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СТАБИЛИЗИРОВАННЫЕ ЯВНЫЕ МЕТОДЫ ТИПА АДАМСА

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Представлены явные многошаговые методы типа Адамса с расширенным интервалом устойчивости, аналогичные явным стабилизированным чебышевским методам типа Рунге – Кутты. Доказано, что для любого $k \geq 1$ существует явный k-шаговый метод типа Адамса первого порядка с интервалом устойчивости длиной $2k$. Коэффициенты и константа погрешности таких методов имеют весьма простой вид. Получена также демпфированная модификация этих методов. В общем случае для построения k-шагового метода порядка p необходимо решить задачу условной оптимизации, в которой целевая функция и p ограничений являются многочленами второй степени от k переменных. Численно построены методы до шестого порядка включительно, проведены несколько вычислительных экспериментов для подтверждения свойств аппроксимации и устойчивости.

Ключевые слова: численное решение ОДУ; жесткость; интервал устойчивости; абсолютная устойчивость; многошаговые методы; методы типа Адамса; явные методы.

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STABILISED EXPLICIT ADAMS-TYPE METHODS

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In this work we present explicit Adams-type multi-step methods with extended stability intervals, which are analogous to the stabilised Chebyshev Runge – Kutta methods. It is proved that for any $k \geq 1$ there exists an explicit k-step Adams-type method of order one with stability interval of length $2k$. The first order methods have remarkably simple expressions for their coefficients and error constant. A damped modification of these methods is derived. In the general case, to construct a k-step method of order p it is necessary to solve a constrained optimisation problem in which the objective function and p constraints are second degree polynomials in k variables. We calculate higher-order methods up to order six numerically and perform some numerical experiments to confirm the accuracy and stability of the methods.

Keywords: numerical ODE solution; stiffness; stability interval; absolute stability; multi-step methods; Adams-type methods; explicit methods.

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Introduction

A k-step explicit Adams-type method for the numerical integration of the ordinary differential equation system

$$y' = f(t, y),\ y(t_0) = y_0,\ y : \mathbb{R} \to \mathbb{R}^n,\ f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n,$$

on a uniform grid has the form

$$y_{m+k} = y_{m+k-1} + \tau\left(\beta_0 f_m + \ldots + \beta_{k-1} f_{m+k-1}\right), \tag{1}$$

where m is the step number, $y_l \approx y(t_0 + l\tau)$, $f_l = f(t_0 + l\tau, y_l)$, $l \geq 0$, τ is a discretisation step, and $\{\beta_j\}$, $j = 0, 1, \ldots, k-1$, are the coefficients for the method.

A conventional means of analysing the linear stability of a multi-step method is through the construction of a stability region $S \subset \mathbb{C}$ such that for all $\lambda\tau \in S$ the numerical solution of the model linear problem

$$y' = \lambda y,\ \lambda \in \mathbb{C},$$

remains bounded for all m. The equivalent requirement is that all roots ζ_j of the characteristic equation

$$\rho(\zeta) - \lambda\tau\sigma(\zeta) = 0 \tag{2}$$

lie within the unit disc on the complex plane, and all the roots of modulus one are simple [1]. Here ρ and σ are the standard generating polynomials which in our case have the form

$$\rho(\zeta) = \zeta^k - \zeta^{k-1},\ \sigma(\zeta) = \sum_{j=0}^{k-1} \beta_j \zeta^j.$$

The stability interval of a method is the largest interval of the real axis of the form $[-\ell, 0]$ contained in S. Here $\ell \geq 0$ is the value which will be referred to as the length of the stability interval. As is known, stability intervals of the classical explicit Adams methods are small and get smaller with the growth of k, so these methods are not suitable for stiff problems. The purpose of the present research is to construct explicit multi-step methods of Adams type (1) of order $p < k$ with increased lengths of stability intervals. Putting it in other words, we develop a multi-step analog of the well-known Chebyshev Runge – Kutta methods [2–5].

The main obstacle for the way of construction of multi-step methods for stiff problems is the dependence of the error constant on the size of stability region, which was investigated by Jeltsch and Nevanlinna [6; 7]. On the one hand, due to [5, theorem 4.2], for any $k > 1$, $\alpha < \frac{\pi}{2}$ and $R > 0$ there exists an explicit linear multi-step method of order $k - 1$ such that the method is stable in the set

$$\{\mu \in \mathbb{C} : |\mu| \leq R,\ |\arg(-\mu)| \leq \alpha\}.$$

Unfortunately, methods which stability regions contain large disks of the form $\{\mu \in \mathbb{C} : |\mu + R| \leq R\}$ are useless in practice due to huge error constants (norms of Peano kernels) [6, theorem 4.1; 1, chapter V.2, theorem 2.6].

On the other hand, in the case of long stability intervals the lower bounds for the error constant are less restrictive. Namely [6, theorem 4.4] gives a lower bound for Peano kernel norms for explicit multi-step methods in the form of $C_k \ell$, where $C_k > 0$. Another interesting fact from [6, theorem 4.7] is that for explicit k-step methods of order $k - 1$ with $\ell > 2$ the error constant has lower bound equal to $\delta_{k-1}\frac{\ell - 2}{2^{k-1}}$, where (δ_k) is a decreasing sequence with $\delta_1 = 0.5$. Thus, we hope that explicit multi-step methods with extended stability interval can have reasonable error constants (see section «Higher order methods»).

The material is organised as follows. In section «Optimisation strategy» we describe the general framework of the method's construction, sections «First order methods» and «First order methods with damping» are devoted to the first order methods and their damped modifications. Higher order methods are discussed in section «Higher order methods», and section «Numerical experiments» contains the results of numerical experiments. In the last section we discuss the obtained results and make final conclusions.

Optimisation strategy

The conventional way of constructing a stability region is to find a root locus curve $\mathcal{C}$ defined as

$$\mathcal{C} = \left\{\mu_\beta\left(e^{i\varphi}\right) : \varphi \in [0, 2\pi)\right\}, \tag{3}$$

where the function $\mu_\beta : \mathbb{C} \to \mathbb{C}$ maps a root of the characteristic equation (2) to the corresponding value of $\lambda\tau$:

$$\mu_\beta(\zeta) = \frac{\rho(\zeta)}{\sigma(\zeta)}. \tag{4}$$

The subscript β indicates the dependence on the coefficients of method (1) which we are to be determined. From the definition of stability region it follows that $\partial S \subseteq \mathcal{C}$ and

$$\ell \leq \mu_\beta(-1),$$

thus the optimisation problem can be stated as

$$\beta^* = \underset{\beta \in \mathcal{F} \cap \mathcal{P}}{\operatorname{argmin}}\, \mu_\beta(-1), \tag{5}$$

where $\mathcal{P}$ is a set of coefficients which satisfy the posed order conditions, and $\mathcal{F}$ is a feasible set of coefficients with a desired shape of the root locus curve. This set is defined as follows.

Primarily we would like to have $\ell = -\mu_\beta(-1)$ for all $\beta \in \mathcal{F}$. To assure this we require the locus curve (3) not to cross the real axis before the parameter φ reaches π. This condition triggers the following definition for the feasible set:

$$\mathcal{F} = \left\{\beta \in \mathbb{R}^k : \operatorname{Im}\mu_\beta\left(e^{i\varphi}\right) \geq 0 \ \forall\varphi \in (0, \pi)\right\}. \tag{6}$$

The main question now is how to find a parametrisation of $\mathcal{F}$ which allows the reduction of (5), (6) to some manageable form. We start by noting that

$$\operatorname{Im}\mu_\beta\left(e^{i\varphi}\right) \geq 0 \Leftrightarrow \nu_\beta(\varphi) \geq 0,$$

where

$$\nu_\beta(\varphi) = \operatorname{Im}\rho\left(e^{i\varphi}\right)\overline{\sigma\left(e^{i\varphi}\right)} = \sum_{j=1}^{k}\left(\beta_{k-j} - \beta_{k-j-1}\right)\sin j\varphi. \tag{7}$$

From here we set $\beta_j = 0$ for all $j < 0$ and $j > k - 1$. By utilising the Chebyshev polynomials of the second kind U_j,

$$U_{j-1}(\cos\varphi)\sin\varphi = \sin j\varphi,$$

and using the power reduction formulae for the powers of $\cos\varphi$, (7) can be represented as

$$\nu_\beta(\varphi) = \sin\varphi\sum_{j=0}^{k-1} a_j \cos j\varphi \tag{8}$$

with some $a_j \in \mathbb{R}$. Since we need $\nu_\beta(\varphi)$ to be non-negative on $(0, \pi)$, the following result from [7, lemma 6.1.3] is useful.

Lemma. *For any non-negative trigonometric polynomial a of the form*

$$A(\varphi) = \sum_{j=0}^{k} a_j \cos j\varphi,\ a_j \in \mathbb{R},$$

there exists a trigonometric polynomial

$$B(\varphi) = \sum_{j=0}^{k} b_j e^{ij\varphi},\ b_j \in \mathbb{R},$$

such that $A(\varphi) = |B(\varphi)|^2$.

From this lemma it follows that all feasible trigonometric polynomials ν_β have the form

$$\nu_\beta(\varphi) = \sin\varphi \left| \sum_{j=0}^{k-1} b_j e^{ij\varphi} \right|^2 = \sin\varphi \sum_{j,l=0}^{k-1} b_j b_l \cos(j-l)\varphi \tag{9}$$

with $b_j \in \mathbb{R}$. To complete the transformation of the optimisation problem we must express the original coefficients $\{\beta_j\}$ in terms of $\{b_j\}$. This can be done by converting (8) to the same basis of $\sin j\varphi$ as (7):

$$\sin\varphi \sum_{j=0}^{k-1} a_j \cos j\varphi = \frac{1}{2} \sum_{j=0}^{k-1} a_j \left(\sin(j+1)\varphi - \sin(j-1)\varphi\right).$$

By equating this expression with (7) it is straightforward to get

$$\beta_j = \frac{1}{2}\left(\tilde{a}_{j-1} + \tilde{a}_j\right),\ j = 0, 1, \ldots, k-2, \tag{10}$$

$$\beta_{k-1} = \tilde{a}_{k-1} + \frac{\tilde{a}_{k-2}}{2}. \tag{10a}$$

Here for clarity $\tilde{a}_j = a_{k-1-j}$, $\tilde{a}_{-1} = 0$. Conversely, from (8), (9) we have

$$\tilde{a}_j = 2\sum_{l=0}^{j} b_l b_{k-1+l-j},\ j = 0, 1, \ldots, k-2, \tag{10b}$$

$$\tilde{a}_{k-1} = \sum_{j=0}^{k-1} b_j^2. \tag{10c}$$

Transformations (10)–(10c) define the required mapping

$$T : b \to \beta,$$

where $b = (b_0, \ldots, b_{k-1})$, $\beta = (\beta_0, \ldots, \beta_{k-1})$.

Now let us derive the form of objective function (5),

$$\mu_\beta(-1) = \frac{2 \cdot (-1)^k}{\sum_{j=0}^{k-1} (-1)^j \beta_j}, \tag{11}$$

in terms of b. By direct application of (10)–(10c) we have

$$\sum_{j=0}^{k-1} (-1)^j \beta_j = (-1)^k \sum_{j=0}^{k-1} b_j^2,$$

so the initial optimisation problem (5), (6) finally takes the surprisingly simple form

$$b^* = \underset{\beta \in \mathcal{P}_p'}{\operatorname{argmin}} \sum_{j=0}^{k-1} b_j^2, \tag{12}$$

where $\mathcal{P}_p'$ is the order p restriction set:

$$\mathcal{P}_p' = \left\{ b \in \mathbb{R}^k : G_q(T(b)) = 0,\ q = 1, 2, \ldots, p \right\}, \tag{12a}$$

$$G_1(\beta) = \sum_{j=0}^{k-1} \beta_j - 1, \tag{12b}$$

$$G_q(\beta) = \sum_{j=0}^{k-1} (1-k+j)^{q-1} \beta_j - \frac{1}{q},\ q > 1. \tag{12c}$$

First order methods

Theorem 1. *For any number of steps $k > 1$ there exists a first order explicit Adams-type method with stability interval of length 2k. The method has the form*

$$y_{k+m} = y_{k+m-1} + \frac{\tau}{k^2}\left(f_m + 3f_{m+1} + \ldots + (2k-1)f_{m+k-1}\right), \tag{13}$$

i. e., $\beta_j = \dfrac{2j+1}{k^2}.$

P r o o f. Directly applying (10)–(10c) to the first order condition (12b) we have

$$\beta_0 + \beta_1 + \ldots + \beta_{k-1} = a_0 + a_1 + \ldots + a_{k-1} = 1.$$

Conversely, by the construction form (8), (9) we have

$$\sum_{j=0}^{k-1} a_j = \sum_{j,\,l}^{k-1} b_j b_l = \left(\sum_{j=1}^{k-1} b_j\right)^2.$$

Thus, the optimisation problem (12)–(12c) in the case of $p = 1$ takes the form

$$b^* = \operatorname*{argmin}_{b \in \mathbb{R}^k}\left(b_0^2 + b_1^2 + \ldots + b_{k-1}^2\right),$$

subject to

$$\left(b_0 + b_1 + \ldots + b_{k-1}\right)^2 = 1.$$

Solving this problem by the method of Lagrange multipliers, we get $b_j^* = k^{-1}$ for all j and then by (10)–(10c) obtain

$$\beta^* = T\left(b^*\right) = \left(\frac{1}{k^2}, \frac{3}{k^2}, \ldots, \frac{2k-1}{k^2}\right).$$

By construction of the method from (11) and since

$$\sum_{j=0}^{k-1}(-1)^j \frac{2j+1}{k^2} = (-1)^k \frac{1}{k}, \tag{14}$$

we have $\ell = -\mu_{\beta^*}(-1) = 2k.$

There is an interesting parity of the above result with the case of s-stage Chebyshev Runge – Kutta methods of order 1, which require s evaluations of f per step and have stability interval equal to $2s^2$ [1; 2]. This allows us to suppose that the achieved length of $2k$ is the largest possible for explicit first order multi-step methods.

Error constant. According to [9] we define the error constant of the multi-step method as

$$C = \frac{C_{p+1}}{\sigma(1)},$$

where

$$C_{p+1} = \frac{1}{(p+1)!}\sum_{j=0}^{k}\left(a_j j^{p+1} - (p+1)\beta_j j^p\right).$$

It is easy to calculate this constant in our case.

Proposition 1. *The error constant of the optimised first order methods is equal to*

$$C = \frac{k}{3} + \frac{1}{6k}.$$

P r o o f. Since $\beta_j = \dfrac{2j+1}{k^2}$, $\alpha_k = 1$, $\alpha_{k-1} = -1$, $\sigma(1) = 1$, we have

$$C = \frac{1}{2}\left(k^2 - (k-1)^2 - \frac{2}{k^2}\sum_{j=0}^{k} j(2j+1)\right) = \frac{k}{3} + \frac{1}{6k}.$$

First order methods with damping

Analogously to the Chebyshev Runge – Kutta methods, in order to pull the root locus curve away from the real axis for $\varphi \in (0, \pi)$ it is necessary to perform a damping transformation with the constructed methods.

Using (7), (8) consider (4) and represent

$$\operatorname{Im}\mu_\beta\left(e^{i\varphi}\right) = Q(\varphi)\sin\varphi,$$

where

$$Q(\varphi) = \frac{\sum_{j=0}^{k-1} a_j \cos j\varphi}{\left|\sigma\left(e^{i\varphi}\right)\right|^2} = \frac{\sum_{j=0}^{k-1} a_j \cos j\varphi}{\sum_{j=0}^{k-1} \delta_j \cos j\varphi}, \tag{15}$$

and

$$\delta_0 = \sum_{j=0}^{k-1} \beta_j^2,\ \delta_j = 2\sum_{l=0}^{j} \beta_l \beta_{j+l}. \tag{16}$$

Recall that the connection between coefficients a_j and β_j is described by the first two equalities of (10)–(10c).

Let $\hat{Q}(\varphi)$ be the damped method's counterpart of (15). We define it as

$$\hat{Q}(\varphi) = \frac{\sum_{j=0}^{k-1} \hat{a}_j \cos j\varphi}{\sum_{j=0}^{k-1} \hat{\delta}_j \cos j\varphi} = C\left(Q(\varphi) + \varepsilon\right),$$

where ε controls the «shift» from the real axis and C is a scaling constant to be determined. Then we have $\hat{a}_j = Ca'_j$,

$$a'_j = a_j + \varepsilon\delta_j.$$

Now we use this equality together with (10)–(10c) and get

$$\beta'_j = \beta_j + \frac{\varepsilon}{2}\left(\delta_{k-j} + \delta_{k-j-1}\right),\ j = 0, 1, \ldots, k-2,$$

$$\beta'_{k-1} = \beta_{k-1} + \frac{\varepsilon}{2}\delta_1 + \varepsilon\delta_0,\ \delta_k = 0.$$

The coefficients $\hat{\beta}_j$ of the sought damped method are expressed as $\hat{\beta}_j = C\beta'_j$. To keep the order of the method equal to one, the constant C should be equal to $\left(\sum_{j=0}^{k-1} \beta'_j\right)^{-1}$. By (16) we have

$$\sum_{j=0}^{k-1} \beta'_j = \sum_{j=0}^{k-1} \beta_j + \varepsilon\sum_{j=0}^{k-1} \delta_j = \sum_{j=0}^{k-1} \beta_j + \varepsilon\sum_{j,l=0}^{k-1} \beta_j\beta_l.$$

Since $\sum_{j=0}^{k-1} \beta_j = 1$ we finally obtain the following formulae for the coefficients of the damped method:

$$\hat{\beta}_j = \frac{\beta_j + \varepsilon\Delta_j}{1+\varepsilon},\ j = 0, 1, \ldots, k-1, \tag{17}$$

where

$$\Delta_j = \frac{1}{2}\left(\delta_{k-j} + \delta_{k-j-1}\right),\ j = 0, 1, \ldots, k-2, \tag{17a}$$

$$\Delta_{k-1} = \frac{1}{2}\delta_1 + \delta_0. \tag{17b}$$

The values of Δ_j for k from 2 to 10 for the optimised first order method (13) are presented in table 1. The stability region boundaries of the one-step methods together with their damped counterparts are displayed in fig. 1.

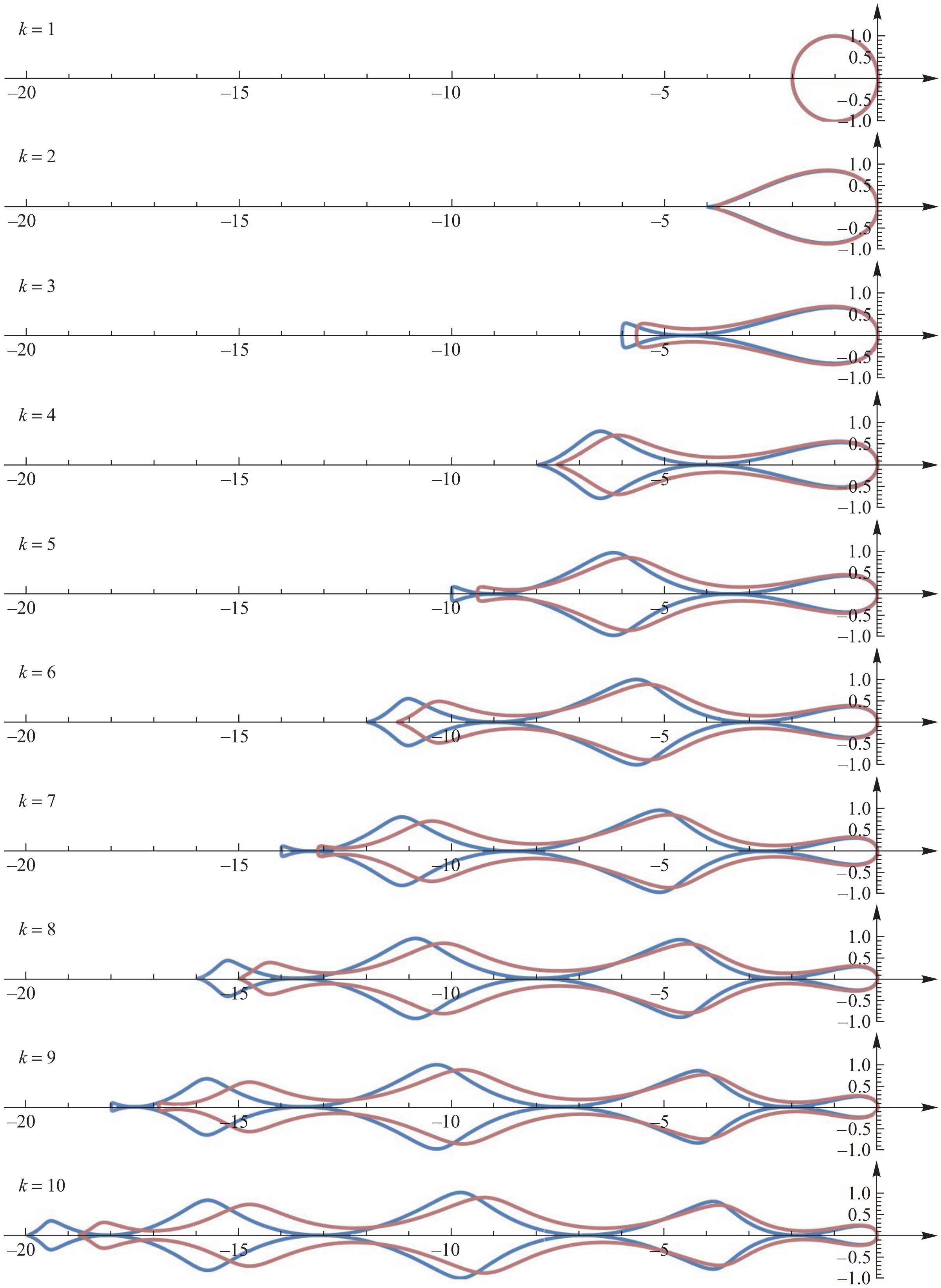

Fig. 1. Stability regions of the optimised first order methods and their damped versions (ε = 0.25) for $k = 1, \ldots, 10$

Table 1

The values of Δ_j for determining the coefficients of the optimised first order methods with damping (17), $\beta_j = \frac{2j+1}{k^2}$

k	Δ_0	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5	Δ_6	Δ_7	Δ_8	Δ_9
2	$\frac{3}{16}$	$\frac{13}{16}$								
3	$\frac{5}{81}$	$\frac{23}{81}$	$\frac{53}{81}$							
4	$\frac{7}{256}$	$\frac{33}{256}$	$\frac{79}{256}$	$\frac{137}{256}$						
5	$\frac{9}{625}$	$\frac{43}{625}$	$\frac{21}{625}$	$\frac{187}{625}$	$\frac{281}{625}$					
6	$\frac{11}{1296}$	$\frac{53}{1296}$	$\frac{131}{1296}$	$\frac{79}{1296}$	$\frac{121}{1296}$	$\frac{167}{1296}$				
7	$\frac{13}{2401}$	$\frac{9}{343}$	$\frac{157}{2401}$	$\frac{41}{343}$	$\frac{445}{2401}$	$\frac{89}{343}$	$\frac{813}{2401}$			
8	$\frac{15}{4096}$	$\frac{73}{4096}$	$\frac{183}{4096}$	$\frac{337}{4096}$	$\frac{527}{4096}$	$\frac{745}{4096}$	$\frac{983}{4096}$	$\frac{1233}{4096}$		
9	$\frac{17}{6561}$	$\frac{83}{6561}$	$\frac{209}{6561}$	$\frac{43}{729}$	$\frac{203}{2187}$	$\frac{289}{2187}$	$\frac{1153}{6561}$	$\frac{1459}{6561}$	$\frac{1777}{6561}$	
10	$\frac{19}{10\,000}$	$\frac{93}{10\,000}$	$\frac{47}{2000}$	$\frac{437}{10\,000}$	$\frac{691}{10\,000}$	$\frac{989}{10\,000}$	$\frac{1323}{10\,000}$	$\frac{337}{2000}$	$\frac{2067}{10\,000}$	$\frac{2461}{10\,000}$

Proposition 2. *The stability interval of the damped method (17)–(17b) with* $\beta_j = \beta_j^* = \frac{2j+1}{k^2}$ *is equal to* $[-\ell_\varepsilon, 0]$, *where*

$$\ell_\varepsilon = \frac{6(1+\varepsilon)k^3}{\varepsilon(4k^2-1)+3k^2}.$$

P r o o f. Let us compute

$$\sum_{j=0}^{k-1}(-1)^j\hat{\beta}_j = (1+\varepsilon)^{-1}\left(\sum_{j=0}^{k-1}(-1)^j\beta_j^* + \varepsilon(-1)^{k-1}\delta_0^*\right).$$

The first term has already been calculated in (14) and the second is determined as

$$\delta_0^* = \sum_{j=0}^{k-1}\left(\beta_j^*\right)^2 = \sum_{j=0}^{k-1}\frac{(2j+1)^2}{k^4} = \frac{4k^2-1}{3k^3}.$$

From here we finally get

$$\mu_{\hat{\beta}}(-1) = \frac{2(-1)^k}{\sum_{j=0}^{k-1}(-1)^j\hat{\beta}_j} = -\frac{6(1+\varepsilon)k^3}{\varepsilon(4k^2-1)+3k^2}.$$

Corollary 1. *The asymptotic length of the damped one-step method is*

$$\lim_{\varepsilon\to\infty}\ell_\varepsilon = \frac{3}{2}k.$$

Higher order methods

To construct a stabilised k-step Adams-type method of order p one should use the general form of the optimisation problem (12)–(12c) with mapping T specified by (10)–(10c). For example, for $k = 5$, $p = 4$, the problem in terms of b_j takes the form

minimise

$$b_0^2 + b_1^2 + b_2^2 + b_3^2 + b_4^2$$

subject to

$$\left(b_0 + b_1 + b_2 + b_3 + b_4\right)^2 = 1,$$

$$b_2 b_3 + \left(3b_2 + b_3\right)b_4 + b_1\left(b_2 + 3b_3 + 5b_4\right) + b_0\left(b_1 + 3b_2 + 5b_3 + 7b_4\right) = -\frac{1}{2},$$

$$b_2 b_3 + \left(5b_2 + b_3\right)b_4 + b_1\left(b_2 + 5b_3 + 13b_4\right) + b_0\left(b_1 + 5b_2 + 13b_3 + 25b_4\right) = \frac{1}{3},$$

$$b_2 b_3 + \left(9b_2 + b_3\right)b_4 + b_1\left(b_2 + 9b_3 + 35b_4\right) + b_0\left(b_1 + 9b_2 + 35b_3 + 91b_4\right) = -\frac{1}{4}.$$

The symbolic solution of this problem yielded by *Wolfram Mathematica* after transforming back to the initial variables β_j is

$$\beta^* = \left(-\frac{1}{4}, \frac{5}{8}, \frac{1}{24}, -\frac{35}{24}, \frac{49}{24}\right)$$

with $\ell = 0.75$, to compare with $\ell = 0.3$ for the classical explicit Adams-type method of order 4. Another neat example is the 5-step method of order 2:

$$\beta^* = \left(-\frac{1}{8}\left(3-\sqrt{5}\right), -\frac{3}{4}\left(\sqrt{5}-2\right), 0, \frac{7}{4}\left(\sqrt{5}-2\right), \frac{9}{8}\left(3-\sqrt{5}\right)\right)$$

with $\ell = 2 + \dfrac{4}{\sqrt{5}} \approx 3.789$. The stability regions of these and the rest of the 5-step methods are shown in the uppermost part of fig. 2.

Unfortunately, it is not always possible to obtain the solution symbolically, thus we compute the coefficients of our methods numerically using *Mathematica's* function `NMinimise`, see the corresponding code in Appendix A. We used 50-digit working precision and computed the (k, p) methods for k from 3 to 10 and p from 2 to k (with the latter value corresponding to the classical Adams methods). The results with 20-digit accuracy are displayed in tables 3 and 4. It is interesting that the (4, 3) method coincides with [9, formula (5.4)]. The stability regions of 5-, 6- and 7-step methods are shown in fig. 2.

To assess the accuracy of the obtained coefficients we checked the magnitude of the order residuals $G_q\left(\beta^*\right)$ see (12b), (12c). In all convergent cases these residuals do not exceed 10^{-19}. Note that *Mathematica's* function `NMinimise` failed to converge in the following cases: $(k, p) = (7, 6)$ and for all $p > 7$. Our hypothesis is that for these (k, p) combinations the Adams-type methods satisfying our restrictions do not exist. Note that (11, 7) method seems to exist and has microscopic $\ell \approx 0.051$ which is just slightly more than $\ell = 0.0465$ for the (7, 7) case. The error constants of all the calculated methods are presented in table 2.

Table 2

Error constants of the stabilised Adams-type methods

k	$p = 1$	$p = 2$	$p = 3$	$p = 4$	$p = 5$	$p = 6$
2	0.75					
3	1.0556	0.66667				
4	1.375	1.0380	0.62500			
5	1.7	1.5208	1.0227	0.59861		
6	2.0278	2.1128	1.5972	1.0120	0.57928	
7	2.3571	2.8134	2.3814	1.6471	1.0032	
8	2.6875	3.6223	3.4092	2.5751	1.6825	0.99505
9	3.0185	4.5392	4.7148	3.8788	2.7235	1.7079
10	3.35	5.5643	6.3328	5.6524	4.2616	2.8403

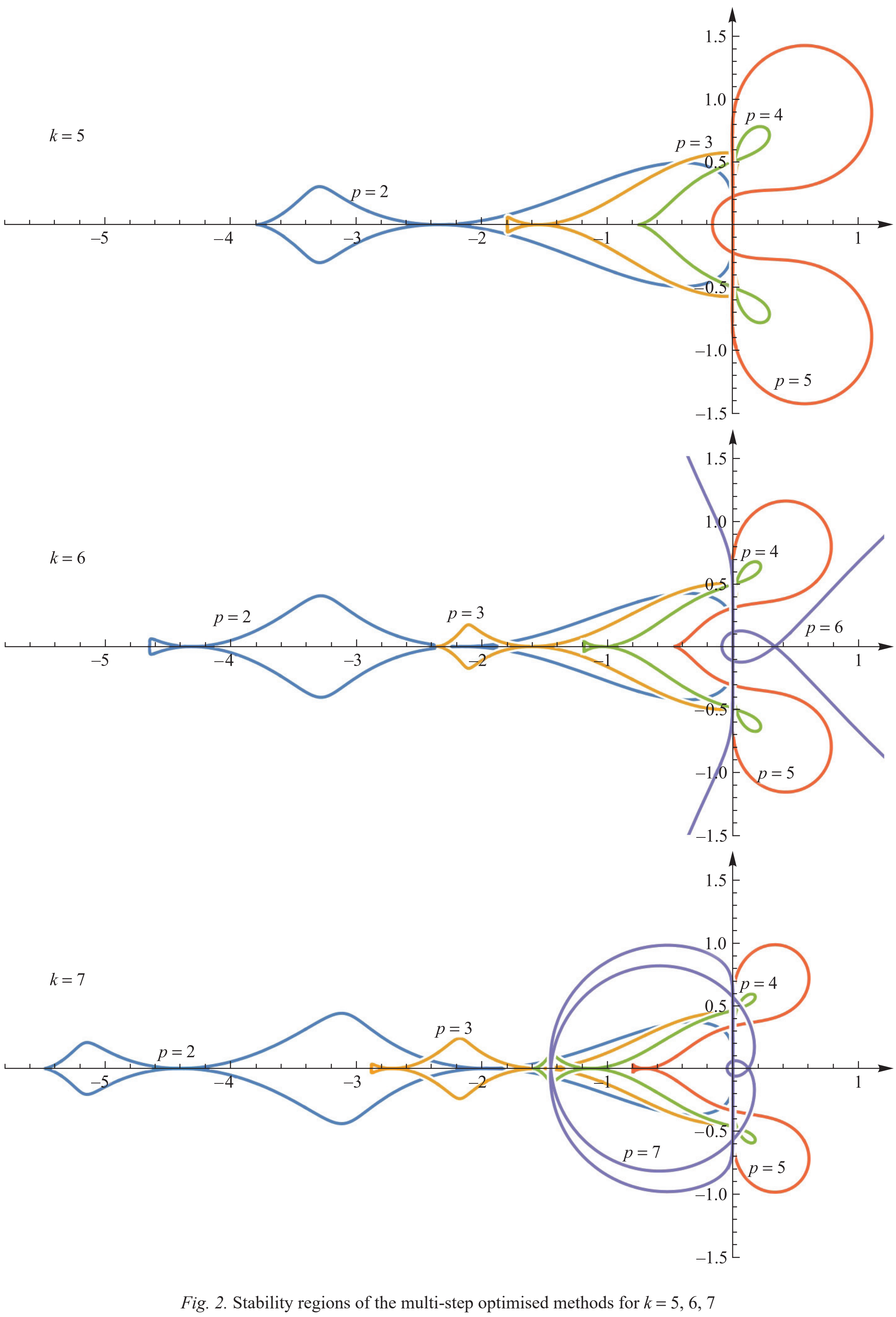

Fig. 2. Stability regions of the multi-step optimised methods for $k = 5, 6, 7$

Coefficients and stability interval lengths

k	Order 2	Order 3
3	ℓ = 2 –0.25 0 1.25	ℓ = 0.545 454 545 454 545 455 0.416 666 666 666 666 666 67 –1.333 333 333 333 333 333 3 1.916 666 666 666 666 666 7
4	ℓ = 2.914 213 562 373 095 –0.146 446 609 406 730 460 69 –0.181 980 515 339 459 636 91 0.303 300 858 899 110 655 90 1.025 126 265 847 079 441 7	ℓ = 1.2 0.25 –0.333 333 333 333 333 333 33 –0.583 333 333 333 333 333 33 1.666 666 666 666 666 666 7
5	ℓ = 3.788 854 381 999 832 –0.095 491 502 812 526 287 949 –0.177 050 983 124 842 272 31 0 0.413 118 960 624 631 968 72 0.859 423 525 312 736 591 54	ℓ = 1.793 779 334 348 686 0.164 376 941 012 461 256 19 –0.009 791 091 775 013 643 927 1 –0.540 221 704 083 059 938 67 –0.047 691 080 558 684 215 630 1.433 326 935 404 296 542 0
6	ℓ = 4.642 734 410 091 836 –0.066 987 298 107 786 995 665 –0.147 114 317 029 978 077 15 –0.089 745 962 155 603 046 598 0.125 644 347 017 869 431 07 0.441 342 951 089 917 564 59 0.736 860 279 185 581 123 75	ℓ=2.347 826 086 956 522 0.115 740 740 740 747 316 06 0.087 962 962 962 956 387 640 –0.287 037 037 037 050 187 68 –0.407 407 407 407 394 256 76 0.245 370 370 370 376 945 69 1.245 370 370 370 363 795 0
7	ℓ = 5.484 476 959 454 063 –0.049 515 566 048 790 436 882 –0.119 125 202 772 785 772 27 –0.110 182 500 025 524 205 85 0 0.198 328 500 045 943 570 54 0.436 792 410 166 881 165 01 0.643 702 358 634 275 679 47	ℓ = 2.877 558 710 633 067 0.085 721 156 820 309 456 282 0.111 546 128 114 633 279 41 –0.117 210 331 348 086 366 45 –0.354 636 657 791 245 849 07 –0.217 440 005 322 052 225 76 0.395 573 727 915 164 329 79 1.096 445 981 611 277 375 8
8	ℓ = 6.318 535 592 272 045 –0.038 060 233 744 366 798 686 –0.096 797 724 520 983 369 102 –0.107 796 952 873 510 886 96 –0.052 994 558 379 770 972 895 0.068 135 860 774 038 963 863 0.237 153 296 321 735 328 73 0.419 456 806 257 518 582 77 0.570 903 506 165 339 152 29	ℓ = 3.391 689 975 797 208 0.065 966 021 983 597 280 828 0.110 324 410 873 232 080 03 –0.022 713 554 363 876 414 313 –0.236 910 211 826 378 789 68 –0.306 342 255 793 388 331 74 –0.055 862 376 110 155 554 778 0.468 251 519 600 799 889 06 0.977 286 445 636 169 840 59
9	ℓ = 7.147 430 550 561 413 –0.030 153 689 607 037 932 268 –0.079 550 128 858 107 345 641 –0.098 407 115 533 249 091 604 –0.073 305 865 502 781 992 742 0 0.115 194 931 504 337 426 25 0.255 858 500 386 456 032 91 0.397 750 644 290 616 707 00 0.512 612 723 319 786 611 24	ℓ = 3.895 290 219 607 647 0.052 301 051 895 272 605 013 0.101 266 962 101 188 747 90 0.026 642 016 446 313 140 531 –0.137 931 929 156 682 986 04 –0.266 954 905 132 604 002 00 –0.219 076 590 372 349 287 46 0.064 279 256 258 874 647 289 0.499 021 276 364 748 587 44 0.880 452 861 595 238 547 33
10	ℓ = 7.972 691 637 812 280 –0.024 471 741 852 422 821 505 –0.066 228 831 765 768 206 903 –0.087 599 164 129 385 382 526 –0.078 738 975 641 538 713 579 –0.034 883 488 233 566 344 682 0.042 635 374 507 685 291 073 0.146 229 526 191 426 841 03 0.262 797 492 388 163 164 20 0.375 296 713 339 364 715 57 0.464 963 095 196 041 457 33	ℓ = 4.391 469 108 714 782 0.042 467 110 956 300 544 552 0.090 440 497 652 067 647 206 0.051 030 056 647 860 180 918 –0.068 250 050 077 061 163 328 –0.199 020 948 512 629 179 34 –0.243 955 170 425 047 826 18 –0.129 131 045 380 918 158 96 0.148 969 943 352 139 819 08 0.506 940 597 805 911 675 08 0.800 509 007 981 376 460 97

Table 3

of the optimised methods of order 2–5

Order 4	Order 5
$\ell = 0.3$ –0.375 000 000 000 000 000 00 1.541 666 666 666 666 666 7 –2.458 333 333 333 333 333 3 2.291 666 666 666 666 666 7	
$\ell = 0.75$ –0.25 0.625 0.041 666 666 666 666 666 667 −1.458 333 333 333 333 333 3 2.041 666 666 666 666 666 7	$\ell = 0.163\,339\,382\,940\,108\,8$ 0.348 611 111 111 111 111 11 –1.769 444 444 444 444 444 4 3.633 333 333 333 333 333 3 –3.852 777 777 777 777 777 8 2.640 277 777 777 777 777 8
$\ell = 1.181\,897\,711\,989\,360$ –0.176 228 059 145 769 668 84 0.217 779 624 303 801 742 76 0.516 162 094 242 489 717 34 –0.676 216 770 425 916 253 54 –0.686 030 943 361 995 271 80 1.804 534 054 387 389 734 1	$\ell = 0.469\,157\,254\,561\,251$ 0.249 421 296 296 296 296 29 –0.898 495 370 370 370 370 36 0.724 768 518 518 518 518 51 1.139 120 370 370 370 370 4 –2.605 671 296 296 296 296 3 2.390 856 481 481 481 481 5
$\ell = 1.586\,803\,103\,995\,642$ –0.130 276 570 699 249 748 82 0.040 823 321 662 060 514 133 0.451 574 102 013 991 105 94 0.016 001 789 308 425 411 316 –0.794 867 969 474 415 111 95 –0.187 023 021 147 214 511 56 1.603 768 348 336 402 340 9	$\ell = 0.792\,362\,028\,995\,767$ 0.184 805 705 228 950 410 08 –0.435 462 017 690 876 205 65 –0.246 164 378 868 764 011 81 1.268 163 587 804 809 902 2 –0.328 303 225 060 673 063 70 –1.594 750 940 737 348 964 2 2.151 711 269 323 901 933 0
$\ell = 1.970\,916\,561\,391\,601$ –0.100 018 782 547 822 773 31 –0.035 748 890 463 804 216 949 0.306 583 717 661 130 874 97 0.277 490 855 549 241 809 02 –0.335 165 400 358 394 580 87 –0.671 991 651 703 567 700 75 0.121 222 314 597 282 248 06 1.437 627 837 265 934 339 8	$\ell = 1.105\,498\,503\,602\,666$ 0.141 608 310 782 164 335 00 –0.194 778 897 037 351 300 08 –0.452 472 522 388 392 286 71 0.576 366 301 237 590 321 03 0.783 547 082 304 835 859 81 –0.919 538 234 654 641 505 58 –0.877 252 163 864 666 963 27 1.942 520 123 620 461 539 7
$\ell = 2.339\,983\,407\,348\,191$ –0.079 129 092 227 346 338 565 –0.067 460 438 055 823 679 907 0.185 229 899 631 699 256 08 0.316 756 417 686 937 500 27 0.007 699 688 785 598 755 599 3 –0.485 616 427 960 531 390 31 –0.486 411 071 972 200 782 01 0.308 966 990 668 254 142 62 1.299 964 033 443 412 536 2	$\ell = 1.405\,151\,117\,615\,213$ 0.111 679 587 452 253 674 79 –0.068 703 909 200 215 014 827 –0.415 591 348 832 787 799 76 0.075 957 984 853 647 800 951 0.789 757 119 684 457 386 45 0.168 798 574 062 768 170 77 –1.038 227 745 131 630 760 2 –0.387 719 877 150 909 038 34 1.764 049 614 262 415 580 2
$\ell = 2.698\,087\,099\,023\,256$ –0.064 133 502 960 306 610 717 –0.078 573 353 260 495 406 661 0.099 782 736 471 490 155 539 0.274 091 499 569 754 023 55 0.175 219 063 810 426 583 79 –0.202 657 937 197 901 007 91 –0.503 462 625 956 399 647 88 –0.307 138 431 963 688 427 39 0.421 961 371 543 814 430 77 1.184 911 179 943 305 906 9	$\ell = 1.692\,885\,048\,664\,239$ 0.090 219 510 737 302 839 601 –0.002 158 456 205 061 795 703 7 –0.321 954 875 526 057 453 95 –0.171 484 785 692 822 685 95 0.474 867 894 821 556 848 85 0.598 397 647 261 845 953 95 –0.276 718 534 444 465 663 97 –0.946 384 003 148 205 677 30 –0.057 121 557 681 252 610 888 1.612 337 159 877 160 245 3

Coefficients and stability interval lengths

k	Order 6	Order 7
6	ℓ = 0.087 719 298 245 614 04 –0.329 861 111 111 111 111 11 1.997 916 666 666 666 666 7 –5.068 055 555 555 555 555 6 6.931 944 444 444 444 444 4 –5.502 083 333 333 333 333 3 2.970 138 888 888 888 888 9	
7	NOT CONVERGED	ℓ = 0.046 513 917 259 370 46 0.315 591 931 216 931 216 93 –2.223 412 698 412 698 412 7 6.731 795 634 920 634 920 6 –11.379 894 179 894 179 894 11.665 823 412 698 412 698 –7.395 634 920 634 920 634 9 3.285 730 820 105 820 105 8
8	ℓ = 0.529 072 293 477 333 5 –0.191 136 896 168 322 945 85 0.658 500 132 899 500 866 28 –0.266 987 088 973 334 445 93 –1.504 164 071 623 426 548 7 1.831 315 884 128 336 433 4 0.753 947 159 797 829 986 77 –2.763 292 764 839 035 425 9 2.481 817 644 778 452 079 9	NOT CONVERGED
9	ℓ = 0.774 504 411 366 456 2 –0.150 724 057 709 530 551 68 0.366 164 179 624 831 523 68 0.264 862 407 421 359 273 31 –1.167 936 096 027 017 846 0 –0.049 706 767 276 153 478 305 1.830 740 825 812 214 481 7 –0.540 064 514 417 873 107 85 –1.820 117 139 586 925 971 6 2.266 781 162 159 095 680 2	NOT CONVERGED
10	ℓ = 1.015 322 150 308 401 –0.121 499 259 815 889 551 61 0.195 020 012 105 151 545 22 0.403 236 549 673 635 503 99 –0.602 004 140 817 800 156 59 –0.798 017 750 437 058 784 58 0.912 988 626 427 640 081 11 1.164 843 723 085 023 816 7 –1.100 111 173 235 220 067 2 –1.133 472 337 616 751 702 8 2.079 015 750 631 269 315 8	NOT CONVERGED

Table 4

of the optimised methods of order 6–9

Order 8	Order 9
ℓ = 0.024 408 513 276 164 89 –0.304 224 537 037 037 037 04 2.445 163 690 476 190 476 2 –8.612 127 976 190 476 190 5 17.379 654 431 216 931 217 –22.027 752 976 190 476 190 18.054 538 690 476 190 476 –9.525 206 679 894 179 894 2 3.589 955 357 142 857 142 9	
NOT CONVERGED	ℓ = 0.012 704 475 963 893 30 0.294 868 000 440 917 107 58 –2.663 168 540 564 373 897 7 10.701 467 702 821 869 489 –25.124 736 000 881 834 215 38.020 414 462 081 128 748 –38.540 361 000 881 834 215 26.310 842 702 821 869 489 –11.884 150 683 421 516 755 3.884 823 357 583 774 250 4
NOT CONVERGED	NOT CONVERGED

Numerical experiments

The purpose of the experiment is to verify accuracy and stability properties of the stabilised Adams-type methods constructed above. We also display results of the classic implicit Adams methods of corresponding orders, which have longer stability intervals than their classical explicit counterparts. In all our experiments we use constant step size and reference solutions computed by *Wolfram Mathematica's* `NDSolve`. The starting points were taken from this reference solution. For each method we perform a series of constant-step integrations with decreasing step size τ and calculate the maximum norm of the error at the endpoint. Missing points on the convergence diagrams mean that the error is too large due to instability of the method for the particular value of τ.

HIRES. This is a classical mildly stiff test system of dimension 8 describing a chemical reaction (see [1, chapter IV.10, formula (10.4)]). All equations except the 6^{th} and 7^{th} are linear. The interval of integration is [0, 40]. Figure 3, *a*, shows the performance of the 6-step stabilised methods of orders 1–6 and the implicit method of order 6. We see that the results agree well with common sense: more accurate methods have shorter stability intervals. Then we compare methods of order 5 and display the results at fig. 3, *b*, where we took *k* from 9 to 15 in order to get larger stability intervals than the implicit method have. There is clear evidence that methods with larger *k* have larger error constants. We do not show the results of the damped first order method, since the difference compared to the simple non-damped methods is negligible for this test problem.

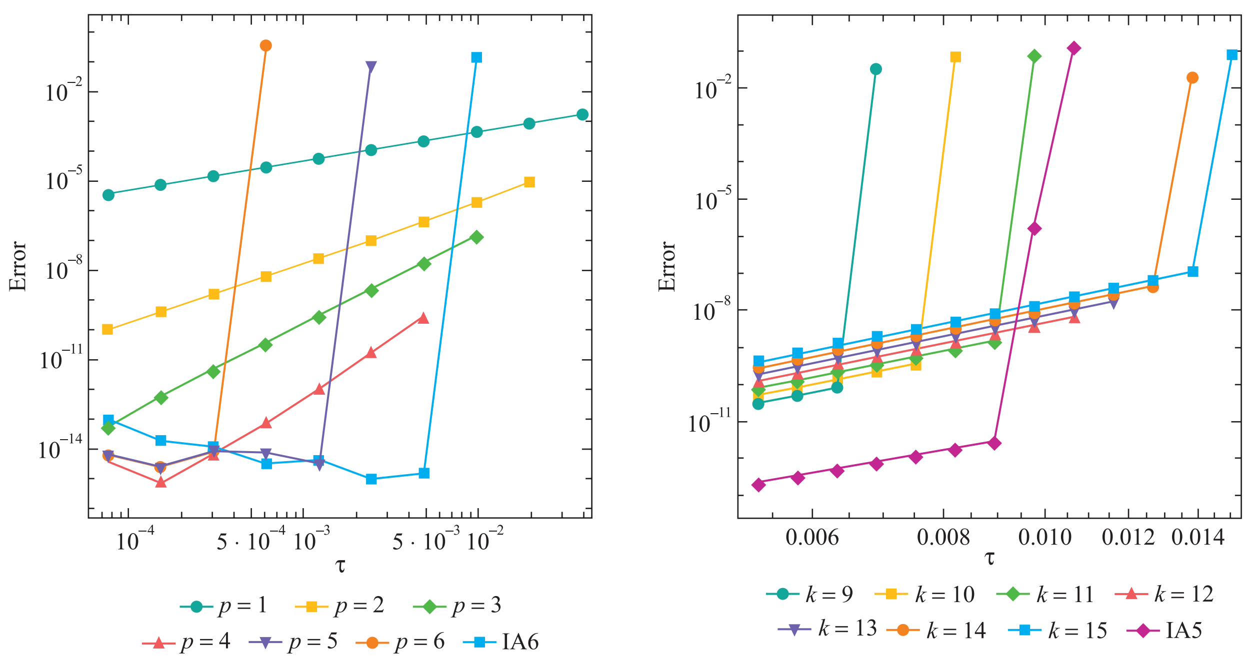

Fig. 3. Numerical experiment with HIRES problem.
Six-step stabilised methods and implicit Adams method of order 6 (*a*).
Stabilised methods of order 5 and implicit Adams method of the same order (*b*)

Burgers' equation. The second problem is taken from [5]. Consider a method of lines discretisation of the one-dimensional non-linear boundary value problem

$$u_t + \left(\frac{u^2}{2}\right)_x = \mu u_{xx},\ x \in [0, 1],\ t \in [0, 0.25],$$
$$u(x, 0) = 1.5x(1 - x)^2, \qquad (18)$$
$$u(0, t) = u(1, t) = 0.$$

The spatial derivatives are approximated by standard central finite differences, the discretisation step is $\Delta x = \frac{1}{501}$, so the dimension of the resulting ordinary differential equation is 500. The Jacobi matrix of this problem is not symmetric and complex eigenvalues occur for sufficiently small values of μ. We took $\mu = 0.005$ for which this is not the case at the starting point, but apparently non-real eigenvalues do emerge during integration.

The first experiment is similar to the one from the previous problem. The results are presented on fig. 4, *a*: we compare six-step methods of different orders. We see that the first order method with damping allows for taking longer time steps than the non-damped one. This indicates that the solution generates non-real eigenvalues of the Jacobi matrix. Hence, it is unlikely to benefit from using stabilized methods with large k and p, for which we do not have damping yet.

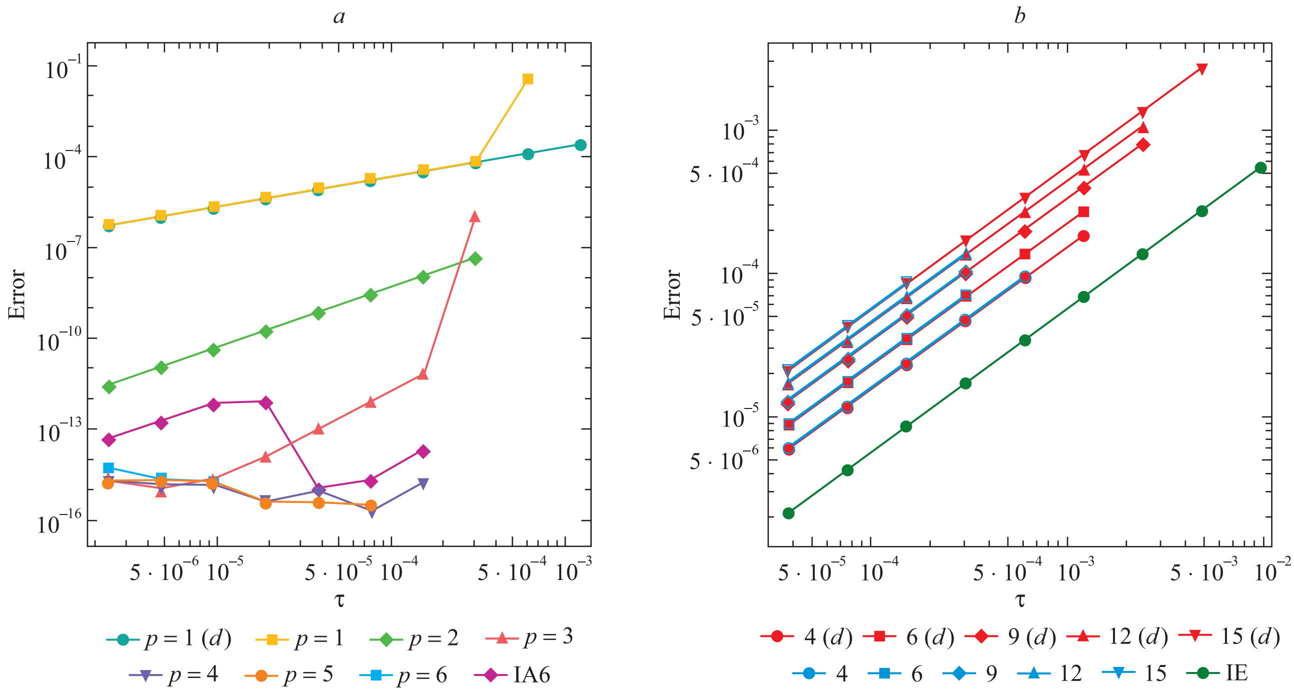

Fig. 4. Numerical experiment with Burgers' equation (18).
Six-step stabilised methods and implicit Adams method of order 6 (*a*).
First order stabilised methods with and without damping
for $\varepsilon = 0.25$, $k = 4, 6, 9, 12, 15$, and the implicit Euler method (*b*)

Indeed, our experiments showed that these methods cannot take larger steps than implicit Adams-type methods of the same order, even if their stability interval is longer. Hence, on fig. 4, *b*, we compare only stabilised explicit methods of order one with the implicit Euler method. This experiment shows that damping is crucial for the general performance of a stabilised method. Another obvious conclusion is that for this particular problem the explicit methods are less accurate than the implicit one.

Conclusion

In this work we presented explicit multi-step methods of Adams type, which possess extended stability intervals. Simple formulae for the first order methods and their error constants are derived. We also applied damping to the first order methods, derived a general scheme for construction of stabilised k-step methods of any order $p < k$, and calculated coefficients for such methods numerically. It was shown that the error constant of the stabilised method grows as the number of steps increases, but this growth is quite slow. Our numerical experiments asserted the theoretical properties of accuracy and stability of the constructed methods and exhibited the importance of damping transformation for the methods.

In our opinion, at present the stabilised Adams-type methods are mostly of theoretical interest, but it cannot be ruled out that they could be useful in practice and become a basis for a competitive solver for mildly stiff problems. From a practical perspective the methods are attractive due to their low cost (just one evaluation of f per step for any k and p) and simplicity of implementation. The weak point is that long stability intervals require a large number of steps, which will entail memory issues, difficulties with the starting values and so on.

Appendix A

Mathematica code for computing the stabilised method's parameters

```
ClearAll[a, b, beta, oc, mu]
k = 5; o = 3;
mu[betas_List] := With[{k = Length@betas}
      , Evaluate[(#^k - #^(k - 1))/(#^Range[0, k - 1]).betas] &
      ];
param = {a[-1] -> 0, a[k] -> 0
      , a[k - 1] -> Sum[b[j]^2, {j, 0, k - 1}]
      , a[j_] :> Sum[b[l] b[l + k - j - 1], {l, 0, j}]
      , beta[k - 1] -> a[k - 1] + a[k - 2]
      , beta[j_] :> a[j - 1] + a[j]
      };
bs = b /@ Range[0, k - 1];
betas = beta /@ Range[0, k - 1];
oc[1] = Total@betas - 1;
oc[p_] := Simplify[betas.Range[1 - k, 0]^(p - 1)] - 1/p;
cons = Thread[(oc /@ Range[o] //. param) == 0];
sol = NMinimize[Prepend[cons, bs.bs], bs
      , Method -> Automatic
      , WorkingPrecision -> 50
      , AccuracyGoal -> 25
      , PrecisionGoal -> 25
      , MaxIterations -> 1000
      ];
betaopt = (betas //. param) /. sol[[2]];
rescond = (oc /@ Range[o]) /. Thread[betas -> betaopt];
<|"k" -> k, "order" -> o, "betas" -> betaopt, "orderres" -> rescond,
"len" -> -mu[betaopt][-1]|>
```

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