

Dense Output for Strong Stability Preserving Runge–Kutta Methods

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Abstract We investigate dense output formulae (also known as continuous extensions) for strong stability preserving (SSP) Runge–Kutta methods. We require that the dense output formula also possess the SSP property, ideally under the same step-size restriction as the method itself. A general recipe for first-order SSP dense output formulae for SSP methods is given, and second-order dense output formulae for several optimal SSP methods are developed. It is shown that SSP dense output formulae of order three and higher do not exist, and that in any method possessing a second-order SSP dense output, the coefficient matrix A has a zero row.

Keywords Runge-Kutta methods · SSP methods · Dense output · Continuous extension

1 Motivation and Goals

Strong stability preserving (SSP) Runge–Kutta (RK) methods are widely used in the time discretization of hyperbolic conservation laws. SSP methods guarantee the preservation of solution properties based on convex functionals, such as monotonicity or contractivity (in arbitrary norms); positivity; and maximum principles. For a review of SSP methods see [4, 5].

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An SSP integrator is chosen usually in order to maximize the allowed step size while guaranteeing some desired property. In practice it frequently happens that the next time step would go beyond a desired output time. In this case, it is common to shorten the step in order to reach the output time exactly. If very frequent output is required, as is often the case in aeroacoustics applications, for instance, then the numerical steps may be much smaller than what the method would otherwise allow. In particular, for SSP methods frequent output may mean that the steps used in practice are much smaller than the SSP step size, which is inefficient. Even if the spacing between output times is much larger than the SSP step size, it may be necessary to use a small step immediately before each output time. In the context of hyperbolic problems, this corresponds to a step with small CFL number, which introduces a larger amount of dissipation.

In order to avoid the need to stop exactly at the output times, a RK method can be designed with a *dense output formula*, also known as a *continuous extension* [3, 12]. Whereas the RK method provides output only at the discrete step times t_1, t_2, \dots , the dense output formula can be used to obtain output at arbitrary times, often without the need for any additional function evaluations. The construction of dense output formulae for general RK methods is well understood. For instance, dense output of at least third order accuracy can be obtained for any RK method using Hermite interpolation, and higher-order formulae can also be derived [6, Section 2.6].

Contractivity of continuous RK methods has been studied previously in [1, 11] and related works. Therein, the interest was primarily in unconditional contractivity for applications to delay differential equations, and a diagonally split Runge–Kutta method was shown to achieve unconditional contractivity (see also [8]).

In the present work, we investigate dense output formulae for explicit SSP RK methods. Naturally, we require that the dense output formula also possess the SSP property, under the same (finite) step-size restriction as the overall method. This turns out to be a very strong requirement: we prove that for any SSP RK method, there exists no SSP dense output formula of order three or higher. On the other hand, we show that for many SSP methods, SSP dense output of order one or two can be constructed in a simple way.

1.1 A Numerical Example

Let us motivate this work by showing what can go wrong if no attention is paid to the SSP property of a dense output formula.

As a test problem, we choose the scalar ODE

$$u'(t) = f(t, u(t)) := \sin(10t) u(t) (1 - u(t)) \quad (1a)$$

$$u(0) = u_0 \quad (1b)$$

with various initial conditions $u_0 \in I_1 := [0, 1]$. It is easily seen that the exact solution of (1)

$$u(t) = u_0 \left(u_0 + (1 - u_0) \exp \left(\frac{\cos(10t) - 1}{10} \right) \right)^{-1}$$

remains in I_1 for any $u_0 \in I_1$ and $t \geq 0$. It is also straightforward to show that applying the forward Euler method

$$u_{n+1} = u_n + hf(nh, u_n)$$

to (1) with an arbitrary starting value $u_0 \in I_1$ and fixed step size $h \in [0, h_{FE}]$ with $h_{FE} := 1$ yields a solution $u_{n+1} \in I_1$.

Now let us apply the following 3-stage, 2nd-order SSP Runge–Kutta method to the same problem:

$$y_1 = u_n \quad (2a)$$

$$y_2 = y_1 + \frac{h}{2} f(t_n, y_1) \quad (2b)$$

$$y_3 = y_2 + \frac{h}{2} f(t_n + h/2, y_2) \quad (2c)$$

$$u_{n+1} = \frac{1}{3} u_n + \frac{2}{3} \left(y_3 + \frac{h}{2} f(t_n + h, y_3) \right). \quad (2d)$$

Since each stage of this method is a convex combination of Euler steps with step size at most $h/2$, it also preserves the invariance of I_1 , under the larger step-size restriction $h \in [0, 2h_{FE}] = [0, 2]$.

In order to evaluate the solution at off-step points, we will consider two dense output formulae. Here $u_{n+\theta}$ is an approximation to $u(t_n + \theta h)$, and we define the solution in a piecewise fashion so that $\theta \in [0, 1]$. The first candidate formula is

$$\begin{aligned} u_{n+\theta} = & \left(1 - 2\theta + \frac{4}{3}\theta^2 \right) u_n + 2(\theta - \theta^2) \left(y_1 + \frac{h}{2} f(t_n, y_1) \right) \\ & + \frac{2}{3}\theta^2 \left(y_3 + \frac{h}{2} f(t_n + h, y_3) \right). \end{aligned} \quad (3)$$

The second candidate formula is

$$u_{n+\theta} = u_n + h \left((2\theta - \theta^2) f(t_n, y_1) + (-2\theta + \theta^2) f(t_n + h/2, y_2) + \theta f(t_n + h, y_3) \right). \quad (4)$$

Both (3) and (4) are 2nd-order accurate. Regarding formula (3), since the coefficient functions $1 - 2\theta + 4\theta^2/3$, $2(\theta - \theta^2)$ and $2\theta^2/3$ are non-negative for $\theta \in [0, 1]$, this formula is also a convex combination of Euler steps, with step size $h/2$. So it also preserves the invariance of I_1 for $h \in [0, 2h_{FE}]$. This is however not true of formula (4).

We integrate (1) with method (2) for a range of initial conditions $u_0 \in I_1$ with step size $h = 1.6$ to obtain the values given by the set of black dots in Fig. 1 (the two sets of dots are the same in both subfigures). The application of the two dense output formulae (3) and (4) to (1) with the same step size $h = 1.6$ now provides us with two sets of piecewise quadratic interpolants. As shown in Fig. 1, the SSP dense output (3) preserves the relation $u_{n+\theta} \in I_1$ while the non-SSP dense output (4) does not. Tests with larger step sizes confirm that dense output using the SSP formula (3) remains in I_1 for $h \in [0, 2h_{FE}]$.

1.2 Outline

In the remainder of the paper, we show how to obtain SSP dense output formulae like (3) and investigate conditions under which such formulae exist. In Sect. 2, we recall algebraic properties of SSP methods and order conditions for Runge–Kutta methods. We also formulate the algebraic conditions for SSP dense output formulae. In Sect. 3, we show by considering the simpler case of quadrature that third-order SSP dense output does not exist. In Sect. 4, we give a first-order SSP dense output for any SSP method and a second-order SSP dense output for certain methods. In the “Appendix” we list some practically useful and simple SSP dense output formulae.

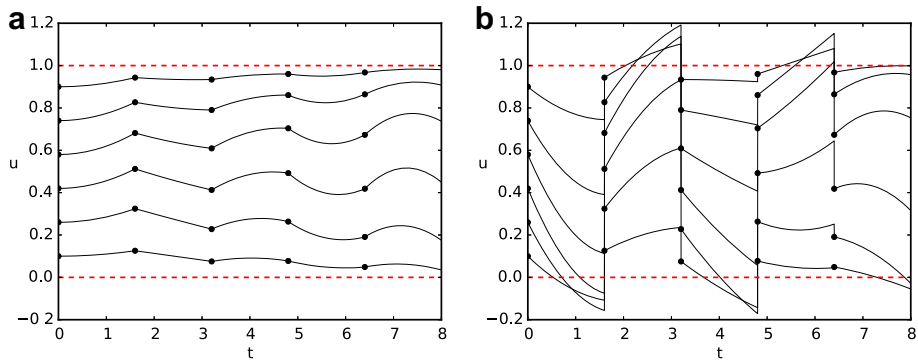


Fig. 1 Numerical solutions of (1) computed using SSP dense output (3) (left figure) and non-SSP dense output (4) (right figure). **a** SSP. **b** Non-SSP

2 Background on Strong Stability Preservation and Dense Output

In this section we review some of the essential algebraic properties of SSP RK methods and dense output that will be used later. For a more general review of SSP theory, see [5]. For a more general review of dense output, see [2].

2.1 Runge–Kutta Methods

An s -stage RK method generates an approximate solution of the initial value problem

$$u'(t) = f(u(t))$$

via the iteration

$$y_i = u_n + h \sum_{j=1}^s a_{i,j} f(y_j) \quad (5a)$$

$$u_{n+1} = u_n + h \sum_{j=1}^s b_j f(y_j). \quad (5b)$$

For simplicity of notation we have assumed the problem is written in autonomous form. The method is defined by the coefficient arrays $A \in \mathbb{R}^{s \times s}$, $b \in \mathbb{R}^s$. We will also refer to the vector c of abscissas, defined by $c_i := \sum_{j=1}^s a_{i,j}$.

The order conditions for a Runge–Kutta method up to order three are

$$\sum_{j=1}^s b_j = 1, \quad (p = 1) \quad (6a)$$

$$\sum_{j=1}^s b_j c_j = \frac{1}{2}, \quad (p = 2) \quad (6b)$$

$$\sum_{j=1}^s b_j c_j^2 = \frac{1}{3}, \quad (p = 3) \quad (6c)$$

$$\sum_{j=1}^s b_j \left(\frac{c_j^2}{2} - \sum_{k=1}^s a_{j,k} c_k \right) = 0, \quad (p = 3). \quad (6d)$$

Any method with more than one row of A equal to zero is (trivially) reducible [7]. Furthermore, a Runge–Kutta method is invariant under permutation of its stages. Therefore, without loss of generality we assume throughout this work that A has at most one row identically equal to zero, and if it has such a row then it is the first row:

$$\text{For each } 2 \leq j \leq s, \text{ row } j \text{ of } A \text{ is not identically zero.} \quad (7)$$

2.2 Strong Stability Preserving Runge–Kutta Methods

Let \mathbf{e} denote the vector of length s with all entries equal to 1. A method is said to be strong stability preserving if there exists $r > 0$ such that

$$A(I + rA)^{-1} \geq 0 \quad rA(I + rA)^{-1}\mathbf{e} \leq 1 \quad (8a)$$

$$b^\top(I + rA)^{-1} \geq 0 \quad rb^\top(I + rA)^{-1}\mathbf{e} \leq 1. \quad (8b)$$

The inequalities are meant componentwise.

The *SSP coefficient* of the method, denoted by $\mathcal{C}(A, b)$, can be defined as follows [5]:

$$\mathcal{C}(A, b) := \sup \{ r \geq 0 : (I + rA)^{-1} \text{ exists and (8) holds} \}$$

if the set in the sup above is not empty, and $\mathcal{C}(A, b) := 0$ otherwise. The following lemma is well known; for a proof see [5, p. 65].

Lemma 1 *Let a RK method (A, b) be given. If the method has positive SSP coefficient $\mathcal{C}(A, b) > 0$, then $a_{i,j} \geq 0$ and $b_j \geq 0$ for all $1 \leq i, j \leq s$.*

2.3 Dense Output for Runge–Kutta Methods

A dense output formula takes the form

$$u_{n+\theta} = u_n + h \sum_{j=1}^s \bar{b}_j(\theta) f(y_j); \quad (9)$$

the weights b_j in (5b) have been replaced by some real-valued functions $\bar{b}_j(\cdot)$. Here $u_{n+\theta}$ is an approximation to the solution at time $t_n + \theta(t_{n+1} - t_n) = t_n + \theta h$, and naturally $\theta \in [0, 1]$. Hence, throughout the work, we assume that the weights \bar{b}_j are defined on the interval $[0, 1]$; in Sect. 3 we will impose some (minimal) smoothness assumptions on \bar{b}_j , and in Sect. 4 we will assume that the weights \bar{b}_j are polynomials (to develop the simplest possible dense output formulae). In some cases it is advantageous to include an additional term proportional to $f(u_{n+1})$ in (9) (but this modification of (9) will not be considered in the present work).

The order conditions for the dense output formula (up to order three) are [6, Section 2.6]

$$\sum_{j=1}^s \bar{b}_j(\theta) = \theta, \quad \forall \theta \in [0, 1] \quad (p = 1) \quad (10a)$$

$$\sum_{j=1}^s \bar{b}_j(\theta) c_j = \frac{\theta^2}{2}, \quad \forall \theta \in [0, 1] \quad (p = 2) \quad (10b)$$

$$\sum_{j=1}^s \bar{b}_j(\theta) c_j^2 = \frac{\theta^3}{3}, \quad \forall \theta \in [0, 1] \quad (p = 3) \quad (10c)$$

$$\sum_{j=1}^s \sum_{k=1}^s \bar{b}_j(\theta) a_{j,k} c_k = \frac{\theta^3}{6}, \quad \forall \theta \in [0, 1] \quad (p = 3). \quad (10d)$$

Conditions (10a)–(10c) [and (6a)–(6c)] are *quadrature conditions*; i.e. they are necessary and sufficient for third-order convergence when the method is applied to a pure quadrature problem $u'(t) = f(t)$.

For a RK method of order p , the convergence rate of the dense output values will be the same as that of the RK step outputs as long as the dense output formula has order $p - 1$ [6].

2.3.1 Continuity at the Endpoints

It is natural to require $\bar{b}_j(0) = 0$ and

$$\bar{b}_j(1) = b_j \quad (11)$$

for a dense output formula, expressing continuity as $\theta \rightarrow 0^+$ and as $\theta \rightarrow 1^-$, respectively, in (9). These assumptions are made in [12] and subsequent works. However, our interest is in applying SSP methods to nonlinear hyperbolic PDEs, whose solutions are not continuous. Indeed, many modern spatial discretizations for hyperbolic PDEs are based on a representation that is discontinuous at every node of the mesh. Thus in our study we allow for extensions that are not continuous at the endpoints. As we will see, the SSP conditions turn out to imply continuity as $\theta \rightarrow 0^+$, and the optimal formulae we find all satisfy continuity also as $\theta \rightarrow 1^-$.

2.4 Strong Stability Preserving Dense Output

We are interested in dense output formulae that also possess the SSP property. To define the *SSP coefficient of the dense output formula* we make use of the following inequalities, which are just (8b) with b replaced by \bar{b} :

$$\bar{b}(\theta)^\top (I + rA)^{-1} \geq 0 \quad r\bar{b}(\theta)^\top (I + rA)^{-1} \mathbf{e} \leq 1 \quad \text{for } 0 \leq \theta \leq 1. \quad (12)$$

Here and in what follows, $\bar{b} : [0, 1] \rightarrow \mathbb{R}^s$ denotes the function $(\bar{b}_1, \dots, \bar{b}_s)$. The SSP coefficient of the dense output formula, denoted by $C(A, \bar{b})$, is defined as follows:

$$C(A, \bar{b}) := \sup \{r \geq 0 : (I + rA)^{-1} \text{ exists and (8a) and (12) hold for all } 0 \leq \theta \leq 1\}$$

if the set in the sup above is not empty, and $C(A, \bar{b}) := 0$ otherwise. We also define the *SSP coefficient of the method with its dense output formula* as

$$C(A, b, \bar{b}) := \min \left(C(A, b), C(A, \bar{b}) \right).$$

This is the coefficient that matters in practice since it dictates the step size that can be used while guaranteeing strong stability of the solution at both the step points and dense output points.

Nonnegativity of the dense output coefficients is necessary in order that the SSP coefficient $\mathcal{C}(A, b, \bar{b})$ be positive.

Lemma 2 *Let a RK method with dense output (A, b, \bar{b}) be given such that $\mathcal{C}(A, b, \bar{b}) > 0$. Then $a_{i,j} \geq 0$, $b_j \geq 0$, and $\bar{b}_j(\theta) \geq 0$ for all $1 \leq i, j \leq s$ and for all $0 \leq \theta \leq 1$.*

The proof of Lemma 2 is similar to that of Lemma 1.

The requirement of continuity as $\theta \rightarrow 0^+$ turns out to be necessary for SSP dense output.

Lemma 3 *Let a RK method with dense output of order at least one be given with coefficients (A, b, \bar{b}) . If $\mathcal{C}(A, b, \bar{b}) > 0$, then*

$$\bar{b}_j(0) = 0 \quad (1 \leq j \leq s). \quad (13)$$

Proof By Lemma 2 we have $\bar{b}_j(\theta) \geq 0$, and condition (10a) implies $\sum_j \bar{b}_j(0) = 0$. \square

Finally, it is clear from the definitions that

$$(11) \implies \mathcal{C}(A, \bar{b}) \leq \mathcal{C}(A, b). \quad (14)$$

3 Restrictions and Non-existence Results

It turns out that certain restrictions on SSP dense output formulae appear already when one considers only quadrature problems. The case of quadrature is considered in Sect. 3.1, and general results for Runge–Kutta methods are deduced in Sect. 3.2.

In this section we are going to impose some smoothness assumptions on the weight functions \bar{b}_j defined on $[0, 1]$. To formulate these, we will use the notation

$$\mathcal{D}^k(0+) \quad (k \in \mathbb{N}^+)$$

to denote the set of real functions that are k times right-differentiable at the origin; the symbols $\bar{b}'_j(0)$ and $\bar{b}''_j(0)$ will denote right-derivatives.

3.1 A Result on Non-negative Quadrature Rules

When we apply a Runge–Kutta method to a problem in which f is independent of u ,

$$u'(t) = f(t), \quad u(t_0) = u_0, \quad (15)$$

the dense output reduces to a quadrature rule

$$u(t_0 + \theta) \approx u_0 + \sum_{j=1}^s \bar{b}_j(\theta) f(t_0 + \theta c_j). \quad (16)$$

We assume, without loss of generality, that the abscissas c_j are distinct (any method (16) with repeated abscissas can be rewritten as a method with distinct abscissas). We show that if the abscissas c_j and weights \bar{b}_j are non-negative, the accuracy of (16) is limited.

Theorem 1 Let a quadrature rule (16) be given with distinct abscissas $c_j \in \mathbb{R}$, and with weight functions $\bar{b}_j \in \mathcal{D}^1(0+)$ that are non-negative in a right neighborhood of zero, i.e.

$$\bar{b}_j(\theta) \geq 0 \quad \forall j \text{ and } \forall \theta \in [0, \epsilon) \text{ with some } \epsilon > 0. \quad (17)$$

If (16) is exact for quadratic polynomials, i.e. if (10a)–(10b) hold, then at least one abscissa is non-positive. If $\bar{b}_j \in \mathcal{D}^2(0+)$, and (16) is exact for cubic polynomials, i.e. if (10a)–(10c) hold, then at least one abscissa is negative.

Proof We suppose in the proof that $c_j \geq 0$ ($1 \leq j \leq s$) (otherwise the proof is complete). Formula (10a) and (17) at $\theta = 0$ imply

$$\bar{b}_j(0) = 0 \quad (1 \leq j \leq s). \quad (18)$$

But then (17) also implies $\bar{b}'_j(0) \geq 0$. Differentiation of (10b) at 0 yields $\sum_{j=1}^s \bar{b}'_j(0)c_j = 0$, so from the non-negativity we get

$$\bar{b}'_j(0) = 0 \text{ or } c_j = 0 \text{ for each } j. \quad (19)$$

Differentiation of (10a) at 0 shows that $\bar{b}'_{j_0}(0) \neq 0$ for some j_0 , hence $c_{j_0} = 0$.

To prove the second statement, we can thus assume that exactly one abscissa is zero (since they are distinct). Let the abscissas be ordered so that $c_1 = 0$; then $c_j > 0$ for $2 \leq j \leq s$. The derivative of (10a) at $\theta = 0$ and (19) now imply

$$\bar{b}'_1(0) = 1 \text{ and } \bar{b}'_j(0) = 0 \text{ for } 2 \leq j \leq s. \quad (20)$$

So from (17) and (18) we obtain that $\bar{b}''_j(0) \geq 0$ for $2 \leq j \leq s$. Since (10c) says

$$\sum_{j=1}^s \bar{b}''_j(0)c_j^2 = \sum_{j=2}^s \bar{b}''_j(0)c_j^2 = 0,$$

we also have $\bar{b}''_j(0) = 0$ for all $2 \leq j \leq s$. But this is incompatible with the second derivative of (10b) at $\theta = 0$. \square

3.2 Restrictions on SSP Dense Output for Runge–Kutta Methods

For a given SSP RK method (A, b) of s stages and order p , we seek to find functions \bar{b}_j ($1 \leq j \leq s$) that satisfy the order conditions (10) up to at least order $p - 1$ and the SSP conditions (12). The next theorem restricts the form of possible formulae and methods with positive SSP coefficient.

Theorem 2 Let an SSP Runge–Kutta method be given with coefficients (A, b) where A satisfies (7), and let (A, \bar{b}) be a dense output formula of order at least two with weight functions $\bar{b}_j \in \mathcal{D}^1(0+)$. Suppose that $C(A, b, \bar{b}) > 0$. Then the first row of A is identically zero and

$$\bar{b}'_1(0) = 1 \quad (21a)$$

$$\bar{b}'_j(0) = 0 \quad \text{for all } 2 \leq j \leq s. \quad (21b)$$

Proof Consider a method that satisfies the assumptions in the theorem. By Lemma 2 we have $\bar{b}_j \geq 0$ and $c_j \geq 0$ ($1 \leq j \leq s$). The method is 2nd-order accurate for quadratures, so we can reread the proof of Theorem 1 up to (20) but omitting the parts written in italics. Note

also that by assumption (7) we have $c_1 = 0$ (and $c_j \neq 0$ for $2 \leq j \leq s$) in the second part of that proof. \square

The next result indicates that no dense output formula of order three or higher exists.

Theorem 3 *Let an SSP Runge–Kutta method (A, b) be given such that A satisfies (7), along with a dense output formula $\bar{b} \in \mathcal{D}^2(0+)$ such that $\mathcal{C}(A, b, \bar{b}) > 0$. Then the order of accuracy of the dense output formula is at most two.*

Proof This follows from Lemma 2 and Theorem 1, which imply that an SSP dense output formula cannot be third order accurate even for quadratures. \square

4 Construction of 1st- and 2nd-Order Formulae

In this section we develop dense output formulae for the optimal SSP Runge–Kutta methods of orders 1 and 2. As always, we assume condition (7). It turns out that dense output formulae of order one or two can be obtained in a simple, general way for many SSP methods.

From now on it is natural to assume that each weight \bar{b}_j is a polynomial whose degree, D , is equal to or greater than the desired order of accuracy of the dense output formula, $p - 1 \leq D$. That is, throughout Sect. 4, we represent \bar{b}_j as

$$\bar{b}_j(\theta) = \sum_{k=0}^D \bar{b}_{j,k} \theta^k \quad (22)$$

with some coefficients $\bar{b}_{j,k} \in \mathbb{R}$ ($1 \leq j \leq s$, $0 \leq k \leq D$).

4.1 First-Order Dense Output

Theorem 4 *Let a Runge–Kutta method of order at least one be given with coefficients (A, b) and SSP coefficient $\mathcal{C}(A, b) > 0$. Then a first-order dense output with the same SSP coefficient $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b)$ is obtained by taking $\bar{b}_j(\theta) := b_j \theta$ ($1 \leq j \leq s$); i.e.*

$$u_{n+\theta} = u_n + h \theta \sum_{j=1}^s b_j f(y_j). \quad (23)$$

Proof It suffices to check that condition (10a) is satisfied and conditions (12) hold with $r = \mathcal{C}(A, b)$. By taking into account $\bar{b}(\theta) = b\theta$ ($\theta \in [0, 1]$), condition (10a) follows from (6a), and conditions (12) follow from the fact that method (A, b) satisfies (8b) with $r = \mathcal{C}(A, b)$. \square

4.2 Second-Order Dense Output

Next we turn our attention to second-order dense output. According to Theorem 2, and applying assumption (7) we have that the first row of A is zero. Motivated by (13), (21), (11) and (10a), and taking $D = 2$ in (22), we see that these conditions yield a unique set of quadratic polynomials \bar{b}_j :

$$\bar{b}_1(\theta) = \theta - (1 - b_1)\theta^2 \quad (24a)$$

$$\bar{b}_j(\theta) = \theta^2 b_j \quad (2 \leq j \leq s). \quad (24b)$$

For many SSP RK methods (A, b) , this choice of \bar{b} gives a second-order SSP dense output formula with $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b)$ (cf. (14)).

Theorem 5 *Let a Runge–Kutta method of order at least two be given with coefficients (A, b) and SSP coefficient $\mathcal{C}(A, b) > 0$. Suppose that the first row of A is zero and let \bar{b} be defined by (24). Then the following statements are true.*

1. (A, \bar{b}) is an SSP dense output formula of order at least two.
2. If

$$b^\top (I + \mathcal{C}(A, b)A)^{-1} \mathbf{e} \leq 1 - \frac{\mathcal{C}(A, b)}{4}, \quad (25)$$

then $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b)$.

3. If $\mathcal{C}(A, b) \leq 2$, then $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b)$.

Proof Since formulae (24) satisfy (11), we have $\mathcal{C}(A, \bar{b}) \leq \mathcal{C}(A, b)$ due to (14). So it suffices to check that the order conditions (10a)–(10b) are satisfied and that the SSP conditions (12) hold with $r = \mathcal{C}(A, b)$.

The order conditions are easily checked, since $\sum_{j=1}^s \bar{b}_j(\theta) = \theta + \theta^2 \left(-1 + \sum_{j=1}^s b_j\right) = \theta$ due to (6a). Similarly, since $c_1 = 0$ because the first row of A is zero, we have $\sum_{j=1}^s \bar{b}_j(\theta)c_j = \sum_{j=2}^s \bar{b}_j(\theta)c_j = \theta^2 \sum_{j=2}^s b_j c_j = \theta^2 \sum_{j=1}^s b_j c_j = \frac{\theta^2}{2}$ due to (6b).

To verify the first SSP condition in (12), we let $M := (I + \mathcal{C}(A, b)A)^{-1}$ and $\mathbf{e}_1 := (1, 0, \dots, 0)^\top$. Since the first row of A is zero, the first row of M is \mathbf{e}_1^\top , hence $\mathbf{e}_1^\top M = \mathbf{e}_1^\top$. Observe that $\bar{b}(\theta) = \theta^2 b + (\theta - \theta^2)\mathbf{e}_1$, so for $0 \leq \theta \leq 1$ we have $\bar{b}(\theta)^\top M = \theta^2 b^\top M + (\theta - \theta^2)\mathbf{e}_1^\top M = \theta^2 b^\top M + (\theta - \theta^2)\mathbf{e}_1^\top \geq \theta^2 b^\top M \geq 0$, because b satisfies (8b).

As for the second SSP condition in (12), we set $\gamma := b^\top M \mathbf{e}$ and $\varphi(\theta) := \mathcal{C}(A, b)(\gamma - 1)\theta^2 + \mathcal{C}(A, b)\theta - 1$ to rewrite it as

$$\begin{aligned} \mathcal{C}(A, b)\bar{b}(\theta)^\top M \mathbf{e} &= \mathcal{C}(A, b)\theta^2 \gamma + \mathcal{C}(A, b)(\theta - \theta^2)\mathbf{e}_1^\top M \mathbf{e} \\ &= \mathcal{C}(A, b)\theta^2 \gamma + \mathcal{C}(A, b)(\theta - \theta^2) = \varphi(\theta) + 1. \end{aligned}$$

Hence $\mathcal{C}(A, b)\bar{b}(\theta)^\top M \mathbf{e} \leq 1$ is equivalent to

$$\varphi(\theta) \leq 0 \quad \forall \theta \in [0, 1]. \quad (26)$$

In what follows we will use

$$\mathcal{C}(A, b) > 0, \quad \gamma \geq 0 \quad \text{and} \quad \mathcal{C}(A, b)\gamma \leq 1 \quad (27)$$

to show (26); the last two inequalities of (27) follow from (8b) again.

- For $\gamma = 1$, we have $\mathcal{C}(A, b) \leq 1$ and $\varphi(\theta) = \mathcal{C}(A, b)\theta - 1$, hence (26) holds and the proof is complete.
- For $\gamma > 1$, the strict global minimum of the parabola φ is attained at $\theta^* = \frac{1}{2(1-\gamma)} < 0$. Hence (26) is equivalent to $\varphi(1) \leq 0$. But $\varphi(1) = \mathcal{C}(A, b)\gamma - 1 \leq 0$ due to (27).
- For $\gamma \in [0, 1)$, the strict global maximum of the parabola φ is attained at $\theta^* = \frac{1}{2(1-\gamma)} > 0$. For $\gamma \in (\frac{1}{2}, 1)$, we have $\theta^* > 1$, so (26) is equivalent to $\varphi(1) \leq 0$, which we have already seen to hold. Finally, for $\gamma \in [0, \frac{1}{2}]$, we see that $\theta^* \in (0, 1]$, so (26) is equivalent to $\varphi(\theta^*) \leq 0$. Here $\varphi(\theta^*) = \frac{\mathcal{C}(A, b) + 4\gamma - 4}{4(1-\gamma)}$, and (25) or $\mathcal{C}(A, b) \leq 2$ implies $\varphi(\theta^*) \leq 0$.

□

4.3 Implicit SSP Methods

First-order SSP dense output for any implicit SSP method can be constructed according to (23). However, since all known optimal implicit SSP methods are diagonally implicit, Theorem 2 implies that they have no second-order SSP dense output with polynomial weights. It is possible that there exist implicit methods with the first row of A equal to zero such that $\mathcal{C}(A, b) > 0$ and some \bar{b} such that $\mathcal{C}(A, \bar{b}) > 0$. However, since such methods will have SSP coefficient even smaller than those of the optimal implicit SSP methods, we have not conducted a search for them.

4.4 Explicit SSP Methods

The theorem in Sect. 4.2 does not settle the question of existence of dense output formulae of order two for particular RK methods of interest. In this section we develop such formulae for some optimal explicit SSP RK methods (A, b) .

One can directly verify that the following optimal explicit SSP methods satisfy condition (25) in Theorem 5, and so (24) provides a 2nd-order SSP dense output formula \bar{b} with $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b) > 0$:

- second-order methods with two [9], three, or four [10] stages;
- third-order methods with three [9] or four [10] stages;
- the fourth-order method with five stages [10].

Coefficients for all of the methods above can be found, for instance in [5, Chapter 6]. Computations show that explicit optimal methods with more stages than those listed above do not satisfy (25) and we have not found a way to construct dense output formulae with SSP coefficient as large as that of the method itself for any of them.

As an illustration, we show in the following subsection that there exists a 2nd-order s -stage dense output formula with $\mathcal{C}(A, \bar{b}) \geq \mathcal{C}(A, b)$ where the weights \bar{b}_j are quadratic polynomials in θ if and only if $s \in \{2, 3, 4\}$.

4.5 Dense Output for Optimal Explicit Second-Order SSP RK Methods

A family of optimal 2nd-order SSP Runge–Kutta methods with s stages (for $s \geq 2$) was introduced in [10]. We have already seen above that (24) gives an SSP dense output with $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b)$ for the members of this family with $s = 2, 3, 4$. In this section we show that no quadratic dense output with $\mathcal{C}(A, \bar{b}) = \mathcal{C}(A, b)$ exists for the members of this family with $s \geq 5$.

We will use the following properties of an optimal 2nd-order SSP RK method (A, b) with s stages [5]: it satisfies (7); it has $b_j = 1/s$ and $c_j = (j - 1)/(s - 1)$ for $1 \leq j \leq s$; $\mathcal{C}(A, b) = s - 1$; and it satisfies

$$(I + \mathcal{C}(A, b)A)^{-1} = \begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}$$

(with zeros elsewhere).

A necessary condition for $\mathcal{C}(A, \bar{b}) \geq \mathcal{C}(A, b)$ is that the SSP conditions (12) with $r := \mathcal{C}(A, b)$ are fulfilled. Thus conditions (12) lead to the inequalities

$$0 \leq \bar{b}_s(\theta) \leq \bar{b}_{s-1}(\theta) \leq \cdots \leq \bar{b}_2(\theta) \leq \bar{b}_1(\theta) \leq \frac{1}{C(A, b)}, \quad \forall \theta \in [0, 1]. \quad (28)$$

On the one hand, by applying Lemma 3, Theorem 2, condition (10a) and the representation (22), we get that

$$\bar{b}_j(\theta) = \bar{b}_{j,2} \theta^2 \quad (2 \leq j \leq s) \quad (29a)$$

$$\bar{b}_1(\theta) = \theta - \theta^2 \sum_{j=2}^s \bar{b}_{j,2} \quad (29b)$$

should hold with some constants $\bar{b}_{j,2}$. Hence (28) evaluated at $\theta = 1$ leads to the necessary conditions

$$0 \leq \bar{b}_{s,2} \leq \bar{b}_{s-1,2} \leq \cdots \leq \bar{b}_{2,2} \leq 1 - \sum_{j=2}^s \bar{b}_{j,2}, \quad (30a)$$

$$1 - \sum_{j=2}^s \bar{b}_{j,2} \leq \frac{1}{s-1}. \quad (30b)$$

On the other hand, the second-order accuracy condition (10b) evaluated at $\theta = 1$ now reads

$$\sum_{j=2}^s \frac{j-1}{s-1} \bar{b}_{j,2} = \frac{1}{2}. \quad (31)$$

One way to satisfy (31) and (30a) is to take

$$\bar{b}_{j,2} = \frac{1}{s} \quad (2 \leq j \leq s). \quad (32)$$

It turns out that this solution is unique.

Lemma 4 Suppose that the real numbers $\bar{b}_{2,2}, \dots, \bar{b}_{s,2}$ satisfy (31) and (30a). Then $\bar{b}_{j,2} = 1/s$ for $2 \leq j \leq s$.

Proof Set $\delta_j := \bar{b}_{j,2} - \frac{1}{s}$. Then from (31) we get

$$\sum_{j=2}^s (j-1) \delta_j = 0, \quad (33)$$

and (30a) becomes

$$-1/s \leq \delta_s \leq \cdots \leq \delta_2 \leq -\sum_{j=2}^s \delta_j. \quad (34)$$

We will show that (33) and (34) imply that $\delta_j = 0$ for each j . Suppose by way of contradiction that $\delta_j \neq 0$ for some j . Then (33) implies that $\delta_j > 0$ for some j , so by (34) we have $\delta_2 > 0$. Hence (34) implies that $\sum_{j=2}^s \delta_j < 0$. This in turn implies recursively that each of the partial sums $\sum_{j=i}^s \delta_j$ (for $i \geq 2$) is negative. But then

$$\sum_{j=2}^s (j-1) \delta_j = \sum_{i=2}^s \sum_{j=i}^s \delta_j < 0,$$

which contradicts (33). \square

We can now give a complete characterization of quadratic 2nd-order SSP dense output formulae for optimal 2nd-order SSP Runge–Kutta methods, satisfying $\mathcal{C}(A, \bar{b}) \geq \mathcal{C}(A, b)$.

Theorem 6 *Consider the optimal 2nd-order SSP RK method with s stages, having SSP coefficient $\mathcal{C}(A, b) = s - 1$. For $2 \leq s \leq 4$, the method possesses a unique 2nd-order accurate SSP dense output formula with quadratic polynomials \bar{b}_j and SSP coefficient $\mathcal{C}(A, \bar{b}) = s - 1$:*

$$\bar{b}_1(\theta) := \theta - \frac{s-1}{s}\theta^2 \quad (35a)$$

$$\bar{b}_j(\theta) := \frac{1}{s}\theta^2 \quad (2 \leq j \leq s). \quad (35b)$$

For $s \geq 5$, there exists no 2nd-order SSP dense output formula quadratic in θ with $\mathcal{C}(A, \bar{b}) \geq s - 1$.

Proof Formulae (29) and Lemma 4 show that any candidate dense output formula must have the form given by (35). But now $b_j = 1/s$ ($1 \leq j \leq s$), hence formulae (35) are identical to formulae (24), and so Theorem 5 is applicable.

For $s \in \{2, 3\}$, we have $\mathcal{C}(A, b) = s - 1 \leq 2$, so Statement 3 of Theorem 5 yields $\mathcal{C}(A, \bar{b}) = s - 1$.

For $s = 4$, we have equality in (25) because both sides are equal to $1/4$, so we again get $\mathcal{C}(A, \bar{b}) = s - 1$.

For $s \geq 5$ however, the inequality $\bar{b}_1(\theta) \leq \frac{1}{\mathcal{C}(A, b)}$ in the necessary condition (28) is violated for $\theta := \frac{s}{2(s-1)} \in (0, 1]$, so there is no corresponding 2nd-order SSP dense output formula with $D = 2$ and $\mathcal{C}(A, \bar{b}) \geq \mathcal{C}(A, b)$. \square

Remark 1 For optimal 2nd-order explicit SSP RK methods (A, b) with $s \geq 5$ stages, Theorem 6 does not preclude the existence of 2nd-order dense output formulae that consist of \bar{b}_j polynomials of degree $D \geq 3$ in (22) and have $\mathcal{C}(A, \bar{b}) \geq \mathcal{C}(A, b) > 0$. But initial searches have failed to yield any such formulae.

Remark 2 The uniqueness in Theorem 6 “almost” follows from the uniqueness stated in the sentence preceding formula (24). However, when deriving (24), the right endpoint condition (11) has been taken into account—whereas when deriving Theorem 6, one does not use (11).

5 Conclusion

We have proved the non-existence of SSP dense output of order three or higher; we have shown that this follows from a more fundamental result on the abscissas of continuously-valued quadrature rules with positive weights. On the other hand, for some of the most common SSP methods it is straightforward to construct dense output of second order using (24).

For methods that do not satisfy condition 2 or 3 of Theorem 5, it may still be possible to develop 2nd-order dense output with $\mathcal{C}(A, \bar{b}) \geq \mathcal{C}(A, b)$.

Theorem 1 naturally suggests the inclusion of negative abscissas in the dense output formula. This can be done most simply by using previous step values u_{n-j} , which is the subject of current research.

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Appendix: Some Complete Methods in Shu–Osher Form

We have worked with methods in Butcher form because of the simplicity of the order conditions in that form. In this “Appendix” we write out some of the methods with dense output in Shu–Osher form, since this is usually the most convenient form for implementation. For the sake of brevity we write the methods in autonomous form and let $\mathcal{C} = \mathcal{C}(A, b, \bar{b})$.

The dense output in Shu–Osher form is

$$u_{n+\theta} = \mu u_n + \sum_{j=1}^s \bar{\beta}_j(\theta) \left(y_j + \frac{h}{C} f(y_j) \right)$$

where

$$\begin{aligned} \bar{\beta}^\top &:= \bar{b}^\top (I + CA)^{-1} \\ \mu &:= 1 - C \bar{b}^\top (I + CA)^{-1}. \end{aligned}$$

We denote each method by SSP(s, p, \bar{p}), where s is the number of stages, p is the order of the method (A, b) , and \bar{p} is the order of the dense output.

SSP(2,2,2)

This method has $\mathcal{C}(A, b, \bar{b}) = 1$.

$$\begin{aligned} y_1 &= u_n \\ y_2 &= y_1 + hf(y_1) \\ u_{n+1} &= \frac{1}{2}u_n + \frac{1}{2}(y_2 + hf(y_2)) \\ u_{n+\theta} &= \left(1 - \theta + \frac{1}{2}\theta^2\right)u_n + (\theta - \theta^2)(y_1 + hf(y_1)) + \frac{1}{2}\theta^2(y_2 + hf(y_2)). \end{aligned}$$

SSP(3,2,2)

This method has $\mathcal{C}(A, b, \bar{b}) = 2$.

$$\begin{aligned} y_1 &= u_n \\ y_2 &= y_1 + \frac{h}{2}f(y_1) \\ y_3 &= y_2 + \frac{h}{2}f(y_2) \\ u_{n+1} &= \frac{1}{3}u_n + \frac{2}{3}\left(y_3 + \frac{h}{2}f(y_3)\right) \\ u_{n+\theta} &= \left(1 - 2\theta + \frac{4}{3}\theta^2\right)u_n + 2(\theta - \theta^2)\left(y_1 + \frac{h}{2}f(y_1)\right) + \frac{2}{3}\theta^2\left(y_3 + \frac{h}{2}f(y_3)\right). \end{aligned}$$

SSP(3,3,2)

This method has $\mathcal{C}(A, b, \bar{b}) = 1$.

$$\begin{aligned} y_1 &= u_n \\ y_2 &= y_1 + hf(y_1) \end{aligned}$$

$$\begin{aligned}
 y_3 &= \frac{3}{4}u_n + \frac{1}{4}(y_2 + hf(y_2)) \\
 u_{n+1} &= \frac{1}{3}u_n + \frac{2}{3}(y_3 + hf(y_3)) \\
 u_{n+\theta} &= \left(1 - \theta + \frac{1}{3}\theta^2\right)u_n + (\theta - \theta^2)(y_1 + hf(y_1)) + \frac{2}{3}\theta^2(y_3 + hf(y_3)).
 \end{aligned}$$

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