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Families of high-order composition methods

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We propose a new rule of thumb for designing high-order composition methods for ODEs: instead of minimizing (some norm of) the principal error coefficients, simply set all the outer stages equal. This rule automatically produces families of minimum error 4th order and corrected 6th order methods, and very good standard 6th order methods, parameterized by the number of stages. Intriguingly, the most accurate methods (evaluated with the total work held fixed) have a very large number of stages.

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1. Composition methods

Ever since high-order composition methods were invented [7,8], a steady stream of papers has appeared extending and refining them. Numerous methods have been announced as 'optimal' in some sense, so that it is difficult to make a final assessment. There are several reasons for this:

- The order conditions are complicated, and it is difficult to find all solution paths. If an error measure is being minimized, it is hard to be sure one has found the global minimum.
- It is possible to add extra stages, which in many cases has been found to decrease the effective error constant. But if enough stages are added, higher order becomes possible, but perhaps not desirable. How should methods be selected then?
- The error criterion depends on choosing a norm in a linear space, for which there is no canonical choice; different norms will give different optimal methods.
- New types of methods (e.g., using a corrector) for different (e.g., near-integrable) problems, have been considered.
- Minimizing the principal error may lead to the increase of higher-order error terms, which may make the 'optimal' method less desirable in practice.

Here we address these issues by studying the order conditions in the most popular and most amenable situation, of 'type SS' methods [5,7,8] (self-adjoint compositions of a family of self-adjoint maps). Let $S(\tau)$ be a self-adjoint integrator of the vector field X_1 with time step τ, so that, up to terms exponentially small in τ,

$$S(\tau) = \exp\bigl(\tau X_1 + \tau^3 X_3 + \tau^5 X_5 + \cdots\bigr).$$

We consider the self-adjoint methods[1]

$$\begin{aligned}\varphi(\tau) &= \left(\prod_{i=1}^{n} S(\alpha_i\tau)\right) S\left(\left(1 - 2\sum_{i=1}^{n}\alpha_i\right)\tau\right)\left(\prod_{i=n}^{1} S(\alpha_i\tau)\right)\\ &= \exp\bigl(\tau X_1 + p_3\tau^3 X_3 + \tau^5(p_5 X_5 + p_{113}X_{113})\\ &\quad + \tau^7(p_7 X_7 + p_{115}X_{115} + p_{313}X_{313} + p_{11113}X_{11113}) + \cdots\bigr)\end{aligned}$$

where we write $X_{113} = [X_1, [X_1, X_3]]$ and the $p_{j_1\ldots}$ are polynomials of degree $\sum_i j_i$ in the α_i. After applying an anti-selfadjoint conjugation or corrector (see, e.g., [2]) of the form

$$\psi(\tau) = \exp\bigl(\tau^4 c_{13}X_{13} + \tau^6(c_{15}X_{15} + c_{1113}X_{1113}) + \cdots\bigr)$$

we have

$$\begin{aligned}\psi\varphi\psi^{-1} = \exp\bigl(&\tau p_1 X_1 + \tau^3 p_3 X_3 + \tau^5\bigl(p_5 X_5 + (p_{113} - c_{13})X_{113}\bigr)\\ &+ \tau^7\bigl(p_7 X_7 + (p_{115} - c_{15})X_{115}\bigr)\\ &+ (p_{313} - p_3 c_{13})X_{313} + (p_{11113} - c_{1113})X_{11113} + \cdots\bigr).\end{aligned}$$

With an appropriate choice of the c_j,

$$\psi\varphi\psi^{-1} = \exp\bigl(\tau X_1 + \tau^3 p_3 X_3 + \tau^5 p_5 X_5 \tau^7\bigl(p_7 X_7 + (p_{313} - p_3 p_{113})X_{313}\bigr) + \cdots\bigr),$$

and when φ is at least 4th order, $p_3 = 0$ so

$$\psi\varphi\psi^{-1} = \exp\bigl(\tau X_1 + \tau^5 p_5 X_5 \tau^7(p_7 X_7 + p_{313}X_{313}) + \cdots\bigr).$$

Crucially,

$$p_j = 2\sum_{i=1}^{n}\alpha_i^j + \left(1 - 2\sum_{i=1}^{n}\alpha_i\right)^j$$

and it is the simple form of these particular order conditions which forms the basis of our study.

We propose that even if a corrector is not being used, one should not include correctable terms in the error coefficients. These errors do not contribute to the qualitative error and it is wasteful to try and minimize them. With this error criterion, our study of

[1] We only consider methods with an odd number of stages, since this means that the consistency condition (total step size is τ) can be satisfied using just the central stage; with an even number of stages enforcing consistency uses up two stages.

fourth order methods suggests the rule of thumb that all outer stages should be set equal. We then test this rule on corrected and uncorrected sixth order methods.

The error when integrating to a fixed time at constant work with a fourth order method of m stages is

$$\mathrm{O}\big(m^4 p_5|X_5| + m^6\big(p_7|X_7| + p_{313}|X_{313}|\big) + \cdots\big).$$

Using the convention that all assessments should be neutral to rescaling the time step (i.e., the methods $\varphi(\tau)$ and $\varphi(\tau/k)^k$ should be rated equally), we use the effective error coefficients

$$e_{j_1\ldots} := m^p |p_{j_1\ldots}|$$

throughout, where p is the order of the method. In this way all error coefficients can be compared to their reference values (either 1 or 0) in the basic method φ. Note that in the past (e.g., in [6]), some measurements, of stability limits for example, have not been scaled by m, which makes them look better than they really are, and may be the reason why the new methods have not been adopted for general use.

2. The rule of thumb

Case 1. Fourth order methods

For fourth order methods, there is only one order condition (p_3) and one uncorrectable principal error coefficient (p_5), so there is no need to choose an error norm. A detailed analysis of the order conditions is possible. We show in proposition 1 that the very simple family of methods introduced by Suzuki in 1990 in one of the first papers on high-order composition methods [7],

$$\varphi = S(\alpha\tau)^n S\big((1-2n\alpha)\tau\big) S(\alpha\tau)^n \tag{1}$$

provides a local minimum of the principal error for any number of stages, and we conjecture that (amongst minima which are critical points) it is a global minimum as well. As $n \to \infty$, $\alpha \to 1/(2n)$ and $1 - 2n\alpha \to 0$, so asymptotically we have a sequence of constant time-step (e.g.) leapfrog steps. The $n = 2$ (5-stage) case of the following proposition was recently found by Blanes [1].

Proposition 1. Amongst all fourth-order self-adjoint composition methods of the form

$$\prod_{i=1}^{2n+1} S(\alpha_i \tau),$$

the method with $\alpha_i = \alpha := 1/((2n) - (2n)^{1/3})$ for $i = 1, \ldots, n$ locally minimizes the uncorrectable component of the principal error.

Proof. Letting $\alpha_{n+1} = \sigma := 1 - 2\sum_{i=1}^{n} \alpha_i$, we have to find extreme points of the error coefficient

$$f(\boldsymbol{\alpha}) = 2\sum_{i=1}^{n} \alpha_i^5 + \sigma^5$$

subject to the constraint

$$g(\boldsymbol{\alpha}) := 2\sum_{i=1}^{n} \alpha_i^3 + \sigma^3 = 0.$$

First we calculate

$$\frac{\partial f}{\partial \alpha_j} = 10\alpha_j^4 - 10\sigma^4,$$
$$\frac{\partial g}{\partial \alpha_j} = 6\alpha_j^2 - 6\sigma^2$$

so that $\alpha_j \equiv \alpha$ is a critical point $f + \lambda g$ where λ is a Lagrange multiplier, and hence a critical point of $f|_{g=0}$. Note that $\nabla g(\alpha \mathbf{1}) = 6(\alpha^2 - \sigma^2)\mathbf{1}$, where $\mathbf{1}$ is the vector containing all 1's. (We also write $\mathbb{1}$ for the matrix containing all 1's.)

We have to calculate the signature of this critical point. We compute this in orthonormal coordinates $v_1, \ldots, v_n$ adapted to the surface $g = 0$, the basis vectors being the columns of Q where $\mathbf{1} = QR$ is the QR factorization of $\mathbf{1}$, the normal vector to $g = 0$ at the critical point. From $v_1^{\mathrm{T}}\mathbf{1} = \sqrt{n}$ and $v_1^{\mathrm{T}} v_j = 0$ for $j > 1$ we have

$$\left(\mathbf{1}^{\mathrm{T}} Q\right)_i = \sqrt{n}\delta_{i1}$$

and

$$\left(Q^{\mathrm{T}} \mathbb{1} Q\right)_{ij} = n\delta_{i1}\delta_{j1}.$$

We shall need the two Hessians

$$F = 40\alpha^3 I + 80\sigma^3 \mathbb{1},$$
$$G = 12\alpha I + 24\sigma^3 \mathbb{1}$$

of f and g at the critical point. Then

$$\begin{aligned} g(\alpha\mathbf{1} + Q\mathbf{v}) &= g(\alpha\mathbf{1}) + \nabla g(\alpha\mathbf{1})^{\mathrm{T}} Q\mathbf{v} + \frac{1}{2}\mathbf{v}^{\mathrm{T}} Q^{\mathrm{T}} G Q\mathbf{v} + \mathrm{O}\left(\mathbf{v}^3\right) \\ &= 6\sqrt{n}\left(\alpha^2 - \sigma^2\right)v_1 + 6\alpha|\mathbf{v}|^2 + 12n\sigma v_1^2 + \mathrm{O}\left(\mathbf{v}^3\right) \end{aligned}$$

so the surface $g = 0$ is nondegenerate at the critical point and is described locally by

$$v_1 = -\frac{\alpha}{\sqrt{n}(\alpha^2 - \sigma^2)}\left(v_2^2 + \cdots + v_n^2\right) + \mathrm{O}\left(\mathbf{v}^3\right).$$

Expressing the objective function in the coordinates $v_2, \ldots, v_n$ gives

$$\begin{aligned} f(\alpha\mathbf{1}+Qv) &= f(\alpha\mathbf{1}) + \nabla f(\alpha\mathbf{1})^{\mathrm{T}} Q\mathbf{v} + \frac{1}{2}\mathbf{v}^{\mathrm{T}} Q^{\mathrm{T}} F Q\mathbf{v} + \mathrm{O}\big(\mathbf{v}^3\big) \\ &= f(\alpha\mathbf{1}) + 10\big(\alpha^4-\sigma^4\big)\sqrt{n}v_1 + 20\alpha^3|\mathbf{v}|^2 + 40n\sigma^3 v_1^2 + \mathrm{O}\big(\mathbf{v}^3\big) \\ &= f(\alpha\mathbf{1}) + \left(20\alpha^3 - 10\frac{(\alpha^4-\sigma^4)\sqrt{n}\alpha}{\sqrt{n}(\alpha^2-\sigma^2)}\right)\big(v_2^2+\cdots+v_n^2\big) + \mathrm{O}\big(\mathbf{v}^3\big). \end{aligned}$$

But

$$20\alpha^3 - 10\frac{(\alpha^4-\sigma^4)\sqrt{n}\alpha}{\sqrt{n}(\alpha^2-\sigma^2)} = 20\alpha^3 - 10\alpha\big(\alpha^2+\sigma^2\big) = 10\frac{1-(2n)^{2/3}}{(2n-(2n)^{1/3})^3} \leqslant 0$$

for all $n \geqslant 1$ so the critical point is a local maximum. Since $f(\alpha\mathbf{1}) = 2n\alpha^5 + (1-2n\alpha)^5 = -(2n)^{-2/3}((2n)^{2/3}-1)^{-4} \leqslant 0$, the error itself is minimized at this point. □

Not only does this family of methods (see table 1) minimize the error, the error itself is very small and the minimum effective error is obtained for surprisingly large n. In terms of $x := (2n)^{1/3}$, the effective error is

$$e(x) = m^4 f(\alpha\mathbf{1}) = \frac{(x^3+1)^4}{x^2(x^2-1)^4}$$

so

$$e'(x) = \frac{2(x+1)(x^2-x+1)^3(x^2-3x+1)}{x^3(x-1)^5}$$

which is negative in $(1, x^*)$ and positive in (x^*, ∞) where $x^* = \frac{1}{2}(3+\sqrt{5})$, corresponding to $x^{*3}+1 \approx 18.944$ stages. The error is minimized by a method of 19 stages!

Table 1
The Suzuki family of 4th order methods, together with their 6th and 8th order effective error coefficients. τ^* is the 'elbow' value of the time step, namely $\sqrt{e_5/e_7}$, at which the 6th and 8th order errors nominally balance. The 19-stage method has the smallest error e_5.

$2n+1$	Method coeff.	Error coefficients				τ^*
	$\alpha = b_1$	e_5	e_{113}	e_7	e_{313}	
3	1.3512	428.60	11.6966	18222.5701	739.44	0.1534
5	0.4145	46.4850	1.5088	702.7579	52.8224	0.2572
7	0.2391	25.8975	2.4816	312.0087	32.9479	0.2881
9	0.1667	20.2500	5.6250	227.8125	30.3750	0.2981
11	0.1275	17.9366	8.9099	198.9201	31.6519	0.3003
13	0.1030	16.8364	12.5428	188.3360	34.5416	0.2990
15	0.0863	16.2981	16.5889	185.8805	38.3817	0.2961
17	0.0742	16.0606	21.0741	187.7303	42.9094	0.2925
19	0.0650	16.0000	26.0101	192.1488	48.0002	0.2886
21	0.0579	16.0507	31.4025	198.2394	53.5871	0.2845

In fact, the critical point of proposition 1 seems to be the only 'interesting' one. In all the others $|\alpha_i|$ takes on at most two distinct nonzero values, but these critical points (with sign changes and zero values) have much larger values of e_5. We therefore make the following conjecture.

Conjecture. The Suzuki method (1) with $n = 19$ achieves the smallest possible effective error over all methods of any number of stages for which the error is a critical point (i.e., excluding higher-order methods for which the error passes through zero).

How can the pattern shown in this excellent family of methods be extended to higher order? Note that the methods have the maximum possible number of equal stages, a property that does generalize.

Proposition 2. The function $p_{2k+3} : \mathbb{R}^n \to \mathbb{R}$ on the surface defined by the k constraints $p_3 = \cdots = p_{2k+1} = 0$ generically has critical points with $n - k$ of the variables equal to any of the other k variables.

Proof. We are seeking critical points of the augmented function

$$p_{2k+3} + \sum_{j=1}^{k} \lambda_j p_{2j+1}.$$

Setting $n-k$ of the variables equal to any of the other k variables, the constraint equations are then k equations in k unknowns, with generically isolated solutions. However, from the symmetry of the p_j, if say $\alpha_1 = \alpha_2$, then $\partial p_j/\partial\alpha_1 = \partial p_j/\partial\alpha_2$. So the remaining $n - k$ equations, $\nabla p_{2k+3} + \sum_{j=1}^{k} \lambda_j \nabla p_{2j+1} = 0$, reduce to k linear equations in k unknowns λ_j, which generically have a solution. □

There can be enormous numbers of these critical points, most of them not minima. However, it seems to be best to repeat only a single value of α_i. For, consider the following class of methods, which can repeat two values, α and β:

$$S(\alpha\tau)^{m/2} S(\beta\tau)^n S(\alpha\tau)^{m/2}.$$

To be fourth order requires

$$m\alpha + n\beta = 1, \qquad m\alpha^3 + n\beta^3 = 0$$

with solution

$$\alpha = \frac{1}{m - (n^2 m)^{1/3}}, \qquad \beta = \frac{1}{n - (m^2 n)^{1/3}}.$$

This solution is a critical point of the error p_5. Clearly, to get the shortest steps, either n or m should be as small as possible (e.g., increasing n from 1 increases α disastrously). But the minimum value of m, namely 2, is greater than the minimum value of n, namely 1, so we should take $n = 1$. This gives the Suzuki family of methods of proposition 1.

If other terms (p_{313} etc.) are included in the constraints or error, the points described in proposition 2 will be no longer critical, and the order of the α_i will become relevant; but these terms seem to be relatively small in the interesting region of parameter space. A study of the 6th-order order conditions $p_3 = p_5 = p_{113} = 0$ suggests that it is the *outer* stages that should be set equal. Therefore we propose the following

Rule of thumb. Set the maximum possible number of outer stages equal to eliminate all free parameters. Find the solution of the order conditions with the smallest stages. Either use the resulting method or use it as a starting point in a full minimization of the error coefficient.

Some evidence for this rule of thumb is found in [1]. His best 6th and 8th order methods have the two outer stages nearly equal. (Only 'nearly' because of the inclusion of extra terms in the principal error.) We find further support when we examine corrected and uncorrected 6th order methods.

Case 2. Corrected sixth order methods

The rule of thumb here gives two order conditions ($p_3 = p_5 = 0$) in two unknowns, which it is possible to reduce to a single real polynomial of degree 15. For each n we tested this polynomial has a single real solution. Furthermore, this solution has nice small α_j's. By proposition 2, it is a critical point of the error p_7, presumably a minimum. As at 4th order, the error p_7 decreases as more stages are added, reaching a minimum at $n = 12$, or 25 stages. The other uncorrectable error term p_{313} can be evaluated on these solutions, and is relatively small (see table 2). Remember, these methods have the advantage that no optimization is needed.

These methods also indicate why it is necessary to consider 4th order methods with $\geqslant 7$ stages, even though 6th order is possible. Consider, say, 9 stages. The Suzuki method does have an error of $e_5 = 20.25$, while other 9 stage methods have $e_5 = 0$; but those have a much larger e_7 (3840 as opposed to 227.8, 17 times as large).

Case 3. Uncorrected sixth order methods

Now there are 3 order conditions ($p_3 = p_5 = p_{113} = 0$) and 7 stages are required, the best 7-stage method being the Yoshida 'A' solution with effective error $7^6 p_7 = 7^6 \cdot 0.8884 = 104518$. With $2n + 1$ stages, we set $b_1 = \cdots = b_{n-2}$, leaving three unknowns b_1, b_{n-1}, and b_n. Unfortunately, the equations seem to be too complicated to reduce to a single polynomial. After trying several methods, the easiest way we found to solve the equations was to regard the smallest real solution of $p_3 = p_5 = 0$ as a function of b_n, and then to evaluate p_{113} on this solution. It is then easy to check if this function of b_n has a zero. This gives a solution for 11, 13, 15, and 17 stages, but not for 9, 19, or 21. The solutions with 11–17 stages, listed in table 3, appear to form a related family, again with decreasing effective error coefficients.

Table 2
Sixth order methods with a corrector, with all outer stages equal. For the given n (i.e. $2n+1$ stages), there is a single real method of this type. The 25-stage method has the smallest error e_7. The coefficients can be found in MATLAB by `syms x y z; z=1-2*y-2*n*x; s=solve(2*n*x^3+2*y^3+z^3,2*n*x^5+2*y^5+z^5); j=find(double(imag(s.x))==0); b1=s.x(j); b2=s.y(j);`.

$2n+1$	Method coefficients		Error coefficients			τ^*
	b_1	b_n	e_7	e_{313}	e_9	
5	1.4522	−2.1506	875520	−32996	2.7×10^8	0.1790
7	0.4312	−0.8342	13551	−276	1.2×10^6	0.1068
9	0.2460	−0.5514	3840	−35	235550	0.1277
11	0.1706	−0.4234	2147	0.38	114534	0.1369
13	0.1300	−0.3489	1572	13	78887	0.1412
15	0.1048	−0.2996	1311	21	64340	0.1429
17	0.0876	−0.2643	1181	27	57574	0.1432
19	0.0752	−0.2377	1109	33	54434	0.1427
21	0.0659	−0.2167	1072	39	53271	0.1419
23	0.0585	−0.1997	1056	44	53315	0.1407
25	0.0527	−0.1856	1053	51	54166	0.1394
27	0.0479	−0.1735	1059	57	55594	0.1380

3. The elbow

In practice, any given method is not used in the limit $\tau \to 0$, for then a higher order method would be more efficient. The errors of all possible methods will form an envelope and users will try to select methods which lie close to this envelope. Somehow, this envelope is contained in the structure of the order conditions, but we know of no direct way to get at it. Here is one way to observe it. If we make the arbitrary assumption that all vector fields X_j have the same order of magnitude, and consider only a single error term e_j at each order, then the effective error scales roughly as $\tau^p e_{p+1}+\tau^{p+2}e_{p+3}+\cdots$ for a method of order p. We define the *elbow*

$$\tau^* := \sqrt{\frac{e_{p+1}}{e_{p+3}}}$$

as the value of the time step below which the asymptotic error behaviour $\mathrm{O}(\tau^p)$ is seen. It corresponds to the corners commonly seen in log–log plots of the error. Indeed, looking at error plots in almost any of the references suggests that the elbow tends to lie close to the envelope. (Is this perhaps the 'rule of elbow'?)

The elbow gives a crude measure of the nonlinear stability of the method: If τ^* is very small, the method is unlikely to ever compete with higher-order methods. Good methods have small e_{p+1} *and* large τ^*. The reference value of τ^* is 1, from the reference method $S(\tau)$. Figure 1 shows typical error curves that might be obtained based on the error coefficients in tables 1 and 2. Clearly, no method is used at time steps

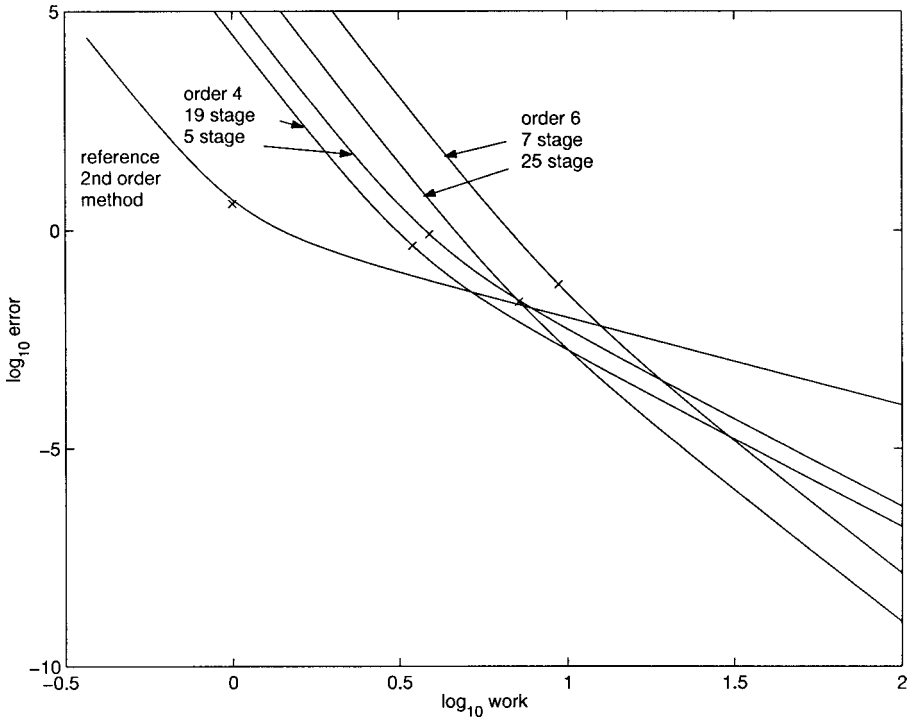

Figure 1. Nominal errors $\sum_j e_j \tau^j$, with positions of the 'elbow' τ^* marked by $\times$. Methods with very large numbers of stages can in principle be competitive.

Table 3
Sixth order methods without a corrector, with all outer stages equal. These methods don't appear to exist for all n, but when then do, they are very accurate. For 7 stages this is the Yoshida 'A' method.

$2n+1$	Method coefficients			Error coefficients			τ^*
	b_1	b_{n-1}	b_n	e_7	e_{313}	e_9	
7	0.7845	0.2356	−1.1777	104518	2116	1.89×10^7	0.0743
11	0.4505	−0.4932	−0.8258	194929	2644	4.07×10^7	0.0692
13	0.2677	−0.3514	−0.5153	26499	2902	3.00×10^6	0.0940
15	0.1887	−0.3026	−0.3521	7895	1964	5.78×10^6	0.1365
17	0.1429	−0.2887	−0.2419	4243	988	2.69×10^5	0.1256

larger than τ^*. What is remarkable about the families of methods in tables 1, 2, and 3, is that the elbows do not decrease with increasing number of stages. We do see, however, that even the largest values of τ^* decrease as the order increases: $\tau^* = 1$, 0.30, and 0.14 for orders 2, 4, and 6, respectively. The tables also indicate that the higher-order errors must increase as the order increases: there is no 4th order method with $e_5 = 1$, its value in the 2nd order method S. Similarly, the minimum value of e_7 for 4th order methods

is 185, but the best we can do with a 6th order method is 1053. It seems likely that this pattern persists for all methods and all orders.

Consider a user trying to get away with, say, leapfrog method at its largest reasonable time step. The user is unhappy with the overall error and wants to choose between decreasing the time step and switching to a higher order method. If, indeed, the higher order methods become competitive at $\tau \sim \tau^*$, then we can say that if the user is willing to to about $1/\tau^*$ more work (i.e., about 3.3 times for 4th order, or 7 times for 6th order) then the higher order method will become advantageous, corresponding to desired error reductions of about 10 and 50, respectively.

We get similar estimates looking at the error coefficients. Second and 4th order methods balance when $\tau^2 \sim 16\tau^4$, or $\tau \sim 0.25$, corresponding to 4 times more work; 2nd and 6th order methods balance when $\tau^2 \sim 1053\tau^6$, or $\tau \sim 0.17$, corresponding to 6 times more work. These encouraging estimates are mainly due to the small error constants of the methods in tables 1 and 2.

Now the same user might complain that it is preposterous to switch from a 1-stage method, say leapfrog, to a 19 or 25 stage method. The work overhead must be 19 or 25 times, which would never be justified. Does not this contradict the previous paragraphs? Perhaps the resolution is that our analysis so far has ignored stability. Leapfrog applied to the harmonic oscillator is stable only for $\tau < 2$, and all of the higher order methods given here have stability limits less than π. (They could perhaps be modified slightly to be stable up to $\tau = 2\pi$ or beyond, although the practical relevance of this is not clear.) When scaled by the number of stages m, their effective stability limits are less than π/m–very small indeed. In problems where the time step is limited by stability, we will indeed have to pay an overhead of about $2m/\pi$ to use these methods.

Example. Rather than a purely numerical example, we present an exact study of the new methods applied to the harmonic oscillator with $p-q$ splitting. This is a worst case for us, since the more nonlinear a problem is, the larger (e.g.) X_7 is compared to X_{313}, since it contains the highest derivatives of the vector field X_1. Writing the methods as $x \mapsto A(\tau)x$, where $A(\tau) \in \mathbb{R}^{2\times 2}$, we compare $\operatorname{tr} A(\tau)$ to its exact value $2\cos(\tau)$. This measures the phase error of the method. Specifically, we expand

$$e(\tau) = \frac{2\cos\tau - \operatorname{tr} A(\tau)}{\tau^2} = \mathrm{O}\big(\tau^p\big)$$

in a Taylor series; to get an effective error, we list in table 4 the coefficients of $e(m\tau)$. By solving $|\operatorname{tr} A(\bar\tau)| = 2$, we can determine the stability limit $\bar\tau$ and the effective stability limit $\bar\tau/m$ of any of the methods.

The results are shown in table 4 and figure 2 and broadly support the general theory, but with some interesting exceptions. The leading order terms do behave as expected. But in all cases the higher order errors are much larger than expected, and grow quite quickly with increasing number of stages m. Consequently, the elbows τ^* in this problem are smaller than predicted and the high order methods are less competitive. Figure 2

Table 4
Taylor series coefficients of the effective phase error for the harmonic oscillator. Here $\bar{\tau}/m$ is the effective stability limit.

m	τ^2	τ^4	τ^6	τ^8	$\bar{\tau}/m$
			Order 2 (leapfrog)		
1	0.0833	−0.0028	5×10^{-5}	-6×10^{-6}	2
			Order 4		
3		−10.715	0.0361	−0.0036	0.524
5		−1.162	7.262	−8.22	0.544
7		−0.647	7.548	−22.67	0.424
9		−0.506	9.275	−47.21	0.339
11		−0.448	11.815	−89.12	0.280
13		−0.420	15.052	−156.43	$\approx\pi/m$
15		−0.407	18.970	−258.91	
17		−0.401	23.585	−408.36	
19		−0.400	28.923	−618.69	
21		−0.401	35.011	−906.09	
			Order 6, with a corrector		
5			46.1	−169	0.275
7			18.4	−173	0.382
9			12.8	−189	0.328
11			11.0	−227	0.276
13			10.4	−285	$\approx\pi/m$
15			10.4	−362	
17			10.7	−461	
19			11.2	−584	
21			11.8	−735	
23			12.6	−916	
25			13.4	−1131	
			Order 6, without a corrector		
7			886.8	−6214	0.324
11			448.6	−11536	0.254
13			188.8	−7798	0.238
15			125.5	−7385	0.207
17			70.2	−6819	0.183

shows that the stability limits, the elbows, and the exchange points (where a higher order method becomes competitive) and all clustered close together. However, it does appear that in the practical regime, the stability limits are not a problem and that the new, large-m methods are competitive. (From table 4 one can see that when the time step is close to the stability limit, the higher-order terms in the error are larger than the leading-order terms, so the method is unlikely to be useful then anyway.)

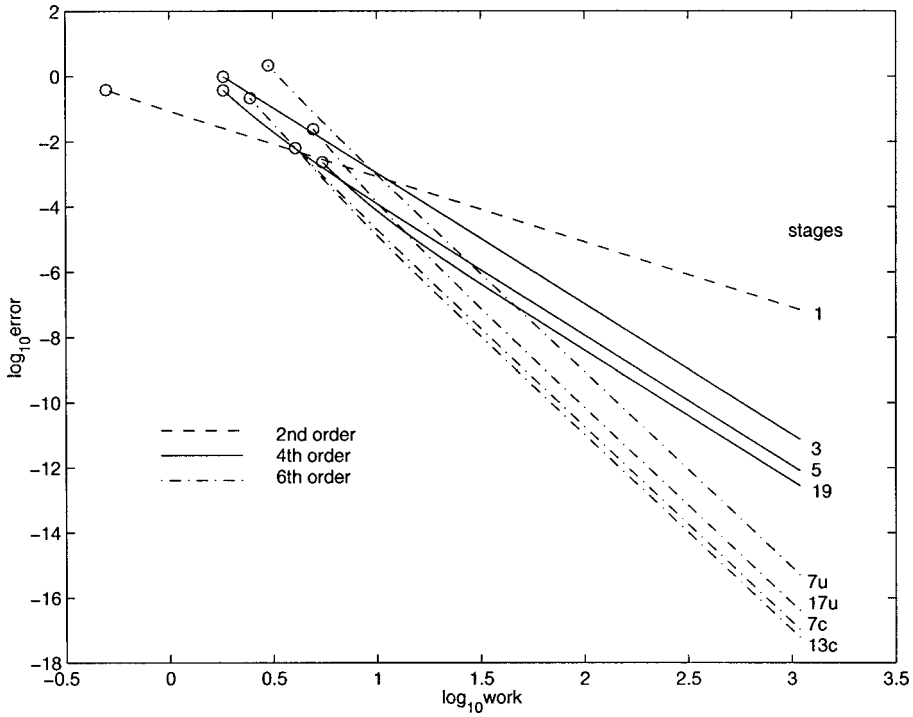

Figure 2. Phase errors for the harmonic oscillator. Here 'work' is just $1/\tau$, and the circles indicate the stability limit of each method. That is, work of W corresponds to $6\pi W$ force evaluations per period. The exchange points (where methods of different orders just balance) depend very sensitively on the choice of method. The new methods with large numbers of stages are very competitive. Strangely, the improvement is largest at 6th order, so much so that the 4th order methods are never competitive for this problem.

With small-m methods (5 stages at 4th order, and 7 at 6th order) it becomes competitive to switch to 4th order at $\tau \sim 0.23$ (i.e., at about $4\times$ more work than the nominal $\tau = 1$), and to 6th order at $\tau \sim 0.037$, or 27 times more work. With the large-m methods, 4th order is never competitive (because the large-m methods have larger 6th order errors, which squeezes them out), but it is now competitive to switch to 6th order at only 4 times more work.

4. Conclusions

We can summarize the best methods found here by crude estimates of their (effective) errors:

$$\begin{aligned}
\text{2nd order:} &\quad \tau^2 + \tau^4 + \tau^6 + \tau^8 + \cdots \\
\text{4th order:} &\quad 16\tau^4 + 192\tau^6 + 2052\tau^8 + \cdots = (2\tau)^4 + (2.4\tau)^6 + (2.6\tau)^8 + \cdots \\
\text{6th order:} &\quad 1053\tau^6 + 54133\tau^8 + \cdots = (3.2\tau)^6 + (3.9\tau)^8 + \cdots \\
\text{8th order:} &\quad 1.11 \times 10^7 \tau^8 + \cdots = (7.6\tau)^8 + \cdots
\end{aligned}$$

which gives some idea of the time steps at which each method becomes competitive (the 8th order method here is taken from [5] and can probably be improved). It is tempting to conjecture that the patterns of increasing coefficients in these tables are inevitable and are implied by the order conditions. The precise values of the coefficients, of course, will scale at each order depending on the problem; it would be interesting to try out these methods on large scale problems (e.g., in molecular dynamics) for which 2nd order methods are commonly used.

In this paper we have considered only one case, of self-adjoint methods composed of self-adjoint, 2nd order stages. It is an important case, but it is possible that the rule of thumb proposed here does not extend to all varieties of composition methods. Proceeding from the general to the particular, we conclude that

- One should not only look for global minima of some error. Local minima may be useful because their parameters and their higher order errors are much smaller. They may also form systematic families. This is true not only for all varieties of composition methods but perhaps also for Runge–Kutta methods as well.
- One should minimize only the non-correctable part of the error. Where would this approach lead for RK methods?
- The rule of thumb not only selects good methods in this case, it gives a definite prescription for the method, independent of any optimization technique and error norm. Can this approach be extended to other cases?
- Error can be minimized by methods with very large number of stages. This is likely to be true for all composition methods and perhaps for RK methods as well. Are these methods useful in practice? If not, what is the appropriate criterion?
- The best elbows found here (a nominal time step of 1 for 2nd order, 0.30 for 4th order, 0.14 for 6th order) indicate fundamental barriers to the application of high order methods and can be used to describe the envelope formed by all methods.
- It is remarkable that the highly accurate Suzuki methods (equation (1)) have been overlooked in the 10 years of research since their discovery.

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