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Construction of diagonally implicit almost collocation methods for Volterra Integral Equations

Abstract. We describe a modification of two-step collocation methods for the numerical solution of Volterra Integral Equations, with particular attention to the construction of efficient and highly stable methods. We present a constructive technique to obtain coefficient matrices having an estabilished structure, e.g. lower triangular or diagonal, and show examples of A-stable methods.

Keywords. Numerical methods for Volterra Integral Equations, Two–step collocation methods, Two–step Runge–Kutta methods, Diagonally–implicit methods.

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1 - Introduction

The present paper summarizes and extends some of the recent works of the authors concering the construction and the analysis of both efficient and highly stable numerical methods for Volterra Integral Equations (VIEs), which arise in many models of evolutionary phenomena with memory. We will particularly consider VIEs of the second kind, having the form

$$y(t) = g(t) + \int_0^t k(t, \tau, y(\tau))d\tau, \quad t \in [0, T], \tag{1}$$

where the *forcing function* $g : \mathbb{R} \to \mathbb{R}^d$ and the *kernel* $k : \mathbb{R}^2 \times \mathbb{R}^d \to \mathbb{R}^d$ are assumed to be sufficiently smooth. Such equations and their classical numerical treatment has been widely described in [3, 4] and the related bibliography. In particular, after defining a uniform mesh

$$I_h = \{t_n := nh, n = 0, ..., N, \ \ h \geq 0, Nh = T\},$$

usually the equation (1) is expressed in the following way

$$y(t) = F^{[n]}(t, y(\cdot)) + \Phi^{[n+1]}(t, y(\cdot)), \quad t \in [t_n, t_{n+1}],$$

where

$$F^{[n]}(t, y(\cdot)) := g(t) + \int_0^{t_n} k(t, \tau, y(\tau))d\tau, \quad \Phi^{[n+1]}(t, y(\cdot)) := \int_{t_n}^{t} k(t, \tau, y(\tau))d\tau$$

are the *lag term* and the *increment term* respectively. A special interest in literature has been reserved to collocation methods, which are based on the idea of approximating the exact solution with a suitable function belonging to a finite dimensional space, usally a piecewise algebraic polynomial, which exactly satisfies the equation on a certain subset of the integration interval, called the set of collocation points. In order to improve the properties of classical one-step collocation methods, Two-Step Almost Collocation (TSAC) methods have been introduced in [9]: the resulting methods possess higher order of convergence without any additional computational cost and preserve strong stability properties.

Let us consider m collocation parameters $c_1, \ldots, c_m$, which identify m internal points $t_{nj} = t_n + c_j h$ inside the generic interval $[t_n, t_{n+1}]$. Then TSAC methods for VIEs [9] assume the form

(2)

$$\begin{cases} P_n(t_n + sh) = \varphi_0(s)y_{n-1} + \varphi_1(s)y_n + \sum\limits_{j=1}^{m} \chi_j(s)Y_j^{[n]} + \sum\limits_{j=1}^{m} \psi_j(s)(F_j^{[n]} + \Phi_j^{[n+1]}) \\ y_{n+1} = P(t_{n+1}), \end{cases}$$

where the algebraic polynomial $P_n(t_n + sh)$, $s \in [0, 1]$, provides a continuous approximation to the solution $y(t_n + sh)$ in the interval $[t_n, t_{n+1}]$. Such polynomial is expressed as linear combination of the basis functions $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$ and $\psi_j(s)$, $j = 1, 2, \ldots, m$, which are determined from the continuous order conditions provided in [9]. Moreover, the polynomial employs the information about the equation on two consecutive steps and suitable sufficiently high order quadrature formulae

(3)

$$F_j^{[n]} = g(t_{nj}) + h \sum_{\nu=1}^{n} \left(b_0 k(t_{nj}, t_{\nu-1}, y_{\nu-1}) + \sum_{l=1}^{m} b_l k(t_{nj}, t_{\nu-1,l}, Y_l^{[\nu]}) + b_{m+1} k(t_{nj}, t_\nu, y_\nu) \right),$$

and

(4)

$$\Phi_j^{[n+1]} = h \left(w_{j0} k(t_{nj}, t_n, y_n) + \sum_{l=1}^{m} w_{jl} k(t_{nj}, t_{nl}, Y_l^{[n+1]}) + w_{j,m+1} k(t_{nj}, t_{n+1}, y_{n+1}) \right),$$

for the discretization of $F^{[n]}(t_{nj}, P(\cdot))$ and $\Phi^{[n+1]}(t_{nj}, P(\cdot))$ respectively, where $Y_i^{[n]} = P_{n-1}(t_{n-1,i})$ are the stage values and b_0, b_l, b_{m+1}, w_{j0}, w_{jl}, $w_{j,m+1}$ are given weights. The polynomial $P_n(t_n + sh)$ is explicitly defined after solving, at each step, the following system of $(m+1)d$ nonlinear equations in the stage values $Y_i^{[n+1]}$ and y_{n+1}, obtained by computing (2) for $s = c_i$, $i = 1, 2, \dots, m$, and $s = 1$:

(5)

$$\begin{cases} Y_i^{[n+1]} = \varphi_0(c_i)y_{n-1} + \varphi_1(c_i)y_n + \sum_{j=1}^{m} \chi_j(c_i)Y_j^{[n]} + \sum_{j=1}^{m} \psi_j(c_i)\Big(F_j^{[n]} + \Phi_j^{[n+1]}\Big), \\ y_{n+1} = \varphi_0(1)y_{n-1} + \varphi_1(1)y_n + \sum_{j=1}^{m} \chi_j(1)Y_j^{[n]} + \sum_{j=1}^{m} \psi_j(1)\Big(F_j^{[n]} + \Phi_j^{[n+1]}\Big), \end{cases}$$

$n = 1, 2, \dots, N-1$. The approximation $P(t)$ of the solution $y(t)$ of (1) on $[0, T]$ is then obtained by considering

$$P(t)|_{(t_n, t_{n+1}]} = P_n(t).$$

The aim of this paper is to describe how to reduce the computational cost associated to the solution of the nonlinear system (5), by suitably extending a widespread strategy used in the context of Ordinary Differential Equations (ODEs). This strategy consists in making the coefficient matrix have a structured shape, e.g. lower triangular or diagonal. In fact, a lower triangular matrix allows to solve the equations in m successive stages, with only a d-dimensional system to be solved at each stage. Moreover, if all the elements on the diagonal are equal, in solving the nonlinear systems by means of Newton-type iterations, one may hope to use repeatedly the stored LU factorization of the Jacobian. If the structure is diagonal, the problem reduces to the solution of m independent systems of dimension d, and can therefore be solved in a parallel environment.

The paper is structured as follows. In Section 2 we recall the main ideas regarding diagonally-implicit TSAC methods [8]. Section 3 is devoted to the presentation of a new constructive technique, while Section 4 contains examples of A-stable methods. Some conclusions and future developements are remarked in Section 5.

2 - Two-step diagonally-implicit almost collocation methods: framework

In this section we recall the main results obtained in [8] regarding the construction of diagonally-implicit TSAC methods belonging to the class (2) such that the coefficient matrix of the nonlinear system (5) has a structured shape, leading to the solution of nonlinear systems of lower dimension d. First of all we recall the order conditions.

Theorem 2.1. *Assume that the kernel $k(t, \eta, y)$ and the function $g(t)$ in (1) are sufficiently smooth. Then the method (2) has uniform order p, i.e.,*

$$\eta(t_n + sh) = O(h^{p+1}), \quad h \to 0,$$

for $s \in [0,1]$, if the polynomials $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$ and $\psi_j(s)$, $j = 1,2,...,m$ satisfy the system of equations

$$(6)\qquad \begin{cases} 1 - \varphi_0(s) - \varphi_1(s) - \displaystyle\sum_{j=1}^{m} \chi_j(s) - \sum_{j=1}^{m} \psi_j(s) = 0, \\ s^k - (-1)^k \varphi_0(s) - \displaystyle\sum_{j=1}^{m} (c_j - 1)^k \chi_j(s) - \sum_{j=1}^{m} c_j^k \psi_j(s) = 0, \end{cases}$$

$s \in [0,1]$, $k = 1,2,...,p$, where

$$(7)\qquad \begin{array}{rcl} \eta(t_n + sh) & = & y(t_n + sh) - \varphi_0(s) y(t_n - h) - \varphi_1(s) y(t_n) \\ & - & \displaystyle\sum_{j=1}^{m} \Big(\chi_j(s) y(t_n + (c_j - 1)h) + \psi_j(s) y(t_n + c_j h) \Big). \end{array}$$

is the local truncation error.

As regards the global error, the method has uniform order of convergence $p^* = \min\{l+1, q, p+1\}$, where l and q are the order of the starting procedure and the order of the quadrature formulas (3)-(4) respectively. Two-step collocation methods are obtained by solving the system of order conditions up to the maximum uniform attainable order $p = 2m+1$, and, in this way, all the basis functions are determined as the unique solution of such system. However, as observed in [9], it is not convenient to impose all the order conditions because it is not possible to achieve high stability properties (e.g. $A-$stability) without getting rid of some of them. Therefore, *almost* collocation methods have been introduced by relaxing a specified number r of order conditions, i.e. by a priori opportunely fixing r basis functions, and determining the remaining ones as the unique solution of the system of order conditions up to $p = 2m + 1 - r$. Within the class of TSAC methods many $A-$stable methods have been constructed [9].

In [8], we considered we considered $w_{j,m+1} = 0$, $j = 1, \ldots, m$, in such a way that (5) becomes a nonlinear system of dimension md only depending on the stage values $Y_i^{[n+1]}$, $i = 1, \ldots, m$, and assumes the following form

$$(8)\qquad \begin{cases} Y_i^{[n+1]} - h \displaystyle\sum_{j=1}^{m} \sum_{l=1}^{m} \psi_j(c_i) w_{jl} k(t_{nj}, t_{nl}, Y_l^{[n+1]}) = B_i^{[n]}, \\ y_{n+1} = P_n(t_{n+1}), \end{cases}$$

where

(9)

$$B_i^{[n]} = \varphi_0(c_i) y_{n-1} + \varphi_1(c_i) y_n + \sum_{j=1}^{m} \chi_j(c_i) Y_j^{[n]} + \sum_{j=1}^{m} \psi_j(c_i) F_j^{[n]} + h \sum_{j=1}^{m} \psi_j(c_i) w_{j0} k(t_{nj}, t_n, y_n).$$

By defining

$$Y^{[n+1]} = \left[Y_1^{[n+1]}, Y_2^{[n+1]}, \ldots, Y_m^{[n+1]} \right]^T, \quad B^{[n]} = \left[B_1^{[n]}, B_2^{[n]}, \ldots, B_m^{[n]} \right]^T,$$

$$\Psi = \big(\psi_j(c_i)\big)_{i,j=1}^{m}, \quad W = \big(w_{jl}\big)_{j,l=1}^{m}, \quad K(t_{nc}, t_{nc}, Y^{[n+1]}) = \Big(K(t_{ni}, t_{nj}, Y_j^{[n+1]}) \Big)_{i,j=1}^{m},$$

the nonlinear system in (8) takes the form

$$Y^{[n+1]} - h(\Psi \otimes I)\big((W \otimes I) \cdot K(t_{nc}, t_{nc}, Y^{[n+1]})\big)e = B^{[n]}, \tag{10}$$

where $\cdot$ denotes the usual Hadamard product, I is the identity matrix of dimension d and e is the unit vector of dimension md. The tensor form (10) clearly shows as the matrices which determine the structure of the nonlinear system (8) are Ψ and W. In [8] we described a strategy to obtain lower triangular or diagonal structures for the matrices Ψ and W: in particular we proposed a quadrature formula of the form

$$\int_0^{c_j} f(s)ds \approx w_{j0} f(0) + \sum_{l=1}^{m} \tilde{w}_{jl} f(c_l - 1) + \sum_{l=1}^{j} w_{jl} f(c_l), \tag{11}$$

for the increment

$$\Phi^{[n+1]}(t_{nj}, P(\cdot)) = h \int_0^{c_j} k(t_{nj}, t_n + sh, P_n(t_n + sh))ds, \tag{12}$$

in addition to the quadrature formula

$$\int_0^{1} f(s)ds \approx b_0 f(0) + \sum_{l=1}^{m} b_l f(c_l) + b_{m+1} f(1), \tag{13}$$

for the approximation of the lag term

$$F^{[n]}(t_{nj}, P(\cdot)) = g(t_{nj}) + h \sum_{\nu=1}^{n} \int_0^{1} k(t_{nj}, t_{\nu-1} + sh, P_{\nu-1}(t_{\nu-1} + sh))ds. \tag{14}$$

We observe that in formula (11), in case of triangular structure, $\tilde{w}_{jl} = 0$, $l = 1, \ldots, j$ while, in case of diagonal structure, $\tilde{w}_{j1} = 0$ and $w_{jl} = 0$, $l = 1, \ldots, j-1$. The determination of the weights in formulae (11) and (13) will be described in the next section.

Assuming that Ψ and W are lower triangular, we obtain the diagonally implicit TSAC methods (DITSAC)

(15)

$$\begin{cases} Y_i^{[n+1]} - h\psi_i(c_i) w_{ii} k(t_{ni}, t_{ni}, Y_i^{[n+1]}) = B_i^{[n]} + \tilde{B}_i^{[n]} + h \sum_{l=1}^{i-1} \sum_{j=l}^{i} \psi_j(c_i) w_{jl} k(t_{nj}, t_{nl}, Y_l^{[n+1]}), \\ y_{n+1} = \varphi_0(1) y_{n-1} + \varphi_1(1) y_n + \sum_{j=1}^{m} \chi_j(1) Y_j^{[n]} + \sum_{j=1}^{m} \psi_j(1) \Big(F_j^{[n]} + \Phi_j^{[n+1]}\Big), \end{cases}$$

where $B_i^{[n]}$ is given by (9),

$$\tilde{B}_i^{[n]} = h \sum_{j=1}^{i} \sum_{l=1}^{m} \psi_j(c_i) \tilde{w}_{jl} k(t_{nj}, t_{n-1,l} Y_l^{[n]}), \tag{16}$$

and $F_j^{[n]}$, $\Phi_j^{[n+1]}$ are approximations of (14) by means of the quadrature formulae (13) and (11).

Concerning the linear stability properties of DITSAC methods (15), i.e. the behaviour of the methods when applied to the basic test equation

$$y(t) = 1 + \lambda \int_0^t y(\tau)d\tau, \quad t \geq 0, \quad \mathrm{Re}(\lambda) \leq 0, \tag{17}$$

the following result holds.

T h e o r e m 2.2. *The stability matrix associated to the two-step collocation method (15) takes the form*

$$R(z) = Q^{-1}(z)M(z), \tag{18}$$

where

$$Q(z) = \begin{bmatrix} 1 & -z\psi^T(1)W & -\psi^T(1) & 0 \\ 0 & I - z\Psi W & -\Psi & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{19}$$

is an invertible matrix for $z < \dfrac{1}{\|\Psi W\|}$ *(for some matrix norm), whose inverse is*

$$Q^{-1}(z) = \begin{bmatrix} 1 & z\psi^T(1)W(I - z\Psi W)^{-1} & -\psi^T(1)(I + zW(I - z\Psi W)^{-1}) & 0 \\ 0 & (I - z\Psi W)^{-1} & -(I - z\Psi W)^{-1}\Psi & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{20}$$

and

$$M(z) = \begin{bmatrix} \varphi_1(1) + z\psi^T(1)w_0 & \chi^T(1) + z\psi^T(1)\tilde{W} & 0 & \varphi_0(1) \\ \varphi_1(c) + z\Psi w_0 & A + z\Psi\tilde{W} & 0 & \varphi_0(c) \\ zb_{m+1}u & zub^T & I & zb_0u \\ 1 & 0 & 0 & 0 \end{bmatrix}. \tag{21}$$

Next section will focus on the determination of the basis functions $\psi_j(s)$, $j = 1, 2, \ldots, m$, and the weights w_{jl} and $\tilde{w}_{jl}$ in (11), in such a way that the matrices Ψ and W exhibit a lower triangular or diagonal shape.

3 - Constructive issues

In order to achieve a lower triangular or diagonal structure for the matrix Ψ, the basis functions $\psi_j(s)$ must satisfy

$$\psi_j(c_i) = 0, \text{for } j > i \text{ or } j \neq i \text{ respectively}, \tag{22}$$

i.e. $\psi_j(s)$ assumes the form

$$\psi_j(s) = \prod_{k=1}^{j-1}(s - c_k)\bar{\psi}_j(s), \ j = 2, \ldots, m \tag{23}$$

or

$$\psi_j(s) = \prod_{\substack{k=1 \\ k\neq j}}^{m}(s - c_k)\tilde{\psi}_j(s), \ j = 1, \ldots, m \tag{24}$$

respectively, where $\bar{\psi}_j(s)$ is a polynomial of degree $p - j + 1$ and $\tilde{\psi}_j(s)$ is a polynomial of degree $p - m + 1$.

In [8] we introduced the following constructive strategy for the determination of the basis functions, i.e. we fixed the polynomial $\varphi_0(s)$ and, eventually, $\varphi_1(s)$, depending on some free parameters. We next derived the remaining basis functions by solving the system of order conditions (6) up to the desired order p. Then we derived some of the free parameters by enforcing the desired structure on the matrix Ψ, i.e. by imposing the form (23) or (24) of the basis functions $\psi_j(s)$, $j = 1, 2, \ldots, m$, and the other free parameters in order to get A-stability. This approach was used in [8] because we observed that, imposing (23) or (24) and computing the remaining basis functions as solution of the system of order conditions, the maximum attainable order would decay to $m + 2$ and $m + 1$ respectively. In fact the following theorem holds.

T h e o r e m 3.1. *Let us suppose that* $r = m - 1$ *or* $r = m$ *basis functions are imposed a priori according to the assumptions (23) and (24) respectively. Then, the resulting system of order conditions up to* $p = 2m + 1 - r$ *admits a unique polynomial solution.*

In the following we will show that actually it is possible to impose *a priori* the conditions (24) without any order reduction, by considering a certain number of $\tilde{\psi}_j(s)$, $j = 1, 2, \ldots, m$, as unknowns of the system of order conditions. First of all, we will show that, in the lower triangular case, this is effectively possible only if the Ψ matrix is actually diagonal.

T h e o r e m 3.2. *Let* $\psi_j(s)$, $j = 2, \ldots, m$, *be chosen as in (23) and assume that* $r < m - 1$ *functions* $\psi_j(s)$, $j = 2, \ldots, r + 1$ *are fixed a priori. Then the resulting system of order conditions in the unknowns* $\varphi_0(s), \varphi_1(s), \chi_j(s), j = 1, 2, \ldots, m, \psi_1(s), \bar{\psi}_j(s), j = r + 2 \ldots, m$ *admits an unique polynomial solution if and only if* $\psi_j(s)$, $j = 1, 2, \ldots, r$, *are of the form (24) and* $\psi_k(c_k) = 1$, $k = 2, \ldots, r + 1$.

P r o o f. If the basis functions $\psi_j(s)$, $j = 2, \ldots, m$, have the form (23) and $\psi_j(s)$, $j = 2, \ldots, r+1$, are fixed a priori, the system of order conditions (6) takes the form

(25)

$$\begin{cases} \varphi_0(s)+\varphi_1(s)+\sum_{j=1}^{m}\chi_j(s)+\psi_1(s)+\sum_{j=r+2}^{m}\prod_{\substack{\ell=1\\ \ell\neq j}}^{m}(s-c_\ell)\bar{\psi}_j(s)=1-\sum_{j=2}^{r+1}\psi_j(s),\\ (-1)^k\varphi_0(s)+\sum_{j=1}^{m}(c_j-1)^k\chi_j(s)+c_1^k\psi_1(s)+\sum_{j=r+2}^{m}c_j^k\prod_{\substack{\ell=1\\ \ell\neq j}}^{m}(s-c_\ell)\bar{\psi}_j(s)=s^k-\sum_{j=2}^{r+1}c_j^k\psi_j(s), \end{cases}$$

or, equivalently,

$$H(s)x(s)=d(s), \tag{26}$$

where

$$\begin{aligned} H(s)&=\left[-1^{(p)},0^{(p)},(c-e)^{(p)},c_1^{(p)},\left(c_i^{(p)}\prod_{k=1}^{i-1}(s-c_k)\right)_{i=r+2}^{m}\right],\\ x(s)&=\left[\varphi_0(s),\varphi_1(s),\left(\chi_j(s)\right)_{j=1}^{m},\psi_1(s),\left(\bar{\psi}_i(s)\right)_{i=r+2}^{m}\right]^T,\\ d(s)&=s^{(p)}-\sum_{j=2}^{r+1}\psi_j(s)c_j^{(p)}, \end{aligned}$$

with the notation

$$\alpha^{(p)}=\begin{bmatrix} 1 & 1 & \dots & 1\\ \alpha_1 & \alpha_2 & \dots & \alpha_n\\ \vdots & \vdots & & \vdots\\ \alpha_1^p & \alpha_2^p & \dots & \alpha_n^p \end{bmatrix}\in\mathbb{R}^{(p+1)\times n},$$

for $\alpha\in\mathbb{R}^n$. We aim to prove that each component of the solution vector $x(s)$ results to be a polynomial. In order to solve the system (26), we apply the Cramer rule, obtaining that

$$x_i(s)=\frac{\det H_i(s)}{\det H(s)},\quad i=1,\dots,2m+2-r,$$

where $H_i(s)$ is the matrix obtained by replacing the i-th column of the matrix $H(s)$ with the vector $d(s)$. By isolating the factors depending on s, we have

$$\det H(s)=\prod_{k=1}^{r+1}(s-c_k)^{m-r-1}\prod_{k=r+2}^{m-1}(s-c_k)^{m-k}\det\bar{H},$$

where $\bar{H}$ is the Vandermonde matrix associated to the abscissa vector $[-1,0,(c-e)^T,c_1,(c_i)_{i=r+1}^{m}]$. For $i=1,\dots,m+3$, it can be easily recognized that

$$x_i(s)=\frac{\det\bar{H}_i(s)}{\det\bar{H}},$$

where $\bar{H}_i(s)$ is the matrix obtained by replacing the i-th column of the matrix $\bar{H}$ with the vector $d(s)$, and therefore $x_i(s)$ is trivially a polynomial. Let us analyze the components

$$x_{m+2+i-r}(s) = \frac{\det H_{m+2+i-r}(s)}{\det H(s)} = \frac{\det \bar{H}_{m+2+i-r}(s)}{\prod_{k=1}^{i-1}(s-c_k)\det \bar{H}},$$

with $i = r+2, \ldots, m$. By setting

$$f_{r,i}(s) = s(s-1)\prod_{k=1}^{m}(s-c_k+1)(s-c_1)\prod_{\substack{k=r+2\\k\neq i}}^{m}(s-c_k),$$

we can write

$$x_{m+2+i-r}(s) = \frac{f_{r,i}(s) - \sum_{j=2}^{r+1}\psi_j(s)f_{r,i}(c_j)}{\prod_{k=1}^{i-1}(s-c_k)f_{r,i}(c_i)},$$

which is a polynomial if and only if

$$f_{r,i}(c_k) - \sum_{j=2}^{r+1}\psi_j(c_k)f_{r,i}(c_j) = 0, \quad k = 1, \ldots, i-1. \tag{27}$$

The condition (27) for $k = 1$ trivially results from (23) and $f_{r,i}(c_1) = 0$. By imposing (27) for $k = 2, \ldots, r+1$, we obtain

$$\psi_k(c_k) = 1 - \sum_{j=2}^{k-1}\frac{f_{r,i}(c_j)}{f_{r,i}(c_k)}\psi_j(c_k), \quad i = r+2, \ldots, m,$$

and, therefore,

$$\psi_j(c_k) = 0, \quad j = 2, \ldots, r, \quad k = j+1, \ldots, r+1, \tag{28}$$

$$\psi_k(c_k) = 1, \quad k = 2, \ldots, r+1. \tag{29}$$

Finally, the condition (27), for $k = r+2, \ldots, i-1$, becomes

$$\sum_{j=2}^{r-1}\psi_j(c_k)f_{r,i}(c_j) = 0, \quad i = r+2, \ldots, m,$$

and, as a consequence,

$$\psi_j(c_k) = 0, \quad j = 2, \ldots, r+1, \quad k = r+2, \ldots, m-1. \tag{30}$$

Conditions (29) and (30), together with the hypothesis (23), are equivalent to (24) which, in addition to (29), conclude the proof. □

As a consequence, the following result holds in the diagonal case.

T h e o r e m 3.3. *Let $\psi_j(s)$, $j = 2, \dots, m$, be chosen as in (24) and assume that $r < m$ functions $\psi_j(s)$, $j = 1, \dots, r$, are fixed a priori. Then the system of order conditions in the unknowns $\varphi_0(s), \varphi_1(s), \chi_j(s), j = 1, 2, \dots, m, \tilde{\psi}_j(s), j = r+1, r+2 \dots, m$, admits an unique polynomial solution if $\psi_k(c_k) = 1$, $k = 1, 2, \dots, r$.*

It is important to underline that, once the condition $\psi_k(c_k) = 1$ involved in the previous theorem is imposed on the basis functions we fix a priori together with $\psi_k(c_\ell) = 0$, $\ell \neq k$, such conditions are automatically inherited by all the other basis functions we determine as solution of the system of order conditions, as it is proved in the following general result.

T h e o r e m 3.4. *Let us define $\xi_1 = -1$, $\xi_2 = 0$, $\xi_{2+j} = c_j - 1$, $\xi_{m+2+j} = c_j$, $j = 1, \dots, m$ and $\Gamma_1(s) = \varphi_0(s)$, $\Gamma_2(s) = \varphi_1(s)$, $\Gamma_{2+j}(s) = \chi_j(s)$, $\Gamma_{m+2+j}(s) = \psi_j(s)$, $j = 1, \dots, m$ and let $i \in \{1, 2, \dots, 2m+2\}$ be a fixed integer. Then, supposing $\xi_i \neq \xi_j$, $i \neq j$,*

i. If $\Gamma_i(\xi_i) = 1$, then $\Gamma_j(\xi_i) = 0$ for all $j \neq i$;

ii. If $\Gamma_i(\xi_\ell) = 0$ with $\ell \neq i$, then $\Gamma_j(\xi_\ell) = \delta_{j\ell}$ for $j \neq i$.

P r o o f. The system of order conditions (6) can be rewritten in terms of ξ_j and $\Gamma_j(s)$ as

$$s^k - \sum_{j=1}^{2m+2} \xi_j^k \Gamma_j(s) = 0, \quad k = 0, 1, \dots, p, \tag{31}$$

where we assume $\xi_2^0 = 1$. We first prove the part *i.* of the thesis. For this purpose, we evaluate (31) in $s = \xi_i$ and, as a consequence, using the assumption *i.* leads to the following linear system

$$\sum_{\substack{j=1 \\ j\neq i}}^{2m+2} \xi_j^k \Gamma_j(\xi_i) = 0, \quad k = 0, 1, \dots, p,$$

which is a Vandermonde type linear system whose unique solution is $\Gamma_j(\xi_i) = 0$ for all $j \neq i$. In analogous way, by evaluating (31) in $s = \xi_\ell$ and taking into account the assumption *ii.*, we obtain the Vandermonde type linear system

$$\xi_\ell^k - \sum_{\substack{j=1 \\ j\neq i}}^{2m+2} \xi_j^k \Gamma_j(\xi_\ell) = 0, \quad k = 0, 1, \dots, p,$$

whose unique solution is $\Gamma_j(\xi_\ell) = \delta_{j\ell}$ for $j \neq i$. □

In addition to the computation of the basis functions, the quadrature formulae (11)-(13) for the approximation of the increment and the lag terms have to be computed: let us focus our attention on the computation of the weights of such formulae. With the purpose of achieving the desired order, quadrature formulae of the form (11) and (13) can be constructed by taking into account that the order of the corresponding increment term and lag term quadrature formulae is at least $O(h^q)$, if they are interpolatory quadrature formulae on $q-1$ and q nodes respectively [4]. Therefore, we impose that lag term quadrature formula (13) exactly integrates the functions

$$f(x) = x^k, \qquad k = 0, 1, \ldots, q-1,$$

while the increment quadrature formula (11) exactly integrates the functions

$$f(x) = x^k, \qquad k = 0, 1, \ldots, q-2.$$

This leads to the following linear systems when $q \leq m+2$:

$$\text{(32)} \qquad \begin{cases} b_0 + \sum\limits_{\ell=1}^{m} b_\ell + b_{m+1} = 1, \\ \sum\limits_{\ell=1}^{m} b_\ell c_\ell^k + b_{m+1} = \frac{1}{k+1}, \quad k = 1, 2, \ldots, q-1, \end{cases}$$

$$\text{(33)} \qquad \begin{cases} w_{j0} + \sum\limits_{\ell=1}^{m} \tilde{w}_{j\ell} + \sum\limits_{\ell=1}^{j} w_{j\ell} = c_j, \\ \sum\limits_{\ell=1}^{m} (c_\ell - 1)^k \tilde{w}_{j\ell} + \sum\limits_{\ell=1}^{j} c_\ell^k w_{j\ell} = \frac{c_j^{k+1}}{k+1}, \quad k = 1, 2, \ldots, q-2, \end{cases}$$

$j = 1, 2, \ldots, m$, whose unique solutions gives the weights of (11) and (13) respectively. If $q > m+2$, we need some additional points in order to preserve the order, then we can fix some additional parameters d_ℓ, $\ell = 1, \ldots, q-2$ and $d_{j\ell}$, $j = 1, \ldots, m$ and $\ell = 1, \ldots, q-j-2$, and determine the weights by solving the system

$$\text{(34)} \qquad \begin{cases} b_0 + \sum\limits_{\ell=1}^{q-2} b_\ell + b_{m+1} = 1, \\ \sum\limits_{\ell=1}^{q-2} b_\ell d_\ell^k + b_{m+1} = \frac{1}{k+1}, \quad k = 1, 2, \ldots, q-1, \end{cases}$$

$$\text{(35)} \qquad \begin{cases} w_{j0} + \sum\limits_{\ell=1}^{q-j-2} \tilde{w}_{j\ell} + \sum\limits_{\ell=1}^{j} w_{j\ell} = d_j, \\ \sum\limits_{\ell=1}^{q-j-\ell} (d_\ell - 1)^k \tilde{w}_{j\ell} + \sum\limits_{\ell=1}^{j} d_\ell^k w_{j\ell} = \frac{d_j^{k+1}}{k+1}, \quad k = 1, 2, \ldots, q-2, \end{cases}$$

$j = 1, 2, \ldots, m$.

4 - Examples of A-stable methods

We present in this section some examples of A-stable DITSAC methods of the form (15), with Ψ and W lower triangular and/or diagonal. We recall that for an A-stable method the roots of the stability polynomial, i.e. characteristic polynomial $p(\omega, z)$ of the stability matrix (18), lie in the unit circle, for all $z \in \mathbb{C}$ such that $\mathrm{Re}(z) \leq 0$. We investigate A-stability using the Schur criterion [22], similarly as it has already been done in [9, 12, 13, 14, 15, 16, 19].

Consider the polynomial

$$\eta(w) = d_k w^k + d_{k-1} w^{k-1} + \cdots + d_1 w + d_0,$$

where d_i are complex coefficients, $d_k \neq 0$ and $d_0 \neq 0$. $\eta(w)$ is said to be a Schur polynomial if all its roots w_i, $i = 1, 2, \ldots, k$, are inside of the unit circle. Define

$$\hat{\eta}(w) = \bar{d}_0 w^k + \bar{d}_1 w^{k-1} + \cdots + \bar{d}_{k-1} w + \bar{d}_k,$$

where $\bar{d}_i$ is the complex conjugate of d_i. Define also the polynomial

$$\eta_1(w) = \frac{1}{w}\Big(\hat{\eta}(0)\eta(w) - \eta(0)\hat{\eta}(w)\Big)$$

of degree at most $k-1$. We have the following theorem.

Theorem 4.1. *(Schur [22]). $\eta(w)$ is a Schur polynomial if and only if*

$$|\hat{\eta}(0)| > |\eta(0)|$$

and $\eta_1(w)$ is a Schur polynomial.

Roughly speaking, the Schur criterion allows us to investigate the stability properties of a k^{th} degree polynomial, looking at the roots of a polynomial of lower degree (i.e. $k-1$). Iterating this process, the last step consists in the investigation of the root of a linear polynomial, plus some additional conditions.

The strategy we carry out in the construction of A-stable methods can be summarized as follows. First of all we set the quadrature formulae (11) and (13), deriving their weights by solving the linear systems (32) and (33) or (34) and (35). Moreover, we assume that the polynomials $\psi_j(s)$ satisfy (23) or (24) and we fix a priori r of them, depending on some free parameters. According to Theorems 3.1–3.3, we have to fix $r = m-1$ basis functions $\psi_k(s)$, $k = 2, \ldots, m$, in the triangular case and we can fix $1 \leq r \leq m$ with $\psi_k(c_k) = 1$, $k = 1, 2, \ldots, r$, in the diagonal case. As a consequence some free parameters must be spent in order to enforce this condition, while the remaining ones will next be used in order to achieve A-stability. We next derive the remaining basis functions by solving the system of order conditions (6) up to p, compute the stability matrix (18) of the resulting method and the corresponding stability polynomial, whose stability properties are investigated by using the Schur criterion.

4.1 - *Examples of methods with $m = 2$ with Ψ and W lower triangular*

We first present the construction of highly stable two-stage DITSAC methods (15), requiring that the matrices Ψ and W are lower triangular. We have already observed in [8, 12] that A-stable methods of maximum uniform order 5 do not exist within this class. Therefore, we next relax one order condition ($r = 1$), and consider DITSAC methods (15) with $m = 2$ and order $p = 2m = 4$. We compute the weights of the quadrature formulae (11) and (13) according to the desired order $p = 4$, obtaining

$$
\begin{aligned}
b_0 &= -\frac{-6c_2c_1 + 2c_1 + 2c_2 - 1}{12c_1c_2}, \quad b = \begin{bmatrix} -\frac{1-2c_2}{12(c_1-1)c_1(c_1-c_2)} & \frac{2c_1-1}{12(c_2-1)c_2(c_2-c_1)} \end{bmatrix}^T, \\
b_3 &= -\frac{-6c_2c_1 + 4c_1 + 4c_2 - 3}{12(c_1-1)(c_2-1)}, \quad w_0 = \left[-\frac{c_1(c_1 - 3c_2 + 3)}{6(c_2 - 1)} \quad -\frac{c_2^2 - 3c_1c_2}{6c_1} \right], \\
W &= \begin{bmatrix} \frac{c_1(2c_1-3c_2+3)}{6(c_1-c_2+1)} & 0 \\ -\frac{c_2^3}{6c_1(c_1-c_2)} & -\frac{2c_2^2-3c_1c_2}{6(c_1-c_2)} \end{bmatrix}, \quad \tilde{W} = \begin{bmatrix} 0 & \frac{c_1^3}{6(c_1-c_2+1)(c_2-1)} \\ 0 & 0 \end{bmatrix}.
\end{aligned}
$$

We next assume that the basis function $\psi_2(s)$ satisfies (23), presenting the form

$$\psi_2(s) = (s - c_1)\tilde{\psi}_2(s),$$

and determine the remaining basis functions $\varphi_0(s), \varphi_1(s), \chi_1(s), \chi_2(s)$ and $\psi_1(s)$ by imposing the system of order conditions (6) up to order $p = 4$. The determined quadrature weights and basis functions now depend on the abscissa vector $c = [c_1, c_2]^T$ which can be regarded as degrees of freedom in order to enforce strong stability properties for the corresponding methods, such as A-stability and, moreover, they also depend on the function $\tilde{\psi}_2(s)$. In particular, we observe that the corresponding stability polynomial depend on the values that the function $\tilde{\psi}_2(s)$ assumes in c_2 and in 1: let us denote these values as $q_0 = \tilde{\psi}_2(c_2)$ and $q_1 = \tilde{\psi}_2(1)$. The degree of the stability polynomial is equal to 6: however, in correspondence of the value

$$q_0 = -\frac{1}{c_1 + c_2},$$

the degree of the stability polynomial becomes equal to 5. We assume for simplicity that $q_1 = 0$ and analyze the stability properties of the resulting polynomial by using the Schur criterion in order to determine the values of the free parameters c_1 and c_2 corresponding to A-stable methods. The result of this analysis is reported in Figure 1.

4.2 - *Examples of methods with $m = 2$ with Ψ and W diagonal*

We now present the construction of highly stable two-stage DITSAC methods (15), requiring that the matrices Ψ and W are diagonal. We have already observed in [8, 12] that no A-stable DITSAC methods with two stages, of order $p = 4, 5$ and such that the matrices Ψ and W are diagonal exist and, therefore, we relax two order conditions, attempting the construction of methods of order $p = 3$. We compute the weights of the quadrature formulae (11) and (13)

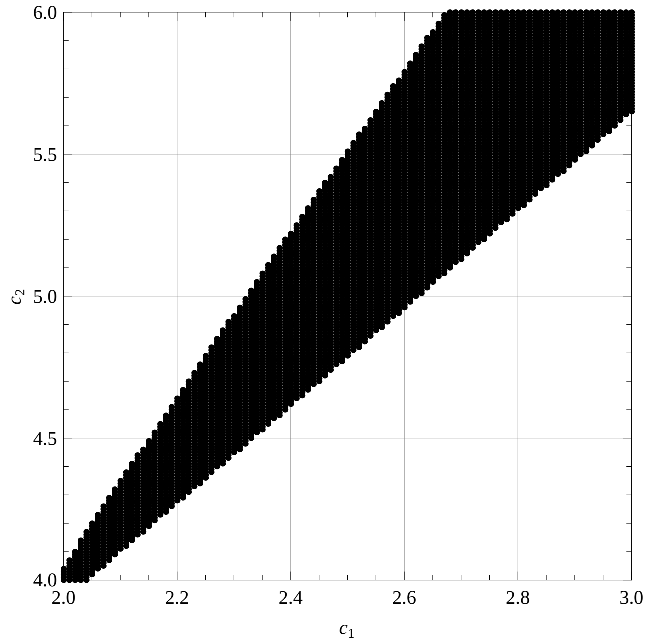

Figure 1: Region of A-stability in the parameter space (c_1, c_2) for DITSAC methods (15), with $m = 2$ and $p = 4$.

corresponding to the diagonal case, obtaining

$$\begin{aligned} b_0 &= -\frac{1-3c_2}{6c_2}, \quad b = \begin{bmatrix} 0 & -\dfrac{1}{6(c_2-1)c_2} \end{bmatrix}^T, \quad b_3 = -\frac{2-3c_2}{6(c_2-1)}, \\ w_0 &= \begin{bmatrix} \frac{c_1}{2} & \frac{c_2}{2} \end{bmatrix}^T, \quad W = \begin{bmatrix} \frac{c_1}{2} & 0 \\ 0 & \frac{c_2}{2} \end{bmatrix}, \quad \tilde{W} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}. \end{aligned}$$

We next assume, according to (24), the following form for $\psi_1(s)$ and $\psi_2(s)$:

$$\begin{aligned} \psi_1(s) &= s(s-c_2)(q_0+q_1 s), \\ \psi_2(s) &= s(s-c_1)(p_0+p_1 s). \end{aligned} \tag{36}$$

The remaining basis functions $\varphi_0(s), \varphi_1(s), \chi_1(s)$ and $\chi_2(s)$ are next determined by imposing the system of order conditions (6) up to $p = 3$. At this point, everything depends on the values of q_0, q_1, p_0, p_1, c_1 and c_2. We next spend some of the parameters in order to enforce some assumptions on the basis functions: in particular, we assume that 1, c_1 and c_2 are roots of the polynomial $\varphi_0(s)$, ensuring that the resulting methods do not depend on y_{n-1}: this choice, as also in the case of two-step Runge–Kutta methods for ODEs, is particularly suitable in order to improve the stability properties of the resulting methods (compare with [19, 20]). We also impose that $\varphi_1(s)$ annihilates in a certain point α that we choose in order to reduce the magnitude of the collocation points, trying to have them as close as possible to the interval [0,1]: in our analysis, we have chosen $\alpha = \frac{1}{4}$. Under these assumptions, a fourth degree stability function arises, which depends on c_1 and c_2. We apply the Schur criterion, in order to determine the values of the free parameters c_1, c_2 achieving A-stability. The results are shown in Figure 2.

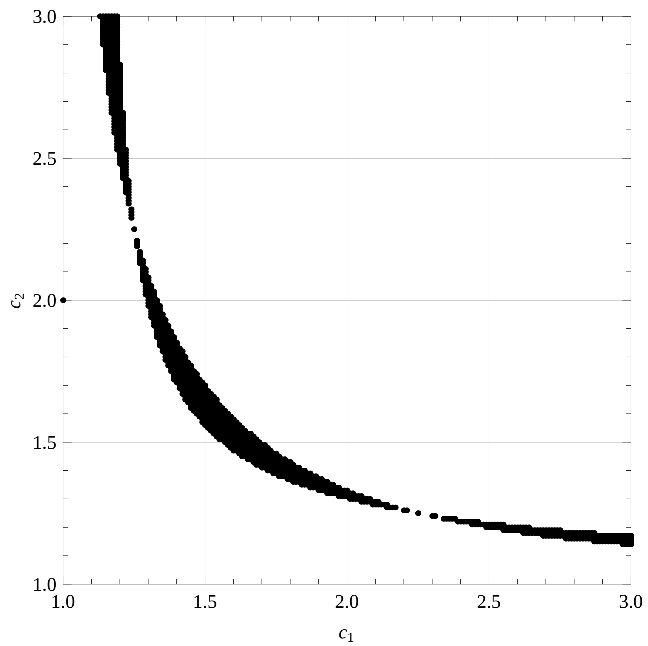

Figure 2: Region of A-stability in the parameter space (c_1, c_2) for DITSAC methods (15), with $m = 2$, $p = 3$ and such that the matrices Ψ and W are diagonal.

We finally present the construction of DITSAC methods (15), with $m = 2$, $p = 3$ and such that the matrices Ψ and W are diagonal and their product is one point spectrum. Also in this case we assume $\psi_1(s)$ and $\psi_2(s)$ of the type (36) and determine all the remaining basis functions as solution of the system of the order conditions. We next derive the values of q_0, q_1 and p_1 such that 1 and c_1 are roots of the polynomial $\varphi_0(s)$, and also impose that $\psi_2(s)$ annihilates in a certain point β we choose in order to reduce the magnitude of the collocation points, trying to have them as close as possible to the interval [0,1]: in our analysis, we have chosen $\beta = -\frac{18}{5}$. We next find p_0 in such a way that the matrix ΨW is also one-point spectrum. As a consequence of our assumptions, a fifth degree stability function arises, which depends on c_1 and c_2: the values of these parameters achieving A-stability are plotted in Figure 3.

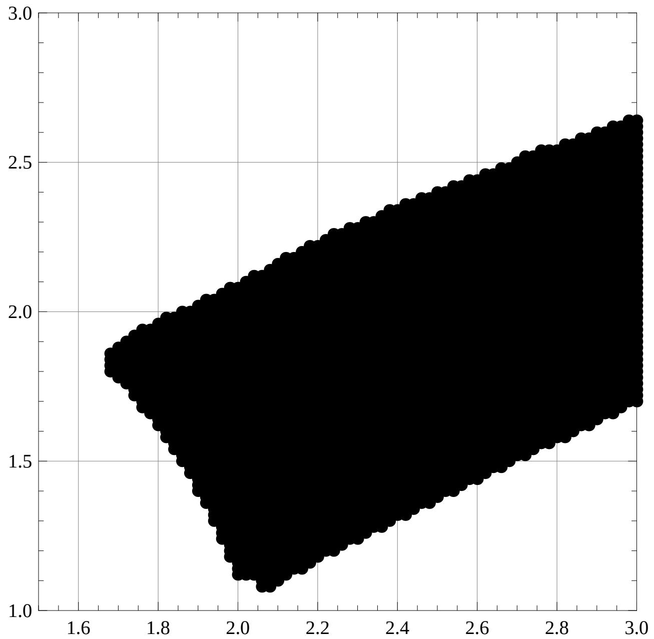

Figure 3: Region of A-stability in the parameter space (c_1, c_2) for DITSAC methods (15), with $m = 2$, $p = 3$ and such that the matrices Ψ and W are diagonal and ΨW is one point spectrum.

4.3 - *Examples of methods with* $m = 3$ *with* Ψ *and* W *lower triangular*

We conclude this section showing the construction of A-stable DITSAC methods (15) with three stages and such that the matrices Ψ and W are lower triangular. We observe that no A-stable methods of order $p = 7, 6$ can be found within this class and, therefore, we relax two order conditions, deriving methods with $m = 3$ and uniform order $p = 5$. We first compute the weights of the quadrature formulae (11) and (13) corresponding to the lower triangular case, obtaining

$$
\begin{aligned}
b_0 &= \frac{-3 + c_2(5 - 10c_3) + 5c_3 + 5c_1\big(1 - 2c_3 + c_2(-2 + 6c_3)\big)}{60c_1c_2c_3}, \\
b &= \begin{bmatrix} \frac{-3+c_2(5-10c_3)+5c_3}{60(-1+c_1)c_1(c_1-c_2)(c_1-c_3)} & \frac{-3+c_1(5-10c_3)+5c_3}{60(-1+c_2)c_2(-c_1+c_2)(c_2-c_3)} & \frac{3-5c_2+5c_1(-1+2c_2)}{60(c_1-c_3)(-1+c_3)c_3(-c_2+c_3)} \end{bmatrix}^T, \\
b_4 &= \frac{-20c_3c_2 + 15c_2 + 15c_3 + 5c_1(-4c_3 + c_2(6c_3 - 4) + 3) - 12}{60(c_1 - 1)(c_2 - 1)(c_3 - 1)}, \\
w_0 &= \begin{bmatrix} \frac{c_1\left(c_1^2-2(c_2+c_3-2)c_1+6(c_2-1)(c_3-1)\right)}{12(c_2-1)(c_3-1)} & \frac{c_2(c_2(c_2-2c_3+2)-2c_1(c_2-3c_3+3))}{12c_1(c_3-1)} & \frac{c_3\left(c_3^2-2c_1c_3-2c_2c_3+6c_1c_2\right)}{12c_1c_2} \end{bmatrix}^T, \\
W &= \begin{bmatrix} \frac{c_1\left(3c_1^2-4(c_2+c_3-2)c_1+6(c_2-1)(c_3-1)\right)}{12(c_1-c_2+1)(c_1-c_3+1)} & -\frac{c_2^3(c_2-2c_3+2)}{12c_1(c_1-c_2)(c_1-c_3+1)} & \frac{(2c_2-c_3)c_3^3}{12c_1(c_1-c_2)(c_1-c_3)} \\ 0 & \frac{c_2(c_1(4c_2-6c_3+6)+c_2(-3c_2+4c_3-4))}{12(c_1-c_2)(c_2-c_3+1)} & \frac{c_3^3(c_3-2c_1)}{12(c_1-c_2)c_2(c_2-c_3)} \\ 0 & 0 & \frac{c_3\left(3c_3^2-4c_1c_3-4c_2c_3+6c_1c_2\right)}{12(c_1-c_3)(c_2-c_3)} \end{bmatrix} \\
\tilde{W} &= \begin{bmatrix} 0 & 0 & 0 \\ \frac{c_1^3(c_1-2c_3+2)}{12(c_1-c_2+1)(c_2-1)(c_2-c_3)} & 0 & 0 \\ \frac{c_1^3(c_1-2c_2+2)}{12(c_1-c_3+1)(c_3-1)(c_3-c_2)} & \frac{c_2^3(c_2-2c_1)}{12(c_1-c_3+1)(c_3-1)(-c_2+c_3-1)} & 0 \end{bmatrix}.
\end{aligned}
$$

We next assume, according to (23), the following form for $\psi_2(s)$ and $\psi_3(s)$:

$$
\begin{aligned}
\psi_2(s) &= (s - c_1)(s - c_3)\tilde{\psi}_2(s), \\
\psi_3(s) &= (s - c_1)(s - c_2)\tilde{\psi}_3(s).
\end{aligned}
$$

The remaining basis functions $\varphi_0(s), \varphi_1(s), \chi_1(s), \chi_2(s), \chi_3(s)$ and $\psi_1(s)$ are next determined by imposing the system of order conditions (6) up to $p = 5$. We next compute the resulting stability polynomial, having degree equal to eight, which depends on the collocation points, but also on some evaluations of the functions $\tilde{\psi}_2(s)$ and $\tilde{\psi}_3(s)$, i.e.

$$q_0 = \tilde{\psi}_2(c_2),\ q_1 = \tilde{\psi}_2(1),\ p_0 = \tilde{\psi}_3(c_3),\ p_1 = \tilde{\psi}_3(1).$$

We impose $q_1 = p_1 = 0$ and compute the values of q_0 and p_0 in order to reduce the degree of the stability polynomial. In this way, a sixth degree stability function arises, which depends on the collocation points. The values of these parameters achieving A-stability are plotted in Figure 4.

5 - Conclusions

We have presented a family of highly-stable diagonally-implicit two-step almost collocation methods for the numerical integration of VIEs (1), and introduced a constructive technique which permits to a priori impose the structure of the coefficient matrices. These methods possess uniform order of convergence on the whole integration interval. We have provided examples of A-stable methods (15) with $m = 2$ and 3, where Ψ and W are lower triangular and/or diagonal

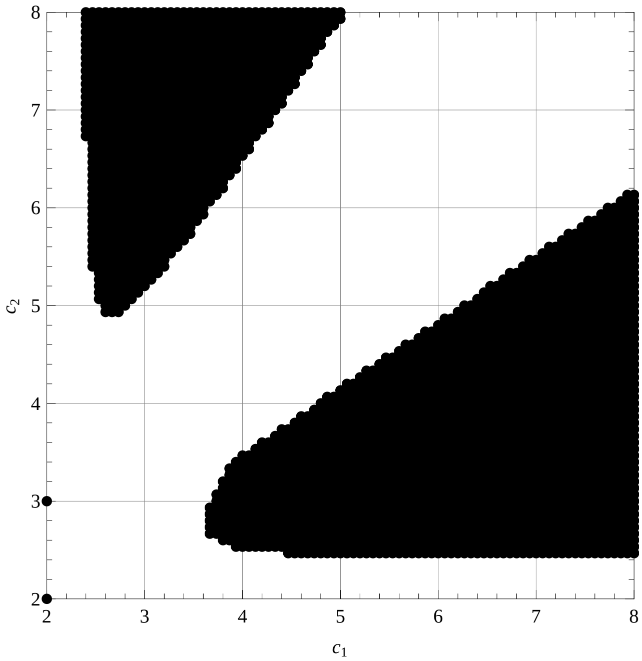

Figure 4: Region of A-stability in the parameter space (c_1, c_2) for DITSAC methods (15), with $m = 3$, $p = 5$, $c_3 = 2$ and such that the matrices Ψ and W are lower triangular.

and, eventually, such that their product is one-point spectrum. Future works will address the construction of highly stable methods (15) depending on more stages and their implementation, in order to exploit their properties to get an efficient variable stepsize-variable order implementation and, eventually, in a parallel environment.

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