NEW NYSTRÖM PAIRS FOR THE GENERAL SECOND-ORDER PROBLEM

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Abstract

We use three different approaches to derive new families of explicit Runge–Kutta Nyström pairs of order 3-4, 4-5 and 5-6 for the general second-order initial value problem. Our aim is two-fold: to add significantly to the theory of Nyström pairs and to obtain pairs that are more efficient and just as reliable as existing pairs.

Résumé

On dérive de nouvelles familles de paires explicites de Runge–Kutta Nyström d'ordre 3-4, 4-5 et 5-6 pour les problèmes à valeurs initiales du second ordre dans le but de développer la théorie des paires de Nyström et d'en obtenir de meilleures.

Keywords: Runge–Kutta Nyström pairs, general second-order initial value problem

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1 INTRODUCTION

Non-stiff initial value ordinary differential equations of the form

$$y'' = f(x, y, y'), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{1}$$

where the prime denotes differentiation with respect to x and $f : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}^n$ have many important applications. These include the Newtonian restricted three-body problem, its recent extensions, relativistic models of the Solar System and models for the orbits of artificial satellites, see for example Roy [18, p. 126], Chandra and Kumar [3], Hallan and Rana [14], Newhall, Standish and Williams [16], and Huang and Liu [15].

Problem (1) can be solved by transforming it to a first-order problem and applying standard integration methods such as explicit Runge–Kutta (ERK) pairs. Alternatively, (1) can be solved directly. One general class of methods for doing so is generalised explicit Runge–Kutta Nyström (ERKNG) pairs. These pairs generate approximations y_i and $\widehat{y}_i$ to $y(x_i)$ and approximations y'_i and $\widehat{y}'_i$ to $y'(x_i)$ at $x_i = x_{i-1} + h$, $i = 1, 2, \ldots$, according to

$$\begin{aligned} y_i &= y_{i-1} + h y'_{i-1} + h^2 \sum_{j=1}^{s} b_j f_j, \quad y'_i = y'_{i-1} + h \sum_{j=1}^{s} b'_j f_j, \\ \widehat{y}_i &= y_{i-1} + h y'_{i-1} + h^2 \sum_{j=1}^{s} \widehat{b}_j f_j, \quad \widehat{y}'_i = y'_{i-1} + h \sum_{j=1}^{s} \widehat{b'}_j f_j, \end{aligned} \tag{2}$$

where $f_1 = f(x_{i-1}, y_{i-1})$,

$$f_j = f(x_{i-1} + c_j h, y_{i-1} + c_j y'_{i-1} + \sum_{k=1}^{j-1} a_{jk} f_k, y'_{i-1} + h \sum_{k=1}^{j-1} a'_{jk} f_k), \quad j = 2, \ldots, s, \tag{3}$$

and the stepsize h can vary from step to step. The coefficients c_j, a_{jk}, a'_{jk}, b_j, $\widehat{b}_j$, b'_j and $\widehat{b'}_j$ are chosen so y_i and y'_i are order p, and $\widehat{y}_i$ and $\widehat{y}'_i$ are order $q < p$. The pair is then referred to as a $q - p$ pair.

For all except possibly low order pairs, the coefficients satisfy the row simplifying assumptions

$$c_i = \sum_{j=1}^{i-1} a'_{ij}, \quad \frac{c_i^2}{2} = \sum_{j=1}^{i-1} a_{ij}, \quad i = 2, \ldots, s. \tag{4}$$

If the coefficients are chosen so that $c_s = 1$, $b_s = b'_s = 0$, $a_{sj} = b_j$, $a'_{sj} = b'_j$, $j = 1, \ldots, s-1$, f_s can be used as f_1 on the next step. This choice, commonly known as FSAL, means the number of derivative evaluations on all accepted steps except the first is $s-1$ and not s.

On each step, the stepsize h is chosen so the norms of the local error estimates $y_i - \widehat{y}_i$ and $y'_i - \widehat{y}'_i$ are less than the local error tolerance TOL.

In marked contrast to ERK pairs, few families of ERKNG pairs of the form (2) have been published. Fine [10] gave a family of ten-stage non-FSAL 5-6 pairs. Later Fine [11] gave a family of five-stage 3-4 non-FSAL pairs and a family of seven-stage 4-5 FSAL pairs. Sharp and Fine [19] presented a family of eight-stage 5-6 non-FSAL pairs.

We use three different approaches to derive new families of 3-4, 4-5 and 5-6 explicit Runge–Kutta Nyström methods for (1). Our aim is to add significantly to the theory of Nyström pairs and to obtain pairs that are more efficient than existing pairs.

The derivation of the new families and the selection of near-optimal pairs from the families is summarised in §2. This is followed in §3 with a summary of our numerical comparisons. We end in §4 with a discussion of our work.

2 DERIVATION

The order conditions for a $q-p$ ERKNG pair consist of those for each of the four formulae in the pair. The derivation of a pair usually starts with the derivative formulae since there are more order conditions than for the solution formulae.

The order conditions for the derivative formulae divide into three sets S1, S2 and S3. S1 consists of the order conditions that do not depend on the a and are those for an ERK pair with the Butcher tableau

$$\begin{array}{c|c} c & A' \\ \hline & b' \\ & \widehat{b'} \end{array} \tag{5}$$

where $c = [0, c_2, \ldots, c_s]^T$, $b' = [b'_1, \ldots, b'_s]$, $\widehat{b'} = [\widehat{b'}_1, \ldots, \widehat{b'}_s]$ and A' is the lower triangular matrix formed from the a'. S2 consists of the order conditions that depend on the a but not on the a'. These order conditions along with the quadrature conditions are those for the derivative formulae in an explicit

Runge–Kutta Nyström method applied to $y'' = f(x, y)$. The Butcher tableau for the derivative formulae is

$$\begin{array}{c|c} c & A \\ \hline & b' \\ & \widehat{b'} \end{array} \tag{6}$$

where A is the lower triangular matrix formed from the a. The remaining set S3 contains the order conditions that depend on the a and the a'. The order conditions for Nyström methods are described in more detail in several references, see for example the monograph of Hairer, Nørsett and Wanner [13, pp. 284-293].

2.1 3-4 PAIRS

Fine [11, 12] presented a family of five-stage 3-4 non-FSAL ERKNG pairs. We show five-stage FSAL ERKNG pairs are possible, reducing the cost of all accepted steps except the first by one derivative evaluation. The FSAL property means $a_{5j} = b_j$, $a'_{5j} = b'_j$, $j = 1, \ldots, 4$, $c_5 = 1$, $b_5 = b'_5 = 0$.

The order conditions for the order four derivative formula are those in S1 along with

$$\sum_{i=3}^{5} \sum_{j=2}^{i-1} b'_i a_{ij} c_j = \frac{1}{24}. \tag{7}$$

The order conditions in S1 are easily solved, see for example Butcher [1], pp. 161-165, to give a family of order four derivative formulae with c_2 and c_3 as free parameters. Equation (7) is then satisfied by taking a_{32} and a_{43} as free parameters and solving for a_{42}.

The order conditions for the order three derivative formula are

$$\widehat{b'}_i c_i^k = (k+1)^{-1}, \quad k = 0, \ldots, 2, \quad \widehat{b'}_i a'_{ij} c_j = \frac{1}{6}, \tag{8}$$

where repeated indices mean summation. Since the c and a' are known or specified as free parameters, the four equations in (8) form a linear system in the five unknowns $\widehat{b'}_i$, $i = 1, \ldots, 5$. We take $\widehat{b'}_5$ as a free parameter and solve for $\widehat{b'}_j$, $j = 1, \ldots, 4$.

The order conditions for the order four solution formula are solved in a similar way to (8) except b_5 is not a free parameter because the FSAL conditions imply $b_5 = 0$. The order conditions for the order three solution formula are satisfied by taking $\widehat{b}_3$, $\widehat{b}_4$ and $\widehat{b}_5$ as free parameters and solving for $\widehat{b}_1$ and $\widehat{b}_2$.

This completes the derivation of our 3-4 family.

2.2 4-5 PAIRS

Fine [11, 12] derived a family of seven-stage 4-5 FSAL ERKNG pairs. The most general family of 4-5 ERK pairs known at the time was the seven-stage FSAL family of Dormand and Prince [5] and Fine used this family as the basis of his 4-5 ERKNG pairs.

Since Fine's work, Sharp and Verner [20] have derived two families of 4-5 ERK pairs that contain existing families as special cases. Sharp and Verner tested near-optimal pairs from the two families and found the pair from the family they labelled $C1()$ was marginally more efficient. We use this family as the basis of our ERKNG pairs.

By definition, pairs from $C1()$ satisfy the order conditions in S1. This gives a family of order four and five derivative formulae with c_2, c_3, c_4, c_5 and $\widehat{b'}_7$ as free parameters. Our derivation then proceeds as follows.

The order conditions in S2 for the order five derivative formula are satisfied by taking a_{32}, a_{43}, a_{53}, a_{54} and a_{65} as free parameters and solving small linear algebraic systems of one to three equations for the remaining a. These linear systems are formed either from the order conditions or the row simplifying assumptions (4). First a_{21} is found, then a_{31}. followed by a_{41} and a_{42}. Next a_{51} and a_{52} are found, then a_{62} and finally a_{61}, a_{63} and a_{64}. The details are available from the authors. Once the order conditions in S1 and S2 have been satisfied, those in S3 are automatically satisfied.

The order conditions for the order five solution formula are satisfied by setting $b_i = (1 - c_i)b'_i$, $i = 1, \ldots, 7$. The three order conditions for the order four solution formula are satisfied by taking $\widehat{b}_5$, $\widehat{b}_6$ and $\widehat{b}_7$ as free parameters and solving for $\widehat{b}_1$, $\widehat{b}_3$ and $\widehat{b}_4$. The simplifying assumptions used to derive $C1()$ imply $\widehat{b}_2 = 0$.

This completes the derivation of our 4-5 family.

2.3 5-6 PAIRS

During the two decades after the work of Verner [21] and Prince and Dormand [17] on eight-stage 5-6 non-FSAL ERK pairs, the derivation of families of 5-6 pairs was a cottage industry, see for example Calvo, Montijano, Rández [2], Dormand, Lockyer, McGorrigan, Prince [4] and Verner [23]. This industry centred on families of nine-stage FSAL 5-6 pairs. The rewards were notable. The structure of ERK pairs of order six is now well understood and near-optimal nine-stage 5-6 FSAL pairs are significantly more efficient than near-optimal eight-stage non-FSAL 5-6 pairs.

The most general family of 5-6 FSAL ERK pairs is that of Verner [23] and we use this for our 5-6 ERKNG pairs. This means the order conditions in S1 for the order five and six derivative formulae are satisfied using the algorithm described in Verner [23]. This gives c_i, $i = 2, \ldots, 7$, a'_{52} and $\widehat{b'}_7$ as free parameters. The order conditions in S2 for the derivative formulae are satisfied in a similar way to that for the 4-5 pairs, with a_{32}, a_{43}, a_{53}, a_{54}, a_{65}, a_{75}, a_{76} and a_{87} as the free parameters. The order conditions for the order five and six solution formulae are then satisfied by setting $b_i = (1 - c_i)b'_i$, $\widehat{b}_i = (1 - c_i)\widehat{b'}_i$, $i = 1, \ldots, 9$.

2.4 NEAR-OPTIMAL PAIRS

We found near-optimal pairs from each of our new families by doing a constrained minimisation over the free parameters. The objective function was

$$\max\{T_{p+1}, T'_{p+1}\}, \tag{9}$$

where T_{p+1} and T'_{p+1} are the L_2 norms of the order $p+1$ error coefficients of the order p solution and derivative formulae. The constraints are intended to ensure the pair is reliable and are described in detailed by Fine [11], and in less detail by Fine [12] and Sharp and Fine [19]. The simplest constraint is the requirement that $c_i \in [0, 1]$, $i = 2, \ldots, s$. The next constraint is a lower bound on the stability intervals S_R and S'_R along the negative real axis for the solution and derivative formula. The remaining constraints are an upper bound on the ratios C and C' of the L_2 norm of the order $p+1$ and p error coefficients for the order $p-1$ solution and derivative formulae, and an upper bound on the maximum magnitude D of a, a', $\widehat{b}$, $\widehat{b'}$, b and b'.

Table 1 lists T_{p+1}, T'_{p+1}, S_R, S'_R, C, C' and D for the most efficient existing 3-4, 4-5 and 5-6 pairs and the three new pairs we obtained from the minimisation. The norm T_5 for Fine's 3-4 pair is zero because Fine intentionally made the formula order five.

The free parameters for the new 3-4 pair have the values $c_2 = 7/20$, $c_3 = 3/5$, $a_{32} = 3/20$, $a_{43} = 1/5$, $\widehat{b}_3 = \widehat{b}_4 = \widehat{b}_5 = 1/20$ and $\widehat{b'}_5 = 1/10$. The free

Table 1: Some properties of the new and existing 3-4, 4-5 and 5-6 pairs. The definitions of T_{p+1}, T'_{p+1}, S_R, S'_R, C, C' and D are given in the text.

Pair	T_{p+1}	T'_{p+1}	S_R	S'_R	C	C'	D
Fine [12] 3-4	0	5.85×10^{-3}	1.50	1.26	1.88	1.98	6.75
New 3-4	1.35×10^{-2}	2.27×10^{-2}	1.44	1.68	2.07	1.52	1.13
Fine [12] 4-5	4.13×10^{-4}	7.09×10^{-4}	1.91	1.65	1.66	2.47	11.36
New 4-5	3.35×10^{-4}	5.44×10^{-4}	1.95	2.06	2.14	2.50	10.42
Sharp & Fine [19] 5-6	5.82×10^{-4}	9.03×10^{-4}	1.97	1.93	1.96	2.00	6.20
New 5-6	4.37×10^{-5}	6.73×10^{-5}	2.43	1.62	1.33	2.00	7.97

parameters for the new 4-5 pair have the values $c_2 = 29/137$, $c_3 = 239/762$, $c_4 = 109/125$, $c_5 = 886/945$, $a_{32} = 8/315$, $a_{43} = 149/747$, $a_{53} = 63/781$, $a_{54} = -73/17541$, $a_{65} = -90/21983$, $\widehat{b}_5 = -3/100$, $\widehat{b}_6 = 1/10$, $\widehat{b}_7 = 1/10$ and $\widehat{b'}_7 = 4/100$, and those for the new 5-6 pair the values $c_2 = 3/26$, $c_3 = 7836/45487$, $c_4 = 7/22$, $c_5 = 39/68$, $c_6 = 59/80$, $c_7 = 277/278$, $a_{32} = 5/671$, $a_{43} = 4/177$, $a_{53} = -2/97$, $a_{54} = 5/71$, $a_{65} = 4/101$, $a_{75} = 2/9$, $a_{76} = 54/703$, $a_{87} = -1/108568$, $a'_{52} = -8/215$ and $\widehat{b'}_7 = -27/80$. The remaining coefficients of the pairs can then be calculated using the derivation described in the previous subsections.

There is nothing sacrosanct about the above choices for the values of the free parameters and it is possible to obtained pairs with smaller error coefficients, particularly if less restrictive constraints are used. Hence we view the pairs we chose as near-optimal and not optimal.

We observe from Table 1 that T'_5 for the new 3-4 pair is approximately four times larger than that for Fine's 3-4 pair. This difference is sufficiently large that the new 3-4 pair will likely be less efficient than Fine's 3-4 pair even though the new pair requires one fewer derivative evaluation on most steps.

We also observe from Table 1 that T_6 and T'_6 for the new 4-5 pair are smaller than those for Fine's 4-5 pair. If we assume the number of derivative evaluations required to achieve a specified accuracy is proportional to $T_6^{1/5}$ or $T_6'^{1/5}$, we expect the new 4-5 pair will be only a few percent more efficient than Fine's 4-5 pair.

The situation is markedly different for the two 5-6 pairs. T_7 and T_7' for the new 5-6 pair are an order of magnitude smaller than for the 5-6 pair of Sharp and Fine [19] (note that the definition of T_7 and T_7' used by Sharp and Fine is different from ours). Hence we expect that the new 5-6 pair will be noticeably more efficient than the existing 5-6 pair on most problems.

3 NUMERICAL COMPARISONS

To test our predictions from the last section, we compared the performance of the three new and three existing pairs on problems E1, E2, E4 and E5 from non-stiff DETEST [6]. The comparisons were done for error tolerances of 10^{-i}, $i = 2, \ldots, 10$. Figures 1, 2 and 3 are $\log_{10} - \log_{10}$ plots of the number of derivative evaluations as a function of the L_2 norm of the end-point global error.

Figure 1 shows that while Fine's [12] pair is usually more efficient than the new 3-4 pair, this is not always the case, partly confounding our prediction from the previous section. One possible explanation for this unexpected behaviour is that using a norm to measure the size of error coefficients can wrongly measure the effect of individual error coefficients and the terms they represent.

In Figure 2, the solid and dashed lines lie close to one another, confirming our prediction that the new 4-5 pair and that of Fine [12] would have similar efficiency. The new 5-6 pair, see Figure 3, is either of similar efficiency or more efficient than the 5-6 pair of Sharp and Fine [19], also confirming our prediction.

4 DISCUSSION

Our aim was to add significantly to the theory of explicit Runge–Kutta Nystrom pairs for the general second order problem and to find pairs that were more efficient than existing pairs. We derived new families of 3-4, 4-5 and 5-6 pairs and performed a constrained minimisation on the error coefficients to find a near-optimal pair for each family. We then used numerical testing to compare the efficiency of the new pairs with existing pairs.

With the 3-4 pairs, we sought to improve the efficiency by reducing the number of derivative evaluations per step. The existing family of 3-4 pairs uses five evaluations per accepted step. We reduced this to four in our family for all accepted steps except the first by re-using the last stage as the first stage on the next step, a technique known as FSAL.

Using FSAL in this way had the drawback of reducing the number of free parameters in the family. This meant the error coefficients of the new near-optimal pair were not as small as that from the existing family. Our numerical testing showed the new pair was often less efficient that the existing pair. We thus have an example of where minimising the cost per step does not maximise the efficiency.

We took a different approach with the 4-5 pairs. The existing family of 4-5 pairs uses seven stages and FSAL. We sought to reduce the size of the error coefficients and hence increase the efficiency by deriving a family of seven-stage FSAL pairs with more free parameters than the existing family. We found such a family and a near-optimal pair in it with smaller error coefficients than the most efficient existing 4-5 pair. However, the reduction in size was not large enough to give a noticeable increase in efficiency.

We used yet another approach for the 5-6 pairs. The existing family of 5-6 pairs has eight stages and does not use FSAL. We sought to improve the efficiency by using nine-stages and FSAL, thus keeping the number of derivative evaluations per step at eight, and reducing the size of the error coefficients. We found a near-optimal pair from the new family whose error coefficients were an order of magnitude smaller than the existing near-optimal 5-6 pair. We confirmed the superior efficiency of the new 5-6 pair numerically.

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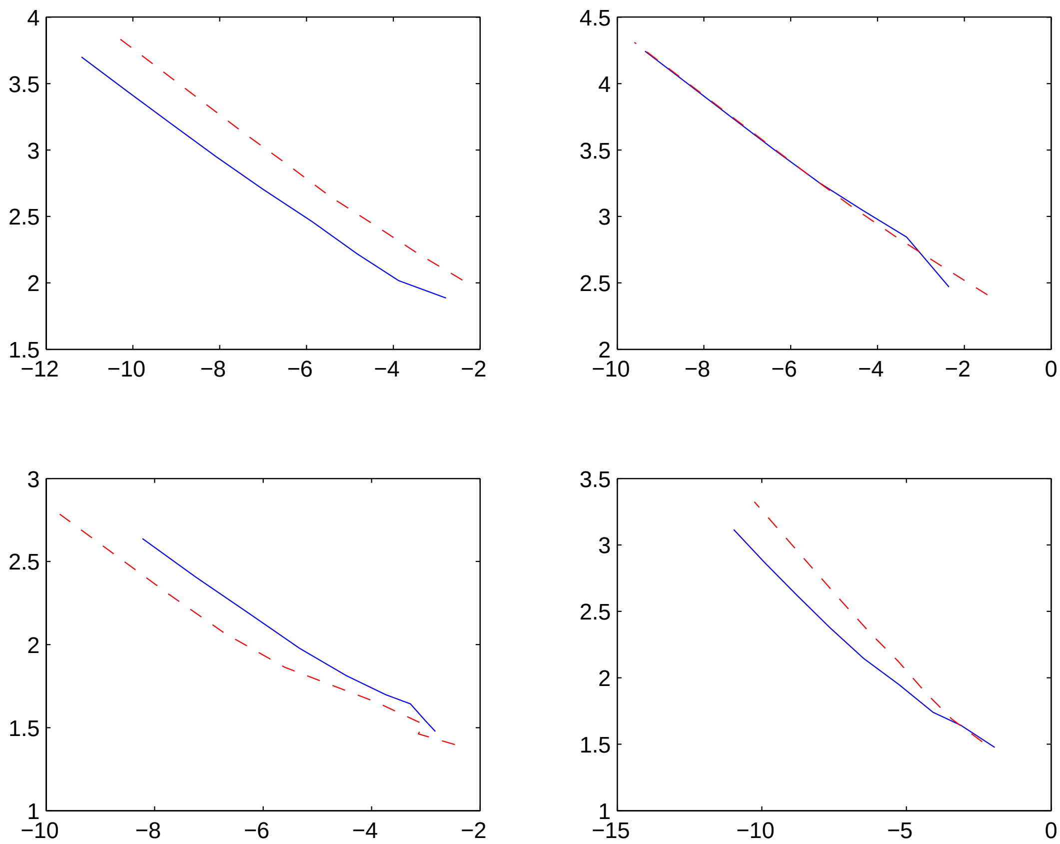

Figure 1: The number of derivative evaluations as a function of the L_2 norm of the end-point global error for Fine's 3-4 pair [12] (solid line) and the new 3-4 pair (dashed line) for problems E1 (top left), E2 (top right), E4 (bottom left) and E5 (bottom right). The horizontal and vertical axes are base-10 logarithms.

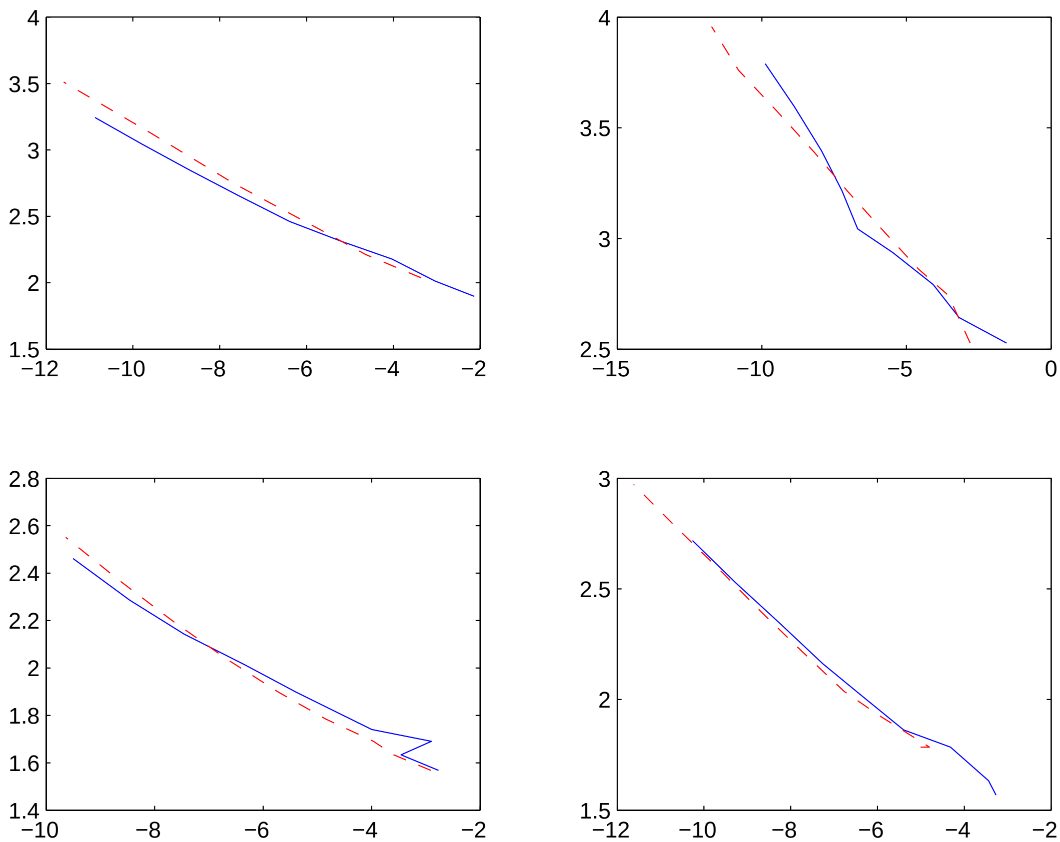

Figure 2: The number of derivative evaluations as a function of the L_2 norm of the end-point global error for Fine's 4-5 pair [12] (solid line) and the new 4-5 pair (dashed line) for problems E1 (top left), E2 (top right), E4 (bottom left) and E5 (bottom right). The horizontal and vertical axes are base-10 logarithms.

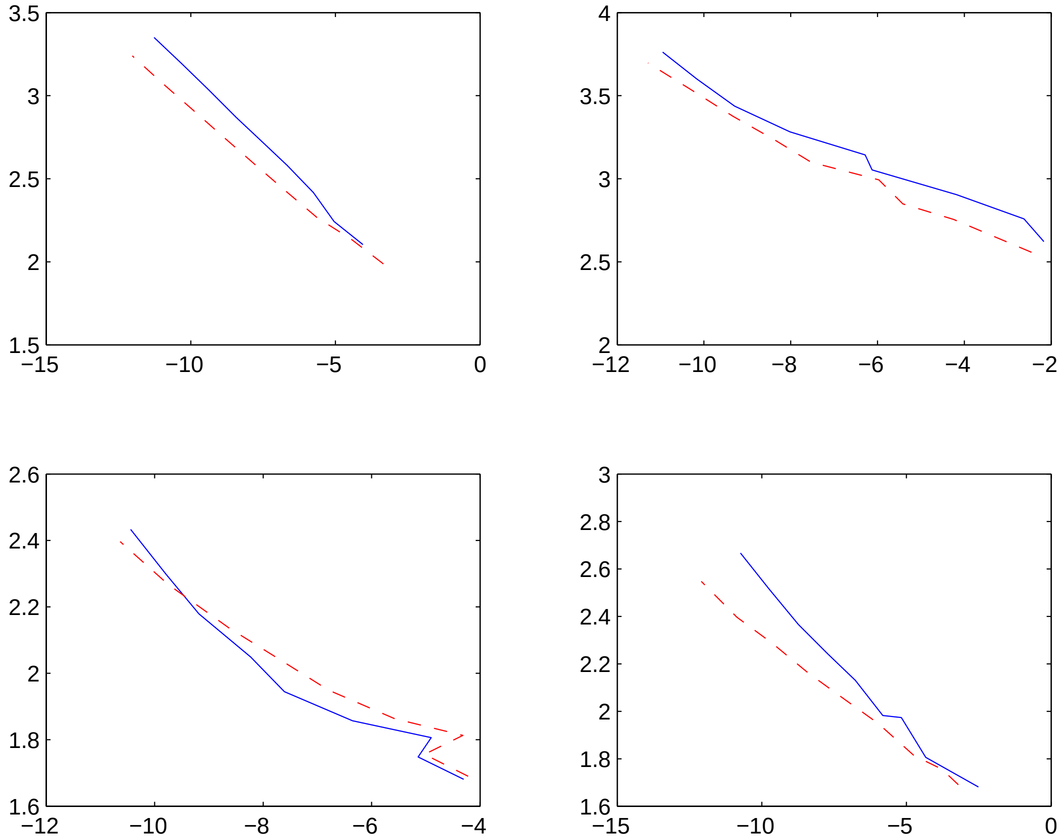

Figure 3: The number of derivative evaluations as a function of the L_2 norm of the end-point global error for Sharp and Fine's 5-6 pair [19] (solid line) and the new 5-6 pair (dashed line) for problems E1 (top left), E2 (top right), E4 (bottom left) and E5 (bottom right). The horizontal and vertical axes are base-10 logarithms.