.0679 - 0.0001\, i$.

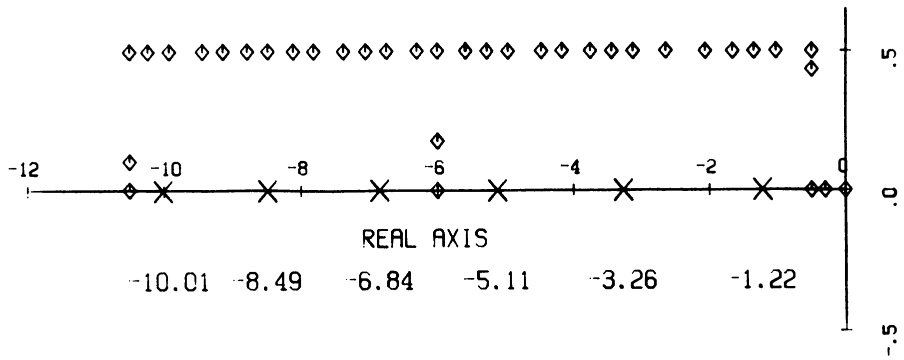

FIGURE 2
Negative poles of the Painlevé equation

Since this method can vault over poles on the real axis, we ask whether it is better to stay far away from the pole or to approach it closely before integrating around it. $y = x^{-2}$, the solution to $y' = -2y/x$, $y(-10) = 0.01$, has no secondary singularities like those which complicated the solution of the Painlevé equation.

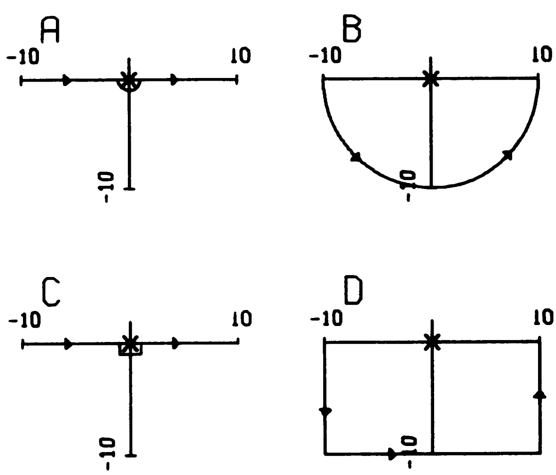

FIGURE 3
Possible paths of integration

This problem was solved along each of the four paths shown in Figure 3 using 30 terms of the series and a variable stepsize of $0.6R_c$. If a fixed stepsize were used, the shortest path, A, would require the fewest steps, but if the stepsize is proportional to the series radius of convergence, the same number of steps are required for the vaulting part of the path regardless of how close to the pole that path is taken. As Table II shows, paths further away from the pole require fewer steps *and* yield more accurate results. Hence, any step approaching the pole on the real axis is wasted. The stepsize on a circular path centered at the pole is constant, so a considerable savings on program overhead compared to the rectangular path is possible. For this problem, the worst relative error for each path occurred at $x = 10$, and the imaginary part of $y(10)$ was typically about 5×10^{-8}.

TABLE II
Comparison of several paths for $y = x^{-2}$

Path	Number of Steps	Worst Relative Error
A	15	6.6×10^{-5}
B	7	1.2×10^{-5}
C	16	4.5×10^{-5}
D	8	1.6×10^{-5}

4. **Singularities in Derivatives.** We have shown that it is possible to integrate around a pole on the real axis. For most problems of interest, however, a pole in the solution has a physical significance, and the solution computed past that pole has no physical relationship to the solution being computed before the pole was encountered. If the pole vaulting technique is to be useful in practice, it must be applied to other types of problems for which solutions exist but are difficult for standard methods to compute.

One such class of problems has solutions with singularities in higher order derivatives not appearing in the differential equation. For example, $y' = f(x, y) = (5/3)y/x$, $y(-1) = -1$, has solution $y = x^{5/3}$, which is defined on the entire real line, but $y'' = (10/9)x^{-1/3}$ has a branch point at $x = 0$. The singularity at $x = 0$ in $f(x, y)$ and in y'' makes this problem difficult, so we view x as a complex variable and vault around the singularity.

Although the solution is known to be real on the entire real line, integrating along paths similar to those shown in Figures 1 or 3 does not yield a real estimate for the solution because the Riemann surface for $y = x^{5/3}$ has three sheets (see Figure 4). Hence we integrated 1½ times around $x = 0$ along the path shown in Figure 5 in 17 steps using a stepsize of $0.6R_c$. Some of the results are given in Table III.

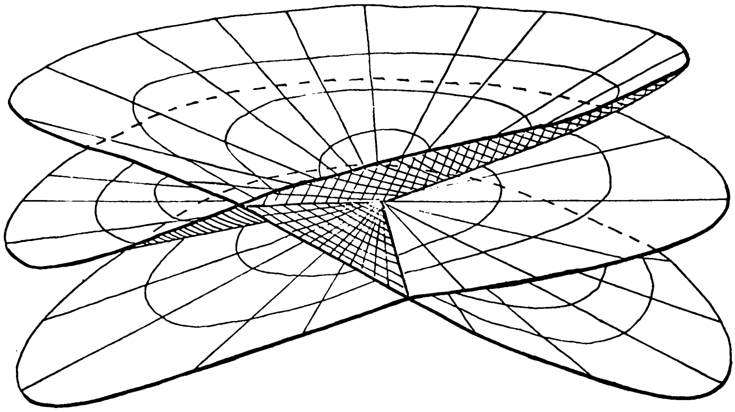

FIGURE 4

Riemann surface for $x^{5/3}$

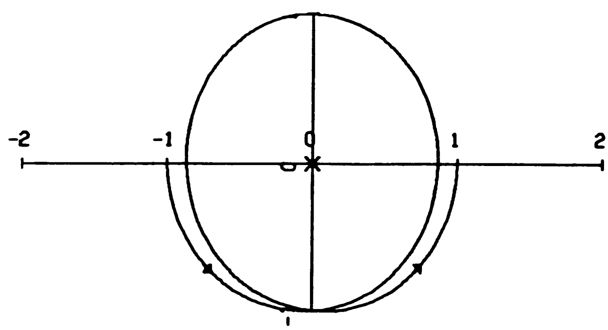

FIGURE 5

Integration path for $y = x^{5/3}$

TABLE III

Integrating $y' = (5/3)y/x$ $1\frac{1}{2}$ *times around* $x = 0$

x	Computed Solution	|Error|
-1.0	-1.0	0.0
$-0.36 - 0.93\,i$	$0.416 - 0.909\,i$	3×10^{-7}
$0.90 + 0.44\,i$	$-0.960 + 0.279\,i$	3×10^{-6}
$-0.96 + 0.28\,i$	$0.839 + 0.544\,i$	5×10^{-6}
$0.52 - 0.85\,i$	$-0.137 - 0.991\,i$	9×10^{-6}
1.0	$1.000 - 9 \times 10^{-6}\,i$	9×10^{-6}

At each step of the analytic continuation, the three-term test yielded the radius of convergence of the series with relative error at most 7×10^{-6} and the order of the singularity with relative error at most 3×10^{-4}. Here the ability to recognize the fractional order accurately is important because this estimate is used to determine the number of sheets of the Riemann surface for the solution and hence the number of times the singularity must be circled in order to return to the real branch of the solution.

5. Conjugate Pairs of Singularities. Another class of problems, which are costly to solve by standard methods, contains problems with conjugate pairs of singularities near the real axis. Very small steps are required near the singularities. For example, [1] solved a celestial mechanics problem which required stepsize changes of 7 orders of magnitude. In this section, we consider two examples in which we vault over the singularities without approaching them closely enough to require a substantial stepsize reduction.

The equation $y' = -2xy^2$, $y(x_0) = 1/(1 + x_0^2)$, has solution $y = 1/(1 + x^2)$ with a pair of simple poles at $x = \pm i$. To integrate directly from -10^4 to 10^4 using a stepsize of $0.6R_c$ requires 33 steps ranging in size from 6×10^3 to 6×10^{-1}. The solution computed in this manner has a relative error at $x = 10^4$ of 10^{-5}, but near 0 the relative error is nearly 100%! By contrast, integrating around a semicircle requires only 7 steps regardless of the diameter. Using the pole vaulting technique to integrate from -10^4 to 10^4 along a semicircle yields the largest relative error at $x = 10^4$ of 10^{-5}. If it is necessary to determine the behavior of the solution near $x = 0$, the direct path of integration must be taken, and small steps must be used. However, if the solution near $x = 0$ is not of interest, pole vaulting at a distance can yield sufficient accuracy, with few enough large steps, to more than compensate for the additional cost of computing in complex arithmetic.

6. Relative Merits of Pole Vaulting. We have given examples to show that a solution to a differential equation can be analytically continued along a path in the complex plane of the independent variable. This technique can be used (1) to extend a solution past a pole on the real axis, (2) to avoid singularities on the real axis in higher derivatives of the solution, or (3) to avoid taking very small integration steps to pass between a conjugate pair of singularities. Taylor series methods work well for this analytic continuation because their high order yields high accuracy, and the radius of convergence can be readily determined so that optimal length steps may be taken. Taylor series methods can be easily adapted to any path, and since the coefficients of the series are computed at each step, the solution may readily be computed not only at the points of expansion but also at any point within the region of convergence of the series.

The pole vaulting technique holds promise for some types of problems, but its efficiency limits its general purpose usage. Complex arithmetic is roughly 4–8 times as expensive as real arithmetic, so its use is justified only if the number of steps required can be substantially reduced. Unless the stepsize used following the real axis varies by several orders of magnitude, pole vaulting should probably not be attempted. For the first example in Section 5, pole vaulting along a semicircle reduced the number of steps from 33 to 7, so the increased cost of complex arithmetic may be justified.

Pole vaulting cannot be attempted without some knowledge of the location and order of the singularities encountered. If this information is available a priori, the path to be followed and even the radius of convergence of the series at any point may be provided. If this information is not available, the estimates from the three-term test may be used to construct the path. In the case of branch points, the structure of the Riemann surface must be determined so that a path may be taken which returns to the real branch of the solution.

The pole vaulting method, using Taylor series for the analytic continuation of the solution along a path in the complex plane, is competitive with standard ODE solving methods for some special problems. Its use for these special applications merits further study.

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