Continuous-stage Runge-Kutta methods based on weighted orthogonal polynomials

Wensheng Tang*

College of Mathematics and Statistics,
Changsha University of Science and Technology,
Changsha 410114, China

Hunan Provincial Key Laboratory of
Mathematical Modeling and Analysis in Engineering,
Changsha 410114, China

Abstract

We develop continuous-stage Runge-Kutta methods based on weighted orthogonal polynomials in this paper. There are two main highlighted merits for developing such methods: Firstly, we do not need to study the tedious solution of multi-variable nonlinear algebraic equations associated with order conditions; Secondly, the well-known weighted interpolatory quadrature theory appeared in every numerical analysis textbook can be directly and conveniently used. By introducing weight function, various orthogonal polynomials can be used in the construction of Runge-Kutta-type methods. It turns out that new families of Runge-Kutta-type methods with special properties (e.g., symplectic, symmetric etc.) can be constructed in batches, and hopefully it may produce new applications in numerical ordinary differential equations.

Keywords: Continuous-stage Runge-Kutta methods; Weighted orthogonal polynomials; Hamiltonian systems; Symplectic methods; Symmetric methods.

1. Introduction

As is well-known, Runge-Kutta (RK) methods have gained a significant place in the field of numerical ordinary differential equations (ODEs) after the pioneering work of Runge (1895) [33]. For over a hundred and twenty years, RK-type methods as well as their numerical theories have been well developed and many relevant applications have been fully explored (see [8, 9, 19, 20] and references therein). Recently, such highly-developed methods are creatively extended by allowing their schemes to be “continuous” with “infinitely many stages”, which then generates the concept of continuous-stage Runge-Kutta (csRK) methods. The most original idea of such special methods was launched by Butcher in 1972 [6] (see also his monograph [9], “386 The element E”, Page 325). Hairer firstly developed it in [22] by using it to interpret and analyze his energy-preserving collocation methods and he created a specific mathematic formulation for csRK methods. Based on these pioneering work, Tang & Sun [42, 43, 47] discovered that Galerkin time-discretization methods for

*Corresponding author.

Email address: tangws@lsec.cc.ac.cn (Wensheng Tang)
ODEs can be closely related to csRK methods in the shape of Hairer’s formalism. More recently, csRK methods have found their own values in the field of geometric numerical integration (i.e., structure-preserving algorithms) [21]. A growing number of structure-preserving algorithms have been developed in the context of csRK methods, which covers symplectic csRK methods [41, 43, 44, 49], conjugate-symplectic (up to a finite order) csRK methods [22, 23, 43, 44], symmetric csRK methods [22, 41, 43, 44, 49], energy-preserving csRK methods [4, 11, 22, 31, 41, 42, 43, 44, 49]. Particularly, in contrast to a negative result given by Celledoni et al [11], showing that there exists no energy-preserving RK methods for general non-polynomial Hamiltonian systems, various classes of energy-preserving methods within the framework of csRK methods can be constructed [22, 29, 30, 31, 41, 44, 49]. Besides, some extensions of csRK methods are developed by Tang et al [46, 48]. It seems that continuous-stage methods provide us a new realm for numerically solving ODEs, and it is expected to further enlarge the application of RK approximation theory in geometric numerical integration [22, 23, 28, 29, 30, 41, 43, 44, 46, 48, 45, 49].

In this paper, we attempt to further develop csRK methods for ODEs, extending the previous study by Tang & Sun [41, 44] to a much more general case. Actually, the previous studies have intensively discussed the construction of csRK methods on the premise of \( B_\tau \equiv 1 \). This paper is devoted to breaking through such limitation and enlarging the family of csRK methods by allowing \( B_\tau \neq 1 \). To achieve this goal, we will develop csRK methods with weighted orthogonal polynomials. There are two main highlighted merits for developing such methods: Firstly, we do not need to study the tedious solution of multi-variable nonlinear algebraic equations associated with order conditions; Secondly, the well-known weighted interpolatory quadrature theory appeared in every numerical analysis textbook can be directly and conveniently used. The conjunction of orthogonal polynomial expansion techniques and weighted interpolatory quadrature theory will help us to realize and attest these merits.

In [7], Butcher gave a survey on many applications of orthogonal polynomials in the field of numerical ODEs (especially those related to accuracy and implementability of RK methods). We recognize that in general numerical integration of various differential equations is closely related to quadrature techniques where the proper employment of orthogonal polynomials is crucial. In this paper, we explore new applications of weighted orthogonal polynomials (e.g., Jacobi polynomials) in the study of csRK methods. Particularly, we are going to discuss their applications in geometric numerical integration. Hopefully, it may produce other new applications in numerical ODEs and probably we can extend their applications to any other relevant fields.

The outline of the paper is as follows. In the next section, we speak out our new idea for extending the previous study of Tang & Sun [41, 44], and then give a few new theoretical results for designing RK-type methods. In section 3, we give some illustrations to expound our approaches for constructing RK-type methods based on Jacobi polynomials. Some discussions about geometric integration by csRK methods will be given in Section 4. At last, we conclude this paper.

2. Continuous-stage Runge-Kutta methods

Let us start with the following initial value problem

\[
\dot{z} = f(t, z), \quad z(t_0) = z_0 \in \mathbb{R}^d, \tag{2.1}
\]

where \( f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d \) is assumed to be sufficiently differentiable.
Definition 2.1. \[22\] Let $A_{\tau, \sigma}$ be a function of two variables $\tau, \sigma \in [0, 1]$, and $B_\tau, C_\tau$ be functions of $\tau \in [0, 1]$. The one-step method $\Phi_h : z_0 \mapsto z_1$ given by

$$
Z_\tau = z_0 + h \int_0^1 A_{\tau, \sigma} f(t_0 + C_\sigma h, Z_\sigma) \, d\sigma, \quad \tau \in [0, 1],
$$

$$
z_1 = z_0 + h \int_0^1 B_\tau f(t_0 + C_\tau h, Z_\tau) \, d\tau,
$$

is called a continuous-stage Runge-Kutta (csRK) method, where $Z_\tau \approx z(t_0 + C_\tau h)$. Here, we always assume

$$
C_\tau = \int_0^1 A_{\tau, \sigma} \, d\sigma,
$$

and often denote a csRK method by a triple $(A_{\tau, \sigma}, B_\tau, C_\tau)$.

Example 2.1 (Hairer’s energy-preserving collocation methods \[22\]). The first example of a computational csRK method is in the following

$$
A_{\tau, \sigma} = \sum_{i=1}^s \frac{1}{b_i} \int_0^\tau \ell_i(x) \, dx \ell_i(\sigma), \quad B_\tau = 1, \quad C_\tau = \tau,
$$

where $\ell_i(x)$ are the Lagrange interpolatory basis polynomials, $b_i = \int_0^1 \ell_i(x) \, dx$ are the interpolatory weights with respect to nodes $c_1, \ldots, c_s$. This method is of superconvergence order (depending on the interpolation) and it can exactly preserve the energy of Hamiltonian systems. Remark that, by approximating the integrals of csRK methods with the interpolatory quadrature formula $(b_i, c_i)_{i=1}^s$, it reduces to a classical collocation method (see \[21\], Page 30).

Instead of using Lagrange interpolatory polynomials as in the example, we will turn to orthogonal polynomials. There are at least two advantages for using orthogonal polynomials: Firstly, orthogonal polynomials are known to be more stable than Lagrange interpolatory polynomials in numerical computation; Secondly, they possess many beautiful properties which is convenient for us to employ them in many aspects.

Our discussions will rely upon the following simplifying assumptions proposed by Hairer in \[22\]

$$
\tilde{B}(\xi) : \quad \int_0^1 B_\tau C_\tau^{\kappa-1} \, d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \xi,
$$

$$
\tilde{C}(\eta) : \quad \int_0^1 A_{\tau, \sigma} C_\sigma^{\kappa-1} \, d\sigma = \frac{1}{\kappa} C_\tau^\kappa, \quad \kappa = 1, \ldots, \eta,
$$

$$
\tilde{D}(\zeta) : \quad \int_0^1 B_\tau C_\tau^{\kappa-1} A_{\tau, \sigma} \, d\tau = \frac{1}{\kappa} B_\sigma (1 - C_\sigma^\kappa), \quad \kappa = 1, \ldots, \zeta.
$$

Based on these conditions, we provide the following result for analyzing the order of csRK methods, which is the counterpart of a classical result by Butcher in 1964 \[3\].

Theorem 2.1. \[22, 44\] If the coefficients $(A_{\tau, \sigma}, B_\tau, C_\tau)$ of method \[22\] satisfy $\tilde{B}(\xi), \tilde{C}(\eta)$ and $\tilde{D}(\zeta)$, then the method is of order at least $\min(\xi, 2\eta + 2, \eta + \zeta + 1)$.

In view of Theorem \[22\] below, the authors in \[44, 49\] have intensively discussed the construction of csRK methods upon the premise of $B_\tau \equiv 1$. However, it may exclude other possibilities of
discovering more new RK-type methods. In this article, we will break through such a limitation but hold on a simple assumption abidingly as done in [22, 44, 49]

\[ C_\tau \equiv \tau, \quad \tau \in [0,1]. \]  

**Theorem 2.2.** [44, 49] Assume a csRK method with coefficients \((A_{\tau,\sigma}, B_\tau, C_\tau)\) satisfies the following two conditions: (a) The one-variable function \(\chi(\xi) = \int_0^\xi B_\tau \, d\tau, \xi \in [0,1]\) has an inverse function and \(B_\tau\) is non-vanishing almost everywhere; (b) The simplifying condition \(\tilde{B}(\xi)\) holds for some integer \(\xi \geq 1\), then the method can always be transformed into a new csRK method with \(B_\tau \equiv 1, \tau \in [0,1]\).

**Lemma 2.1.** Under the assumption (2.6), the simplifying assumptions \(\tilde{B}(\xi), \tilde{C}(\eta)\) and \(\tilde{D}(\zeta)\) are equivalent to

\[
\tilde{B}(\xi) : \int_0^1 B_\tau p(\tau) \, d\tau = \int_0^1 p(x) \, dx, \quad \text{for } \forall p \text{ with } \deg(p) \leq \xi - 1, \tag{2.7}
\]

\[
\tilde{C}(\eta) : \int_0^1 A_{\tau,\sigma} p(\sigma) \, d\sigma = \int_0^\tau p(x) \, dx, \quad \text{for } \forall p \text{ with } \deg(p) \leq \eta - 1, \tag{2.8}
\]

\[
\tilde{D}(\zeta) : \int_0^1 B_\tau A_{\tau,\sigma} p(\tau) \, d\tau = B_\sigma \int_\sigma^1 p(x) \, dx, \quad \text{for } \forall p \text{ with } \deg(p) \leq \zeta - 1, \tag{2.9}
\]

where \(\deg(p)\) stands for the degree of polynomial function \(p\).

**Proof.** It is observed that \(\tilde{B}(\xi), \tilde{C}(\eta)\) and \(\tilde{D}(\zeta)\) can be recast as

\[
\tilde{B}(\xi) : \int_0^1 B_\tau \tau^{\kappa - 1} \, d\tau = \int_0^1 x^{\kappa - 1} \, dx, \quad \kappa = 1, \ldots, \xi,
\]

\[
\tilde{C}(\eta) : \int_0^1 A_{\tau,\sigma} \sigma^{\kappa - 1} \, d\sigma = \int_0^\tau x^{\kappa - 1} \, dx, \quad \kappa = 1, \ldots, \eta,
\]

\[
\tilde{D}(\zeta) : \int_0^1 B_\tau \tau^{\kappa - 1} A_{\tau,\sigma} \, d\tau = B_\sigma \int_\sigma^1 x^{\kappa - 1} \, dx, \quad \kappa = 1, \ldots, \zeta.
\]

Therefore, these formulae are satisfied for all monomials like \(x^\iota\) with degree \(\iota\) no larger than \(\xi - 1, \eta - 1\) and \(\zeta - 1\) respectively. Consequently, the final result follows from the fact that any polynomial function \(p\) can be expressed as a linear combination of monomials. \(\square\)

For further discussion, we have to introduce the concept of weight function and revisit the relevant theory of orthogonal polynomials.

**Definition 2.2.** A non-negative (or positive almost everywhere) function \(w(x)\) is called a weight function on \([a,b]\), if it satisfies the following two conditions:

(a) The \(k\)-th moment \(\int_a^b x^k \, w(x) \, dx, \ k \in \mathbb{N}\) exists;

(b) For \(\forall \, u(x) \geq 0, \int_a^b u(x) \, w(x) \, dx = 0 \implies u(x) \equiv 0.\)

\(^1\)This condition is always fulfilled for a csRK method of order at least 1.
By available polynomial theory \[40\], for a given weight function \(w(x)\), there exists a sequence of orthogonal polynomials in the weighted function space (Hilbert space)

\[
L^2_w[a, b] = \{ u \text{ is measurable on } [a, b] : \int_a^b |u(x)|^2 w(x) \, dx < +\infty \}
\]

with respect to the inner product

\[
(u, v)_w = \int_a^b u(x)v(x)w(x) \, dx.
\]

Actually, starting from the monomials \(1, x, x^2, \ldots\), we can always use the Gram-Schmidt procedure to construct a system of orthogonal polynomials \(\{P_n^*(x)\}_{n=0}^\infty\) such that the degree of \(P_n^*(x)\) is exact \(n\). It is known that the monic polynomials with orthogonality property should satisfy the following recursion formula

\[
P_0^*(x) = 1, \quad P_1^*(x) = x - \alpha_0, \quad P_{n+1}^*(x) = (x - \alpha_n)P_n^*(x) - \beta_n P_{n-1}^*(x), \quad n = 1, 2, 3, \ldots
\]

where

\[
\alpha_n = \frac{(x P_n^*, P_n^*)_w}{(P_n^*, P_n^*)_w}, \quad n = 0, 1, 2, \ldots, \quad \text{and} \quad \beta_n = \frac{(P_n^*, P_n^*)_w}{(P_{n-1}^*, P_{n-1}^*)_w}, \quad n = 1, 2, 3, \ldots.
\]

By setting

\[
P_n(x) = \frac{P_n^*(x)}{\|P_n^*(x)\|_w}, \quad n = 0, 1, 2, \ldots,
\]

we get a family of normalized orthogonal polynomials \(\{P_n(x)\}_{n=0}^\infty\) which becomes a complete orthogonal set in the Hilbert space \(L^2_w[a, b]\). It is known that \(P_n(x)\) has exactly \(n\) real simple zeros in the open interval \((a, b)\).

Assume \(A_{\tau, \sigma}\) and \(B_{\tau}\) have the following decompositions

\[
A_{\tau, \sigma} = \tilde{A}_{\tau, \sigma} w(\sigma), \quad B_{\tau} = \tilde{B}_{\tau} w(\tau),
\]

where \(w\) is a weight function defined on \([0, 1]\), and then the csRK method (2.2) can be written as

\[
Z_\tau = z_0 + h \int_0^1 \tilde{A}_{\tau, \sigma} w(\sigma) f(t_0 + \sigma h, Z_\sigma) \, d\sigma, \quad \tau \in [0, 1],
\]

\[
z_1 = z_0 + h \int_0^1 \tilde{B}_{\tau} w(\tau) f(t_0 + \tau h, Z_\tau) \, d\tau.
\]  \hfill (2.10)

**Theorem 2.3.** Suppose \(\tilde{B}_{\tau}, \tilde{A}_{\tau, \sigma}, (\tilde{B}_{\tau} A_{\tau, \sigma}) \in L^2_w[0, 1]\), then, under the assumption (2.6) we have

(a) \(\tilde{B}(\xi)\) holds \(\iff\) \(B_{\tau}\) has the following form in terms of the normalized orthogonal polynomials in \(L^2_w[0, 1]\):

\[
B_{\tau} = \left( \sum_{j=0}^{\xi-1} \int_0^1 P_j(x) \, dx P_j(\tau) + \sum_{j \geq \xi} \lambda_j P_j(\tau) \right) w(\tau),
\]  \hfill (2.11)

where \(\lambda_j\) are any real parameters;

---

\(^2\)The notation \(A_{\tau, \sigma}\) stands for the one-variable function in terms of \(\sigma\), and \(A_{\tau, \star}, \tilde{A}_{\tau, \sigma}\) can be understood likewise.
(b) $\hat{C}(\eta)$ holds $\iff A_{\tau,\sigma}$ has the following form in terms of the normalized orthogonal polynomials in $L^2_w[0,1]$: 

$$A_{\tau,\sigma} = \left(\sum_{j=0}^{\eta-1} \int_0^\tau P_j(x) \, dx P_j(\sigma) + \sum_{j=0}^{\eta-1} \phi_j(\tau) P_j(\sigma)\right)w(\sigma),$$ (2.12)

where $\phi_j(\tau)$ are any $L^2_w$-integrable real functions;

(c) $\hat{D}(\zeta)$ holds $\iff B_{\tau} A_{\tau,\sigma}$ has the following form in terms of the normalized orthogonal polynomials in $L^2_w[0,1]$: 

$$B_{\tau} A_{\tau,\sigma} = \left(\sum_{j=0}^{\zeta-1} B_{\sigma} \int_\sigma^1 P_j(x) \, dx P_j(\tau) + \sum_{j=0}^{\zeta-1} \psi_j(\sigma) P_j(\tau)\right)w(\tau),$$ (2.13)

where $\psi_j(\sigma)$ are any $L^2_w$-integrable real functions.

Proof. For part (a), consider the following orthogonal polynomial expansion in $L^2_w[0,1]$ 

$$\hat{B}_{\tau} = \sum_{j \geq 0} \lambda_j P_j(\tau) \iff B_{\tau} = \hat{B}_{\tau} w(\tau) = \sum_{j \geq 0} \lambda_j P_j(\tau) w(\tau), \quad \lambda_j \in \mathbb{R},$$

and substitute the formula above into (2.7) (with $p$ replaced by $P_j$) in Lemma 2.1 then it follows 

$$\lambda_j = \int_0^1 P_j(x) \, dx, \quad j = 0, \cdots, \xi - 1,$$

which gives (2.11). For part (b) and (c), consider the following orthogonal expansions of $\hat{A}_{\tau,\sigma}$ with respect to $\sigma$ and $\hat{B}_{\tau} A_{\tau,\sigma}$ with respect to $\tau$ in $L^2_w[0,1]$, respectively,

$$\hat{A}_{\tau,\sigma} = \sum_{j \geq 0} \phi_j(\tau) P_j(\sigma) \iff A_{\tau,\sigma} = \hat{A}_{\tau,\sigma} w(\sigma) = \sum_{j \geq 0} \phi_j(\tau) P_j(\sigma) w(\sigma), \quad \phi_j(\tau) \in L^2_w(I),$$

$$\hat{B}_{\tau} A_{\tau,\sigma} = \sum_{j \geq 0} \psi_j(\sigma) P_j(\tau) \iff B_{\tau} A_{\tau,\sigma} = \hat{B}_{\tau} w(\tau) A_{\tau,\sigma} = \sum_{j \geq 0} \psi_j(\sigma) P_j(\tau) w(\tau), \quad \psi_j(\sigma) \in L^2_w(I),$$

and then substitute them into (2.8) and (2.9), which then leads to the final results. 

It is crystal clear that to construct a csRK method is to settle the triple $(A_{\tau,\sigma}, B_{\tau}, C_{\tau})$. Theorem 2.3 provides us a guideline to design Butcher coefficients so as to fulfill the order conditions, especially for $A_{\tau,\sigma}$ and $B_{\tau}$, observing that $C_{\tau}$ is known by the premise (2.6). In general, for the sake of practical use, we have to derive finite forms of $A_{\tau,\sigma}$ and $B_{\tau}$ by truncating the series suitably. By doing so, $\hat{A}_{\tau,\sigma}$ and $\hat{B}_{\tau}$ thereupon become polynomials with finite degrees.

As for practical computation, the integrals of csRK schemes need to be approximated by using an $s$-point weighted interpolatory quadrature formula 

$$\int_0^1 \Phi(x) w(x) \, dx \approx \sum_{i=1}^s b_i \Phi(c_i), \quad c_i \in [0,1],$$ (2.14)

where 

$$b_i = \int_0^1 \ell_i(x) w(x) \, dx, \quad \ell_i(x) = \prod_{j=1, j \neq i}^s \frac{x - c_j}{c_i - c_j}, \quad i = 1, \cdots, s.$$
Here, we remark that for the simplest case $s = 1$, we define $\ell_1(x) = 1$.

Thus, by applying a weighted quadrature formula (2.14) to the csRK method (2.10), it brings out an $s$-stage standard RK method

$$\hat{Z}_i = z_0 + h \sum_{j=1}^{s} b_j \hat{A}_{c_i} f(t_0 + c_j h, \hat{Z}_j), \quad i = 1, \ldots, s,$$

$$z_1 = z_0 + h \sum_{i=1}^{s} b_i \hat{B}_{c_i} f(t_0 + c_i h, \hat{Z}_i),$$

(2.15)

where $\hat{Z}_i \approx Z_{c_i}$. The following result is an extension of the previous result by Tang et al [44, 46].

**Theorem 2.4.** Assume the underlying quadrature formula (2.14) is of order $p$, and $\hat{A}_{\tau,\sigma}$ is of degree $\pi^\tau_A$ with respect to $\tau$ and of degree $\pi^\sigma_A$ with respect to $\sigma$, and $\hat{B}_{\tau}$ is of degree $\pi^\tau_B$. If all the simplifying assumptions $\hat{B}(\xi)$, $\hat{C}(\eta)$ and $\hat{D}(\zeta)$ in (2.5) are fulfilled, then the standard RK method (2.15) is at least of order

$$\min(\rho, 2\alpha + 2, \alpha + \beta + 1),$$

where $\rho = \min(\xi, p - \pi^\tau_B)$, $\alpha = \min(\eta, p - \pi^\sigma_A)$ and $\beta = \min(\zeta, p - \pi^\tau_A - \pi^\tau_B)$.

**Proof.** A well-known result given by Butcher in 1964 [5] shows that if an $s$-stage RK method with Butcher coefficients $(a_{ij}, b_i, c_i)$ satisfies the following classical simplifying assumptions

$$B(\rho) : \sum_{i=1}^{s} b_i c_i^{\kappa - 1} = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \rho,$$

$$C(\alpha) : \sum_{j=1}^{s} a_{ij} c_j^{\kappa - 1} = \frac{c_i^{\kappa}}{\kappa}, \quad i = 1, \ldots, s, \quad \kappa = 1, \ldots, \alpha,$$

$$D(\beta) : \sum_{i=1}^{s} b_i c_i^{\kappa - 1} a_{ij} = \frac{b_j}{\kappa}(1 - c_j^{\kappa}), \quad j = 1, \ldots, s, \quad \kappa = 1, \ldots, \beta,$$

then the method is at least of order

$$\min\{\rho, 2\alpha + 2, \alpha + \beta + 1\}.$$

Now we consider to what degree the Butcher coefficients of (2.15) will fulfill these classical simplifying assumptions. The idea of proof relies upon the approximation of those integrals of $\hat{B}(\xi)$, $\hat{C}(\eta)$, $\hat{D}(\zeta)$ by the quadrature rule. Here we take the first condition $\hat{B}(\xi)$ as an example. After applying the quadrature rule of order $p$ to $\hat{B}(\xi)$ in (2.5), it gives

$$\sum_{i=1}^{s} (b_i \hat{B}_{c_i}) c_i^{\kappa - 1} = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \rho.$$  

(2.17)

Next, let us determine what $\rho$ would be. Now that the order of the quadrature formula is $p$, which means it is exact for any polynomial with degree up to $p - 1$, and thus we have

$$\pi^\tau_B + (\rho - 1) \leq p - 1,$$
where the left-hand side of the inequality stands for the highest degree of the polynomial part \( \tilde{B}_\tau \kappa - 1 = \tilde{B}_\tau \kappa - 1 \) of integrand in \( \tilde{B}(\xi) \). On the other hand, we have \( \rho \leq \xi \).

As a result, \( \rho \) can be taken as \( \rho = \min(\xi, p - \pi_B^\tau) \).

Undoubtedly, a suitable quadrature rule is of great importance for constructing standard RK methods with the approach above. As far as we know, the optimal quadrature technique is the well-known Gauss-Christoffel’s, which can be stated as follows (see, for example, [1, 38]). It is well to be reminded that other suboptimal quadrature rules (e.g., Gauss-Christoffel-Radau type, Gauss-Christoffel-Lobatto type etc.) can also be used [38].

**Theorem 2.5.** If \( c_1, c_2, \cdots, c_s \) are chosen as the \( s \) distinct zeros of the normalized orthogonal polynomial \( P_s(x) \) of degree \( s \) in \( L_2^w[0,1] \), then the interpolatory quadrature formula (2.14) is exact for polynomials of degree \( 2s - 1 \), i.e., of the optimal order \( p = 2s \). If \( \Phi \in C^{2s} \), then it has the following error estimate

\[
\int_{-1}^{1} \Phi(x)w(x) \, dx - \sum_{i=1}^{s} b_i \Phi(c_i) = \frac{\Phi^{(2s)}(\xi)}{(2s)!\mu_s^2},
\]

for some \( \xi \in [0,1] \), where \( \mu_s \) is the leading coefficient of \( P_s(x) \).

### 3. RK-type methods based on Jacobi polynomials

A family of well-known orthogonal polynomials called Jacobi polynomials [14, 40] which constitute a complete orthogonal set in \( L_2^w[-1,1] \) are based on the following weight function

\[
w^{(\alpha,\beta)}(x) = (1-x)^\alpha (1+x)^\beta, \quad \alpha > -1, \ \beta > -1.
\]

Specifically, the Jacobi polynomial of degree \( n \), denoted by \( P_n^{(\alpha,\beta)}(x), x \in [-1,1] \), can be explicitly computed by the Rodrigue’s formula [14, 40]

\[
P_0^{(\alpha,\beta)}(x) = 1, \quad P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n! (1-x)^\alpha (1+x)^\beta} \frac{d^n}{dx^n} \left((1-x)^{\alpha+n}(1+x)^{\beta+n}\right), \quad n \geq 1.
\]

An important property of Jacobi polynomials is that they are orthogonal to each other with respect to the \( L_2^w \) inner product on \([-1,1]\)

\[
\int_{-1}^{1} w^{(\alpha,\beta)}(x) P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x) \, dx = \epsilon_n \delta_{nm}, \quad n, m = 0, 1, \cdots,
\]

where\(^3\)

\[
\epsilon_0 = \frac{2^{\alpha+\beta+1} \Gamma(\alpha+1) \Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}, \quad \epsilon_n = \frac{2^{\alpha+\beta+1} \Gamma(n+\alpha+1) \Gamma(n+\beta+1)}{(2n+\alpha+\beta+1) \Gamma(n+\alpha+\beta+1)n!}, \quad n \geq 1,
\]

\(^3\)Many literatures conducted a minor error by unifying \( \epsilon_0 \) into the formula of \( \epsilon_n (n \geq 1) \). In fact, in the case of \( n = 0 \), when we take \( \alpha + \beta = -1 \), it will make no sense with the denominator of \( \epsilon_n \) becoming zero.
and here
\[ \Gamma(s) = \int_0^{+\infty} x^{s-1}e^{-x} \, dx, \quad s \in \mathbb{R}^+, \]
is the well-known Gamma function. Then, we can get the so-called normalized shifted Jacobi polynomial of degree \( n \) by setting
\[ P_n^{(\alpha,\beta)}(x) = \frac{P_n^{*(\alpha,\beta)}(2x-1)}{\sqrt{\epsilon_n/2}}, \quad n = 0, 1, 2, \ldots, \]
that is,
\[ P_0^{(\alpha,\beta)}(x) = \frac{1}{\sqrt{\epsilon_0/2}}, \quad P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{n!\sqrt{\epsilon_n/2}} \frac{d^n}{d\tau^n} \left[(1-x)^{\alpha+n}x^{\beta+n}\right], \quad n \geq 1, \quad (3.1) \]
which satisfy the orthogonality on \([0, 1] \)
\[ \int_0^1 w^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)P_m^{(\alpha,\beta)}(x) \, dx = \delta_{nm}, \quad n, m = 0, 1, 2, \ldots, \]
and the associated weight function is
\[ w^{(\alpha,\beta)}(x) = w^{*(\alpha,\beta)}(2x-1) = 2^{\alpha+\beta}(1-x)^{\alpha}x^{\beta}, \quad \alpha > -1, \beta > -1. \]

A useful formula that relates shifted Jacobi polynomials and their derivatives is
\[ \frac{d}{dx} P_n^{(\alpha,\beta)}(x) = 2\sqrt{n(n+\alpha+\beta+1)} P_{n-1}^{(\alpha+1,\beta+1)}(x), \quad n \geq 1, \quad (3.2) \]
and we have a symmetry relation
\[ P_n^{(\alpha,\beta)}(1-x) = (-1)^n P_n^{(\beta,\alpha)}(x), \quad n \geq 0. \quad (3.3) \]

If we take \( \beta = \alpha > -1 \), then a special class of Jacobi polynomials called Gegenbauer polynomials or ultraspherical polynomials are gained. Particularly, from (3.2) and (3.3) it gives the following identity
\[ \int_0^1 P_n^{(\alpha,\alpha)}(x) \, dx = 0, \quad \forall \alpha > 0 \text{ and } n \text{ is odd.} \quad (3.4) \]

A basic but taken-for-granted rule for constructing a traditional RK method is that the order of the scheme should be required as high as possible for a given stage \([10, 9]\). On this account, it is naturally expected to design \( \hat{B}_r \) with a low degree, as revealed by Theorem 2.3 and Theorem 2.4. The property (3.1) can help us in this respect. Another case in point will be shown later associated with Legendre polynomials \((w(x) \equiv 1)\), where \( B_r(= \hat{B}_r) \) can be greatly reduced (see the formula (3.16) later).

**Theorem 3.1.** Let \( \{P_j(x)\}_{j \in \mathbb{Z}} \) be Gegenbauer polynomials based on weight function \( w(x) = 2^{2\alpha}(1-x)^{\alpha}x^{\alpha} \) with \( \alpha > 0 \). If we take
\[ A_{r,\sigma} = \sum_{j=0}^{r-1} \int_0^1 P_j(x) \, dx \int_0^1 P_{j}(\sigma) \, w(\sigma), \quad B_r = \sum_{j=0}^{r-1} \int_0^1 P_j(x) \, dx \int_0^1 P_{j}(\tau) \, w(\tau), \quad C_r = \tau, \quad (3.5) \]
as the coefficients of a csRK method, and use an \( s \)-point \((s \geq r - 1)\) Gauss-Christoffel’s quadrature rule to get an \( s \)-stage standard RK method \((2.15)\), then we have the following statements:
(a) If \( r \) is odd, then the RK method is at least of order
\[
    p = \begin{cases} \ r + 1, & s \geq r, \\ \ r - 1, & s = r - 1. \end{cases}
\]  
(3.6)

(b) If \( r \) is even, then the RK method is at least of order \( p = r, s \geq r - 1 \).

Proof. Since part (b) can be proved similarly, here we only prove part (a).

By (2.12) of Theorem 2.3, \( A_{\tau, \sigma} \) satisfies \( \tilde{C}(r) \). By hypothesis the Gegenbauer polynomials satisfy the property (3.4) and notice that \( r \) is odd, it yields
\[
    B_{\tau} = \sum_{j=0}^{r-1} \int_{0}^{1} P_{j}(x) \, dx \, P_{j}(\tau)w(\tau),
\]
which implies \( \tilde{B}(r+1) \). It is not clear whether \( \tilde{D}(\zeta) \) is satisfied and to what degree it will be fulfilled (due to lack of further information). Under the worst situation, \( \tilde{D}(\zeta) \) offers no contributions to the order accuracy. Nonetheless, at least the associated csRK method is of order \( r + 1 \) by Theorem 2.1, and we remark that the resulting standard RK methods will arrive at such order when we use quadrature rules with enough nodes (namely of high enough order), but it may not be higher than \( r + 1 \).

When \( s \geq r \), it suffices to consider the case of \( s = r \). Observe that
\[
    \pi_A^\sigma = r - 1, \quad \pi_B^\tau = r - 1,
\]
and now the Gauss-Christoffel’s quadrature is of order \( 2r \), then we can directly use Theorem 2.4 and Theorem 2.5 to draw the conclusion.

When \( s = r - 1 \), taking into account that \( P_{r-1}(c_i) = 0, i = 1, \cdots, r - 1 \) with \( c_i \) as the quadrature nodes of Gauss-Christoffel’s rule, we can consider the following coefficients instead of (3.5)
\[
    A_{\tau, \sigma} = \sum_{j=0}^{r-2} \int_{0}^{\tau} P_{j}(x) \, dx \, P_{j}(\sigma)w(\sigma), \quad B_{\tau} = \sum_{j=0}^{r-2} \int_{0}^{1} P_{j}(x) \, dx \, P_{j}(\tau)w(\tau), \quad C_{\tau} = \tau.
\]  
(3.7)

This is because after using the quadrature rule it leads to the same RK coefficients (c.f., (2.15)) from (3.7) and (3.5). Therefore, we actually have
\[
    \pi_A^\sigma = r - 2, \quad \pi_B^\tau = r - 2,
\]
and obviously \( \tilde{B}(r - 1), \tilde{C}(r - 1) \) are fulfilled by (3.7), which implies the final result by Theorem 2.4.

Remark 3.1. The csRK method with coefficients (3.5) can also be interpreted as an extended form of the local Fourier expansion methods presented in [4]. That is, a local Fourier expansion of the continuous problem is truncated after a finite number of terms. Here, we truncate the expansion series with \( r \) terms and introduce a weight function, while [4] considered a special case in terms of Legendre polynomials with weight function \( w(x) = 1 \).

---

4 Actually, for the case of Legendre polynomials, (3.5) fulfills \( \tilde{D}(\zeta) \) with \( \zeta = r - 1 \). But, for small \( r \), e.g., \( r = 1 \), (3.5) fails to fulfill \( \tilde{D}(\zeta) \) for any positive integer \( \zeta \). Other type orthogonal polynomials are generally in the worse situation.
By slightly changing the upper limit of summation of $A_{\tau,\sigma}$ and $B_\tau$ in (3.5), it leads to the following results, which can be proved similarly.

**Theorem 3.2.** We consider the following

$$A_{\tau,\sigma} = \sum_{j=0}^{r} \int_{0}^{\tau} P_j(x) \, P_j(\sigma) \, w(\sigma) \, dx, \quad B_\tau = \sum_{j=0}^{r-1} \int_{0}^{1} P_j(x) \, dx \, P_j(\tau) \, w(\tau), \quad C_\tau = \tau, \quad (3.8)$$

as the coefficients of a csRK method, where $\{P_j(x)\}_{j \in \mathbb{Z}}$ are Gegenbauer polynomials (see also (3.4) with $\alpha > 0$). If we use an $s$-point $(s \geq r - 1)$ Gauss-Christoffel’s quadrature rule, then it gives an $s$-stage standard RK method satisfying

(a) If $r$ is odd, then the method is at least of order

$$p = \begin{cases} 
  r + 1, & s \geq r, \\
  r - 1, & s = r - 1.
\end{cases} \quad (3.9)$$

(b) If $r$ is even, then the method is at least of order

$$p = \begin{cases} 
  r, & s \geq r, \\
  r - 1, & s = r - 1.
\end{cases} \quad (3.10)$$

**Theorem 3.3.** We consider the following

$$A_{\tau,\sigma} = \sum_{j=0}^{r-1} \int_{0}^{\tau} P_j(x) \, dx \, P_j(\sigma) \, w(\sigma), \quad B_\tau = \sum_{j=0}^{r} \int_{0}^{1} P_j(x) \, dx \, P_j(\tau) \, w(\tau), \quad C_\tau = \tau, \quad (3.11)$$

as the coefficients of a csRK method, where $\{P_j(x)\}_{j \in \mathbb{Z}}$ are Gegenbauer polynomials (see also (3.4) with $\alpha > 0$). If we use an $s$-point $(s \geq r - 1)$ Gauss-Christoffel’s quadrature rule, then it gives an $s$-stage standard RK method satisfying

(a) If $r$ is odd, then the method is at least of order

$$p = \begin{cases} 
  r + 1, & s \geq r, \\
  r - 1, & s = r - 1.
\end{cases} \quad (3.12)$$

(b) If $r$ is even, then the method is at least of order

$$p = \begin{cases} 
  r, & s \geq r, \\
  r - 1, & s = r - 1.
\end{cases} \quad (3.13)$$

**Remark 3.2.** Remark that if we consider a general type of weighted orthogonal polynomials to make up (3.5), and use an $s$-point $(s \geq r - 1)$ Gauss-Christoffel’s quadrature rule, then we get an $s$-stage RK method (2.15) of order at least

$$p = \begin{cases} 
  r, & s \geq r, \\
  r - 1, & s = r - 1.
\end{cases} \quad (3.14)$$

Other cases can be similarly discussed and some counterparts of the above results can be obtained.
3.1. RK-type methods based on Legendre polynomials

The simplest case for shifted Jacobi polynomials (as well as Gegenbauer polynomials) must be the well-known shifted Legendre polynomials denoted by \( L_n(x) := P_n^{(0,0)}(x) \), which can be explicitly calculated with

\[
L_0(x) = 1, \quad L_n(x) = \frac{\sqrt{2n + 1}}{n!} \frac{d^n}{dx^n} \left( x^n(x - 1)^n \right), \quad n \geq 1.
\]

It is known that such special polynomials are orthogonal on \([0, 1]\) in terms of weight function \( w(x) := w^{(0,0)}(x) = 1 \), and they satisfy the following integration formulae \([20, 44]\)

\[
\int_0^x L_0(t) \, dt = \xi_1 L_1(x) + \frac{1}{2} L_0(x), \\
\int_0^x L_n(t) \, dt = \xi_n L_{n+1}(x) - \xi_n L_{n-1}(x), \quad n = 1, 2, 3, \ldots, \\
\int_x^1 L_n(t) \, dt = \delta_{n0} - \int_0^x L_n(t) \, dt, \quad n = 0, 1, 2, \ldots,
\]

where \( \xi_n = \frac{1}{2\sqrt{4n^2 - 1}} \). Taking into account that

\[
\int_0^1 L_0(x) \, dx = 1, \quad \int_0^1 L_j(x) \, dx = 0, \quad j \geq 1,
\]

the formula \([2.11]\) given in Theorem \([2.3]\) becomes

\[
B_\tau = 1 + \sum_{j \geq \xi} \lambda_j L_j(\tau),
\]

(3.16)

where \( \lambda_j \) are any real parameters. However, it is not a practical option to construct those csRK methods with a high-degree \( B_\tau \). A very simple choice is to get rid off the tail of \((3.16)\) and let \( B_\tau = 1 \). In such a case, Theorem \([2.3]\) can be reduced by using \((3.15)\) (for more details, see \([44]\)), and it leads to the existing result previously given by Tang & Sun \([41, 44]\). Here we state it again in the following theorem.

**Theorem 3.4.** \([41, 44]\) Let \( B_\tau \equiv 1, \quad C_\tau = \tau, \quad \text{and} \quad A_{\tau, \sigma} \in L^2([0,1] \times [0,1]), \) then the following two statements are equivalent to each other: (a) Both \( C(\alpha) \) and \( D(\beta) \) hold; (b) The coefficient \( A_{\tau, \sigma} \) has the following form in terms of Legendre polynomials

\[
A_{\tau, \sigma} = \frac{1}{2} + \sum_{j=0}^{N_1} \xi_{j+1} L_{j+1}(\tau) L_j(\sigma) - \sum_{j=0}^{N_2} \xi_{j+1} L_{j+1}(\sigma) L_j(\tau) + \sum_{i \geq \beta, j \geq \alpha} \alpha_{(i,j)} L_i(\tau) L_j(\sigma),
\]

(3.17)

where \( N_1 = \max(\alpha - 1, \beta - 2), \) \( N_2 = \max(\alpha - 2, \beta - 1), \) \( \xi_j = \frac{1}{2\sqrt{4j^2 - 1}} \) and \( \alpha_{(i,j)} \) are any real parameters.

By Theorem \([2.1]\) a csRK method with \( B_\tau \equiv 1, \quad C_\tau = \tau \) and \( A_{\tau, \sigma} \) given by \((3.17)\) is of order at least \( \min(\infty, 2\alpha + 2, \alpha + \beta + 1) = \min(2\alpha + 2, \alpha + \beta + 1) \). It has been shown in \([41, 42, 44, 46]\) that by using suitable quadrature formulae (c.f., Theorem \([2.4]\)) a number of classical high-order RK methods can be retrieved, such as Gauss-Legendre RK schemes, Radau IA, Radau IIA, Radau IB, Radau IIIB, Lobatto IIIA, Lobatto IIIB, Lobatto IIIIC and so forth. It turns out that this approach \([41, 44]\) is comparable to the W-transformation technique proposed by Hairer & Wanner \([20]\).
Table 3.1: Three A-stable RK methods of order 2, 4, 4, derived from (3.18) with \( r = 1, 2, 2 \) respectively, based on Chebyshev-Gauss-Lobatto quadrature rules.

Example 3.1. If we take

\[
A_{\tau, \sigma} = \sum_{j=0}^{r-1} \int_{0}^{\tau} L_j(x) \, dx \, L_j(\sigma), \quad B_{\tau} \equiv 1, \quad C_{\tau} = \tau,
\]

and use the \( r \)-point Gauss quadrature rule, then we regain the famous Gauss-Legendre RK scheme which is of the optimal order \( 2r \) (see, [42]). It is known that such scheme is A-stable and its stability function is a diagonal Padé approximation to \( e^z \) [20].

Additionally, by using the Chebyshev-Gauss-Lobatto quadrature rules with abscissae [50]

\[
c_i = \frac{1}{2} \left( 1 + \cos \left( \frac{s - i}{s - 1} \pi \right) \right), \quad i = 1, 2, \ldots, s.
\]

we obtain other three RK methods which are shown in Table 3.1. Their stability functions are given by, respectively,

\[
R_1(z) = \frac{2 + z}{2 - z}, \quad R_2(z) = \frac{12 + 6z + z^2}{12 - 6z + z^2}, \quad R_3(z) = \frac{12 + 6z + z^2}{12 - 6z + z^2},
\]

where \( z = \lambda h \). Observe that these schemes share the same stability functions with Gauss-Legendre RK methods, hence all of them are A-stable. We find that the former two RK methods are exactly corresponding to the relevant schemes given by Vigo-Aguiar & Ramos (see (4.2) and (4.3) in [50]), but our third scheme is completely different from their scheme (4.4) (though the same quadrature rule is used).

It is worth mentioning that the csRK method with coefficients given by (3.18) is also known as an energy-preserving integrator for solving Hamiltonian systems, and it exactly corresponds to the \( \infty \)-HBVMs [4], Hairer’s highest-order energy-preserving collocation methods [22] as well as continuous time finite element methods [42]. Moreover, such method has been proved to be conjugate to a symplectic method up to order \( 2r + 2 \) [23].

3.2. RK-type methods based on three simple types of Jacobi polynomials

A little more complex orthogonal polynomials of the Jacobi type are the so-called Jacobi type I, II and III polynomials which can be found in [7]. These orthogonal polynomials are based on the following weight functions, respectively,

\[\text{footnote}[5]{Actually, one can prove that if an interpolatory quadrature rule of order no less than \( 2r \) is used, then the resulting RK scheme is always A-stable [43].}\]

\[\text{footnote}[6]{Here our weight functions have a different form compared with those given in [7], except for some tuned constant factors.}\]
Table 3.2: From left to right: Gauss-Christoffel-Jacobi I, Gauss-Christoffel-Jacobi II, Gauss-Christoffel-Jacobi III RK methods of order 2, derived from (3.5) with $r = 2$, by using Jacobi type I, II and III polynomials respectively.

|            | $6 - \sqrt{6}$ | $24 - \sqrt{6}$ | $4 - \sqrt{6}$ | $24 - \sqrt{6}$ | $5 - \sqrt{6}$ | $5 + \sqrt{6}$ | $5 - \sqrt{6}$ |
|------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| $10$       | $12 + 3\sqrt{6}$ | $12 + 7\sqrt{6}$ | $12 - 3\sqrt{6}$ | $12 + 11\sqrt{6}$ | $10$          | $10$          | $20$           |
| $10$       | $6 + \sqrt{6}$       | $12 - 7\sqrt{6}$ | $12 + 3\sqrt{6}$ | $12 + 11\sqrt{6}$ | $10$          | $10$          | $20$           |
| $10$       | $6 + \sqrt{6}$       | $12 - 7\sqrt{6}$ | $12 + 3\sqrt{6}$ | $12 + 11\sqrt{6}$ | $10$          | $10$          | $20$           |

Table 3.3: From left to right: Gauss-Christoffel-Jacobi III of order 2, 2 and 4, derived from (3.5) with $r = 1, 2, 3$ respectively, by using Jacobi type III polynomials.

|            | $6 - \sqrt{6}$ | $24 - \sqrt{6}$ | $4 - \sqrt{6}$ | $24 - \sqrt{6}$ | $5 - \sqrt{6}$ | $5 + \sqrt{6}$ | $5 - \sqrt{6}$ |
|------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| $10$       | $12 + 3\sqrt{6}$ | $12 + 7\sqrt{6}$ | $12 - 3\sqrt{6}$ | $12 + 11\sqrt{6}$ | $10$          | $10$          | $20$           |
| $10$       | $6 + \sqrt{6}$       | $12 - 7\sqrt{6}$ | $12 + 3\sqrt{6}$ | $12 + 11\sqrt{6}$ | $10$          | $10$          | $20$           |
| $10$       | $6 + \sqrt{6}$       | $12 - 7\sqrt{6}$ | $12 + 3\sqrt{6}$ | $12 + 11\sqrt{6}$ | $10$          | $10$          | $20$           |

(a) $w^{(0,1)}(\tau) = 2\tau$ for Jacobi type I;
(b) $w^{(1,0)}(\tau) = 2(1 - \tau)$ for Jacobi type II;
(c) $w^{(1,1)}(\tau) = 4(1 - \tau)\tau$ for Jacobi type III.

Observe that Jacobi type III actually is a special case of Gegenbauer type polynomials. We can easily gain these polynomials by using the Rodrigues’ formula (3.1). By using Theorem 3.1-3.3 and Remark 3.2, we can construct many standard RK schemes based on Gauss-Christoffel’s quadrature rules, some of which as examples are listed in Table 3.2 and 3.3. For convenience, we call them Gauss-Christoffel-Jacobi I, Gauss-Christoffel-Jacobi II, Gauss-Christoffel-Jacobi III families of RK methods, respectively. These schemes (except for the first method shown in Table 3.3 which is the well-known implicit midpoint rule [21]) are completely new and do not correspond to any schemes appeared in the existing literature.

3.3. RK-type methods based on Chebyshev polynomials

In this part, we will consider two types of Chebyshev polynomials, namely, Chebyshev polynomials of the first kind and the second kind. As a subclass of Jacobi polynomials, they are frequently used in various fields especially in the study of spectral methods (see [17, 18, 52, 51] and references therein). Particularly, Chebyshev nodes are often used in polynomial interpolation because the resulting interpolation polynomial minimizes the effect of Runge’s phenomenon.

Firstly, let us consider the shifted normalized Chebyshev polynomials of the first kind denoted by $T_n(x)$, i.e.,

$$T_0(x) = \frac{\sqrt{2}}{\sqrt{\pi}}, \quad T_n(x) = \frac{2\cos(n \arccos(2x - 1))}{\sqrt{\pi}}, \quad n \geq 1,$$

which is also a special subclass of Gegenbauer polynomials with $\alpha = \beta = -1/2$. These Chebyshev...
Theorem 3.1-3.3 can be directly applied, because $U$ can be obtained for this case. Some RK methods based on Table 3.5: From left to right: Gauss-Christoffel-Chebyshev II of order 2, 2, 4, derived from (3.5) with $P$ respectively, by using $T$ polynomials have the following properties:

\[
\int_0^1 T_n(t) \, dt = \begin{cases} 
\frac{1}{2} + \frac{\sqrt{2}}{8} & \text{if } n \text{ is odd,} \\
\frac{\sqrt{2}}{8}, & \text{if } n \text{ is even,} \\
\frac{2}{\sqrt{2}\pi}, & \text{if } n = 0.
\end{cases} 
\]  

(3.19)

It is seen that such polynomials also satisfy the relation (3.2), though they do not fall into the family of Gegenbauer polynomials $P_{\alpha}(x)$ with $\alpha > 0$. Obviously, the same results of Theorem 3.3 can be obtained for this case. Some RK methods based on $T_n(x)$ are given in Table 3.4.

Secondly, let us consider the shifted normalized Chebyshev polynomials of the second kind denoted by $U_n(x)$, i.e.,

\[
U_n(x) = \frac{\sin \left( (n + 1) \arccos(2x - 1) \right)}{\sqrt{\pi (x - x^2)}} = \frac{T'_{n+1}(x)}{2(n + 1)}, \quad n \geq 0.
\]

Theorem 3.3 can be directly applied, because $U_n(x)$ are Gegenbauer polynomials with $\alpha = 1/2 > 0$. Some RK methods based on $U_n(x)$ are given in Table 3.5.

4. Geometric integration by csRK methods

In recent years, numerical solution of Hamiltonian systems and time-reversible systems has been placed on a central position in the field of geometric integration [21, 35, 27]. The well-known Hamiltonian systems are usually written in the compact form

\[
\dot{z} = J^{-1} \nabla H(z), \quad z(t_0) = z_0 \in \mathbb{R}^{2d},
\]  

(4.1)
where $J$ is a standard structure matrix, $H$ is the Hamiltonian function (often stands for the total energy). Symplecticity (Poincaré 1899) is known as a characteristic property of Hamiltonian systems (see [21], page 185). It is natural to search for numerical methods that share this geometric property, thereupon symplectic methods were created [13, 21, 27, 34, 35] and afterwards symplectic RK methods were discovered independently by three authors [36, 39, 26], while energy-preserving methods were developed parallelly and deemed to be of interest in some fields (e.g., classical mechanics, molecular dynamics, chaotic dynamics and so forth) [24, 25, 32, 21, 27]. Usually, symplectic methods can produce many excellent numerical behaviors including linear error growth, long-time near-conservation of first integrals, and existence of invariant tori [21, 37]. Besides, symmetric methods are popular for solving reversible Hamiltonian problems arising in various fields, and they share many similar excellent long-time properties with symplectic methods [21].

4.1. Symplectic methods

In this part, we discuss the construction of symplectic methods based on weighted orthogonal polynomials. As examples, the construction of symplectic schemes based on Chebyshev polynomials will be presented.

**Lemma 4.1.** [49] If the coefficients of a csRK method (2.2) satisfy

$$B_\tau A_{\tau,\sigma} + B_\sigma A_{\sigma,\tau} \equiv B_\tau B_\sigma, \quad \tau, \sigma \in [0, 1],$$

then it is symplectic. In addition, if the coefficients of the underlying symplectic csRK method satisfy (4.2), then the RK scheme derived by using numerical quadrature is always symplectic.

**Theorem 4.1.** Under the assumption (2.6), for a symplectic csRK method with coefficients satisfying (4.2), we have the following statements:

(a) $\check{B}(\xi)$ and $\check{C}(\eta) \Rightarrow \check{D}(\zeta)$, where $\zeta = \min\{\xi, \eta\}$;

(b) $\check{B}(\xi)$ and $\check{D}(\zeta) \Rightarrow \check{C}(\eta)$, where $\eta = \min\{\xi, \zeta\}$.

**Proof.** Here we only provide the proof of (a), while (b) can be similarly obtained. By multiplying $\sigma^{\kappa-1}$ from both sides of (4.2) and taking integral, it gives

$$B_\tau \int_0^1 A_{\tau,\sigma} \sigma^{\kappa-1} d\sigma + \int_0^1 B_\sigma \sigma^{\kappa-1} A_{\sigma,\tau} d\sigma = B_\tau \int_0^1 B_\sigma \sigma^{\kappa-1} d\sigma, \quad \kappa = 1, 2, \cdots, \zeta. \tag{4.3}$$

Now let $\zeta = \min\{\xi, \eta\}$, which implies $\zeta \leq \xi$ and $\zeta \leq \eta$, and thus $\check{B}(\zeta)$ and $\check{C}(\zeta)$ can be used for calculating the integrals of (4.3). As a result, we have

$$B_\tau \frac{\tau^{\kappa}}{\kappa} + \int_0^1 B_\sigma \sigma^{\kappa-1} A_{\sigma,\tau} d\sigma = B_\tau \frac{1}{\kappa}, \quad \kappa = 1, 2, \cdots, \zeta,$$

which can be reduced to

$$\int_0^1 B_\sigma \sigma^{\kappa-1} A_{\sigma,\tau} d\sigma = \frac{B_\tau}{\kappa} (1 - \tau^\kappa), \quad \kappa = 1, 2, \cdots, \zeta.$$

Finally, by exchanging $\tau \leftrightarrow \sigma$ in the formula above, it gives $\check{D}(\zeta)$ with $\zeta = \min\{\xi, \eta\}$. \hfill \Box

---

7 Generally, we cannot have a numerical method which exactly preserves symplecticity and energy at the same time for a general nonlinear Hamiltonian system [12, 16].

8 Note that here we can use weighted or non-weighted interpolatory quadrature formula.
Remark 4.1. A counterpart result for classical symplectic RK methods can be similarly obtained.

In what follows, with the help of Lemma 4.1 and Theorem 4.1 we present two techniques to construct symplectic methods separately.

4.1.1. Construction of symplectic methods: Technique I

Observe that by Theorem 2.3 we can easily design the coefficients $B_\tau$ and $A_{\tau,\sigma}$ so as to satisfy $\tilde{B}(\xi)$ and $\tilde{C}(\eta)$, and it is possible for us to get symplectic methods by further requiring the symplectic condition (4.2), where the free parameters $\lambda_j$ and $\phi_j(\tau)$ should be carefully tuned. By this way, the statement (a) of Theorem 4.1 tells us that the resulting symplectic methods are at least of order $\min\{\xi, 2\eta + 2, \eta + \zeta + 1\} = \min\{\xi, \eta + \zeta + 1\}$ with $\zeta = \min\{\xi, \eta\}$. More precisely, we can arrive at the following result.

Theorem 4.2. Suppose the simplifying assumptions $\tilde{B}(\xi)$, $\tilde{C}(\eta)$ and $\tilde{D}(\zeta)$ hold with $\xi, \eta, \zeta \geq 1$. Let $r = \min\{\xi, \eta, \zeta\}$, and with the premise (2.6), we have the following ansatz

\[
B_\tau = \sum_{j=0}^{r-1} \int_0^1 P_j(x) \, dx P_j(\tau) w(\tau) + \sum_{j \geq r} \lambda_j P_j(\tau) w(\tau),
\]

\[
A_{\tau, \sigma} = \sum_{j=0}^{r-1} \int_0^\tau P_j(x) \, dx P_j(\sigma) w(\sigma) + \sum_{j \geq r} \phi_j(\tau) P_j(\sigma) w(\sigma),
\]

\[
B_\tau A_{\tau, \sigma} = \sum_{j=0}^{r-1} B_\sigma \int_0^1 P_j(x) \, dx P_j(\tau) w(\tau) + \sum_{j \geq r} \psi_j(\sigma) P_j(\tau) w(\tau),
\]

where

\[
\lambda_j = \int_0^1 P_j(x) \, dx, \quad r \leq j \leq \xi - 1,
\]

\[
\phi_j(\tau) = \int_0^\tau P_j(x) \, dx, \quad r \leq j \leq \eta - 1,
\]

\[
\psi_j(\sigma) = B_\sigma \int_\sigma^1 P_j(x) \, dx, \quad r \leq j \leq \zeta - 1,
\]

whenever “$\xi > r$” or “$\eta > r$” or “$\zeta > r$” holds. For the csRK method with (4.4) as its coefficients, if additionally

\[
B_\sigma (\lambda_j - \phi_j(\sigma)) = \psi_j(\sigma), \quad j \geq r,
\]

then the method is symplectic.

Proof. It suffices for us to consider whether the symplectic condition (4.2) is fulfilled by the Butcher coefficients. By exchanging $\tau \leftrightarrow \sigma$ in the second formula of (4.4) and multiplying $B_\sigma$ from both sides, it gives

\[
B_\sigma A_{\sigma, \tau} = \sum_{j=0}^{r-1} B_\sigma \int_0^\sigma P_j(x) \, dx P_j(\tau) w(\tau) + \sum_{j \geq r} B_\sigma \phi_j(\sigma) P_j(\tau) w(\tau).
\]

Then, by using the resulting formula above with the first and third formula of (4.4) it is easy to verify the symplectic condition (4.2) with the premise (4.5).

\[\square\]
Table 4.1: Two symplectic RK methods of order 2, based on Chebyshev polynomials of the first kind.

|      |         |         |         |         |
|------|---------|---------|---------|---------|
| $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{2-\sqrt{2}}{4}$ | $\frac{1}{4}$ | $\frac{1-\sqrt{2}}{4}$ |
| $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{2+\sqrt{2}}{4}$ | $\frac{1}{4}$ | $\frac{1+\sqrt{2}}{4}$ |

Remark 4.2. We emphasize that (4.5) alone does not provide a “sufficient” condition for symplecticity, recognizing that $\lambda_j, \phi_j(\sigma), \psi_j(\sigma)$ are also restricted by the simultaneous system of (4.4). Moreover, it cannot be used independently, for example, if we take $\xi = \eta = \zeta = r$ and let $\lambda_j = \phi_j(\sigma) = \psi_j(\sigma) \equiv 0$, $j \geq r$ so as to satisfy the condition (4.5), then the first two formulae generally contradict with the third formula of (4.4). This implies that, condition (4.5) can only be used as a “necessary” condition in the construction of symplectic methods.

Example 4.1. If we take $\xi = 2$, $\eta = 1$ for satisfying $\bar{B}(\xi)$ and $\bar{C}(\eta)$, then it allows us to make the following ansatz (with the premise $C_\tau = \tau$)

\[
B_\tau = \sum_{j=0}^{1} \int_{0}^{1} T_j(x) dx T_j(\tau) \omega(\tau) + \lambda_2 T_2(\tau) \omega(\tau),
\]

\[
A_{\tau, \sigma} = \int_{0}^{\tau} T_0(x) dx T_0(\sigma) \omega(\sigma) + \phi_1(\tau) T_1(\sigma) \omega(\sigma),
\]

where $T_n(x)$ are Chebyshev polynomials of the first kind. After some elementary calculations, we find that if one chooses $\lambda_2 = 0$, $\phi_1(\tau) = -\sqrt{n}/2\pi$, $\psi_1(\sigma) = 1/(2\sqrt{n^3} \sigma (1 - \sigma))$, that is,

\[
A_{\tau, \sigma} = \frac{\tau - \sigma + \frac{1}{2}}{\pi \sqrt{\sigma (1 - \sigma)}}, \quad B_\tau = \frac{1}{\pi \sqrt{\tau (1 - \tau)}}, \quad C_\tau = \tau,
\]

then it gives a 2-order symplectic csRK method. By using Gauss-Christoffel quadrature rules we get two symplectic RK methods of order 2, which is shown in Table 4.1. The first scheme corresponds to the well-known implicit midpoint rule which is a symplectic method firstly discovered by K. Feng [15].

4.1.2. Construction of symplectic methods: Technique II

In fact, the first technique above has a drawback that it needs to consider the solution of the simultaneous system in terms of $\lambda_j, \phi_j(\tau)$ and $\psi_j(\sigma)$, conducting complex computation and elusive
choice of free parameters. To get rid off this drawback, we present another easier and enforceable technique below, which is based on the following result.

**Theorem 4.3.** Suppose that $A_{\tau,\sigma}/B_\sigma \in L^2_{w}([0, 1] \times [0, 1])$, then symplectic condition (4.1) is equivalent to the fact that $A_{\tau,\sigma}$ has the following form in terms of the orthogonal polynomials $P_n(x)$ in $L^2_{w}[0, 1]

$$A_{\tau,\sigma} = B_\sigma \left( \frac{1}{2} + \sum_{0<i+j \in \mathbb{Z}} \alpha(i,j) P_i(\tau) P_j(\sigma) \right), \quad \alpha(i,j) \in \mathbb{R},$$

where $\alpha(i,j)$ is skew-symmetric, i.e., $\alpha(i,j) = -\alpha(j,i)$, $i + j > 0$.

**Proof.** Recognizing that for a practical csRK method, $B_\tau$ must not vanish, otherwise it fails to fulfill the simplifying assumption $\tilde{B}(\xi)$ which then gives no order accuracy. Hence we always assume $B_\tau \neq 0$. Consequently, by dividing $B_\tau A_{\tau,\sigma}$ from both sides of (4.2), we arrive at

$$\frac{A_{\tau,\sigma}}{B_\sigma} + \frac{A_{\sigma,\tau}}{B_\tau} \equiv 1.$$  

(4.7)

Now that $\{P_i(\tau) P_j(\sigma)\}_{i,j \in \mathbb{Z}}$ forms a complete orthogonal basis in the Hilbert space $L^2_{w}([0, 1] \times [0, 1])$, we consider expanding $A_{\tau,\sigma}/B_\sigma$ as

$$A_{\tau,\sigma}/B_\sigma = \sum_{0 \leq i, j \in \mathbb{Z}} \alpha(i,j) P_i(\tau) P_j(\sigma),$$

(4.8)

where $\alpha(i,j)$ are real parameters. By exchanging $\tau \leftrightarrow \sigma$, we have

$$A_{\sigma,\tau}/B_\tau = \sum_{0 \leq i, j \in \mathbb{Z}} \alpha(i,j) P_i(\sigma) P_j(\tau) = \sum_{0 \leq i, j \in \mathbb{Z}} \alpha(j,i) P_i(\tau) P_j(\sigma).$$

(4.9)

Take notice that $P_0(x)$ as a 0-degree polynomial is a nonzero constant. By plugging (4.8) & (4.9) into (4.7) and afterwards collecting like terms, it gives

$$\alpha_{(0,0)} P_0(\tau) P_0(\sigma) = \frac{1}{2} \quad \text{and} \quad \alpha(i,j) = -\alpha(j,i), \quad i + j > 0,$$

which then leads to the final result by (4.8).

Consequently, our second technique to construct symplectic methods can be described as follows:

**Step 1.** Make an ansatz for $B_\tau$ which satisfies $\tilde{B}(\xi)$ with $\xi \geq 1$, noticing that now $\lambda_j$ can be freely embedded in the formula;

**Step 2.** Suppose $A_{\tau,\sigma}$ is in the form (according to Theorem 4.3)

$$A_{\tau,\sigma} = B_\sigma \left( \frac{1}{2} + \sum_{0<i+j \in \mathbb{Z}} \alpha(i,j) P_i(\tau) P_j(\sigma) \right), \quad \alpha(i,j) = -\alpha(j,i),$$

where $\alpha(i,j)$ are kept as parameters with a finite number, and for the sake of settling $\alpha(i,j)$, we then substitute it into $\tilde{C}(\eta)$ (see (2.8), usually we let $\eta < \xi$):

$$\int_0^1 A_{\tau,\sigma} P_\kappa(\sigma) \, d\sigma = \int_0^\tau P_\kappa(x) \, dx, \quad \kappa = 0, 1, \cdots, \eta - 1.$$

Alternatively, another way is to consider substituting $B_\tau$ and $A_{\tau,\sigma}$ into the order conditions instead of the simplifying assumptions, as done in (4.10);

**Step 3.** Write down $B_\tau$ and $A_{\tau,\sigma}$ (satisfy $\tilde{B}(\xi)$ and $\tilde{C}(\eta)$ automatically), which results in a symplectic csRK method of order at least $\min\{\xi, \eta + \zeta + 1\}$ with $\zeta = \min\{\xi, \eta\}$. 

19
Example 4.2. Let $\xi = 3$, $\eta = 1$ for satisfying $\tilde{B}(\xi)$ and $\tilde{C}(\eta)$, and make the following ansatz in terms of $T_n(x)$ (Chebyshev polynomials of the first kind)

$$B_\tau = \sum_{j=0}^{2} \int_{0}^{1} T_j(x) dx T_j(\tau) w(\tau), \quad C_\tau = \tau, \quad \tau \in [0, 1],$$

$$A_{\tau, \sigma} = B_\sigma \left( \frac{1}{2} + \mu T_1(\sigma) - \mu T_1(\tau) + \nu T_1(\sigma) T_2(\sigma) - \nu T_2(\tau) T_1(\sigma) \right).$$

Substituting $A_{\tau, \sigma}$ into $\tilde{C}(1)$, it easily gives (hint: $\tilde{B}(\xi)$ is helpful in the calculation of integrals)

$$\mu + \frac{2\nu}{3\sqrt{\pi}} = -\frac{\sqrt{\pi}}{4}.$$

Let $\mu = -2\nu/(3\sqrt{\pi}) - \sqrt{\pi}/4$, then we get a family of one-parameter symplectic csRK methods of order $\geq 3$. Actually, we find that they are also symmetric and thus they possess an even order 4. By using the 3-point Gauss-Christoffel quadrature rule we get a family of 3-stage 4-order symplectic RK methods which are shown in Table 4.2, with $\omega := \frac{4\sqrt{3}}{2\sqrt{\pi}}$.

Generally, it is not very convenient and optimal to construct “high-order” symplectic RK methods via using a general weighted orthogonal polynomials. However, if we restrict ourselves to using Legendre polynomials, then it is much easier to design symplectic methods of arbitrarily high order, which has been previously investigated by Tang et al [41, 43, 44, 46, 49]. The following theorem, which can be viewed as a corollary of Theorem 4.3, shows a simpler but useful feature for symplecticity.

**Theorem 4.4.** [46] A csRK method with $B_\tau = 1$, $C_\tau = \tau$ is symplectic if $A_{\tau, \sigma}$ has the following form in terms of Legendre polynomials

$$A_{\tau, \sigma} = \frac{1}{2} + \sum_{0 \leq i+j \in \mathbb{Z}} \alpha_{(i,j)} L_i(\tau) L_j(\sigma), \quad \alpha_{(i,j)} \in \mathbb{R}, \quad (4.10)$$

where $\alpha_{(i,j)}$ is skew-symmetric, i.e., $\alpha_{(i,j)} = -\alpha_{(j,i)}$, $i + j > 0$.

Actually, by putting Theorem 3.4 and Theorem 4.4 together we can establish symplectic csRK methods of arbitrarily high order. Symplectic RK methods are then easily obtained with the help of any numerical quadrature rule (see Lemma 4.1).
4.2. Symmetric methods

Symmetric methods are preferable for solving reversible Hamiltonian systems, and one of their attractive properties is that they possess an even order which has important application value on study of splitting and composition methods [21]. The concept of such methods can be found in [21]. In this part, we present some new results for constructing symmetric methods based on weighted orthogonal polynomials.

Lemma 4.2. [49] Under the assumption \((2.3)\) and we suppose \(\bar{B}(\xi)\) holds with \(\xi \geq 1\) (which means the method is of order at least 1), then a csRK method is symmetric if

\[
A_{\tau, \sigma} + A_{1-\tau, 1-\sigma} \equiv B_\sigma, \; \tau, \sigma \in [0,1].
\]  

(4.11)

Particularly, for the weighted csRK method \((2.10)\), the symmetric condition \((4.11)\) becomes

\[
\hat{A}_{\tau, \sigma}w(\sigma) + \hat{A}_{1-\tau, 1-\sigma}w(1-\sigma) \equiv \hat{B}_\sigma w(\sigma), \; \tau, \sigma \in [0,1].
\]  

(4.12)

If additionally require \(w(\sigma) = w(1-\sigma)\), then the corresponding symmetric condition reduces to

\[
\hat{A}_{\tau, \sigma} + \hat{A}_{1-\tau, 1-\sigma} \equiv \hat{B}_\sigma, \; \tau, \sigma \in [0,1].
\]  

(4.13)

Besides, if the coefficients of the underlying csRK method \((2.10)\) satisfy \((4.13)\), then the RK scheme \((2.15)\) derived by numerical quadrature is symmetric, provided that the quadrature weights and abscissae (see \((2.14)\)) satisfy \(b_{s+1-i} = b_i\) and \(c_{s+1-i} = 1 - c_i\) for all \(i\).

Theorem 4.5. Let \(\{P_j(x)\}_{j\in\mathbb{Z}}\) be Gegenbauer polynomials based on weight function \(w(x) = 2^{2\alpha}(1-x)^\alpha x^\alpha\) with \(\alpha > 0\), and suppose the simplifying assumptions \(\bar{B}(\xi), \bar{C}(\eta)\) hold. With the premise \((2.6)\) and \(r = \min\{\xi, \eta\}\), we set the following ansatz

\[
B_\tau = \sum_{j=0}^{r-1} \int_0^1 P_j(x) dx P_j(\tau) w(\tau) + \sum_{j \geq r} \lambda_j P_j(\tau) w(\tau),
\]  

(4.14)

\[
A_{\tau, \sigma} = \sum_{j=0}^{r-1} \int_0^\tau P_j(x) dx P_j(\sigma) w(\sigma) + \sum_{j \geq r} \phi_j(\tau) P_j(\sigma) w(\sigma),
\]

where

\[
\lambda_j = \int_0^1 P_j(x) dx, \; r \leq j \leq \xi - 1,
\]

\[
\phi_j(\tau) = \int_0^\tau P_j(x) dx, \; r \leq j \leq \eta - 1,
\]

whenever \(\xi > r\) or \(\eta > r\) holds. For the csRK method with \((4.14)\) as its coefficients, if we additionally require

\[
\phi_j(\tau) + (-1)^j \phi_j(1-\tau) = \lambda_j, \; j \geq r,
\]  

(4.15)

then the method is symmetric. Moreover, an s-stage standard RK method \((2.15)\) based on any quadrature rules with symmetric weights and abscissae is also symmetric.
Proof. We only prove the first statement about csRK methods, while the second statement is trivial by the second statement of Lemma 4.2. The proof relies upon the verification of the symmetric condition (4.11).

Observe that \( w(1 - \sigma) = w(\sigma) \) and the symmetry relation (3.3) implies

\[
P_n^{(\beta, \beta)}(1 - \tau) = (-1)^n P_n^{(\beta, \beta)}(\tau), \quad \beta > -1, \quad n \geq 0,
\]

as a result, we have

\[
B_\sigma = \sum_{j=0}^{r-1} \int_0^1 P_j^{(\alpha, \alpha)}(x) \, dx \, P_j^{(\alpha, \alpha)}(\sigma) w(\sigma) + \sum_{j \geq r} \lambda_j P_j^{(\alpha, \alpha)}(\sigma) w(\sigma),
\]

\[
A_{\tau, \sigma} = \sum_{j=0}^{r-1} \int_0^\tau P_j^{(\alpha, \alpha)}(x) \, dx \, P_j^{(\alpha, \alpha)}(\sigma) w(\sigma) + \sum_{j \geq r} \phi_j(\tau) P_j^{(\alpha, \alpha)}(\sigma) w(\sigma),
\]

\[
A_{1-\tau, 1-\sigma} = \sum_{j=0}^{r-1} (-1)^j \int_0^{1-\tau} P_j^{(\alpha, \alpha)}(x) \, dx \, P_j^{(\alpha, \alpha)}(\sigma) w(\sigma) + \sum_{j \geq r} (-1)^j \phi_j(1-\tau) P_j^{(\alpha, \alpha)}(\sigma) w(\sigma),
\]

where, for convenience, we have denoted the \( j \)-degree Gegenbauer polynomial by \( P_j^{(\alpha, \alpha)}(x) \) \((\alpha > 0)\). Besides, from (3.2) it gives

\[
\int_0^\tau P_j^{(\alpha, \alpha)}(x) \, dx = \frac{1}{\mu_j} \left( P_{j+1}^{(\alpha-1, \alpha-1)}(\tau) - P_{j+1}^{(\alpha-1, \alpha-1)}(0) \right),
\]

\[
\int_0^{1-\tau} P_j^{(\alpha, \alpha)}(x) \, dx = \frac{1}{\mu_j} \left( P_{j+1}^{(\alpha-1, \alpha-1)}(1-\tau) - P_{j+1}^{(\alpha-1, \alpha-1)}(0) \right),
\]

\[
\int_0^{1} P_j^{(\alpha, \alpha)}(x) \, dx = \frac{1}{\mu_j} \left( P_{j+1}^{(\alpha-1, \alpha-1)}(1) - P_{j+1}^{(\alpha-1, \alpha-1)}(0) \right),
\]

with \( \mu_j = 2\sqrt{(j+1)(j+2\alpha)} \), and by virtue of (4.16) the last two formulae become

\[
\int_0^{1-\tau} P_j^{(\alpha, \alpha)}(x) \, dx = \frac{1}{\mu_j} \left( (-1)^{j+1} P_{j+1}^{(\alpha-1, \alpha-1)}(\tau) - P_{j+1}^{(\alpha-1, \alpha-1)}(0) \right),
\]

\[
\int_0^{1} P_j^{(\alpha, \alpha)}(x) \, dx = \frac{1}{\mu_j} \left( (-1)^{j+1} P_{j+1}^{(\alpha-1, \alpha-1)}(0) - P_{j+1}^{(\alpha-1, \alpha-1)}(0) \right),
\]

which can lead us into the final result.

Remark 4.3. Theorem 4.5 still holds true when \( \alpha = 0 \) and \( \alpha = -1/2 \) which are corresponding to Legendre polynomials and Chebyshev polynomials of the first kind respectively. This can be easily verified by using (3.15) and (3.19).

Example 4.3. As a practical application of the result above, Table 3.1, 3.3, 3.4 and 3.5 actually have presented good examples for symmetric methods, and all of them share an even order.

The following result is not restricted for the use of Gegenbauer polynomials, which can be applied to a wider class of weighted orthogonal polynomials.
Theorem 4.6. Suppose that \( A_{\tau,\sigma}/B_{\sigma} \in L^2_w([0,1] \times [0,1]) \), then symmetric condition \((4.11)\) is equivalent to the fact that \( A_{\tau,\sigma} \) has the following form in terms of the orthogonal polynomials \( P_n(x) \) in \( L^2_w([0,1]) \)

\[
A_{\tau,\sigma} = B_{\sigma} \left( \frac{1}{2} + \sum_{\substack{i+j \text{ odd} \,\, 0 \leq i,j \in \mathbb{Z}}} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right), \quad \alpha_{(i,j)} \in \mathbb{R},
\]

\((4.17)\)

with \( B_{\sigma} \equiv B_{1-\sigma} \), where \( \alpha_{(i,j)} \) can be any real parameters for odd \( i+j \), provided that the orthogonal polynomials \( P_n(x) \) satisfy

\[
P_n(1-x) = (-1)^n P_n(x), \quad n \in \mathbb{Z}.
\]

Proof. We only give the proof for the necessity, seeing that the sufficiency part is rather trivial. Obviously, \((4.11)\) implies \( B_{\sigma} \equiv B_{1-\sigma} \) in \([0,1]\). Then, \((4.11)\) can be recast as

\[
\frac{A_{\tau,\sigma}}{B_{\sigma}} + \frac{A_{1-\tau,1-\sigma}}{B_{1-\sigma}} \equiv 1.
\]

\((4.18)\)

The remaining process of proof is very similar to that of Theorem 4.3.

By using the similar technique for constructing symplectic methods (c.f., technique II), we get a simple way to derive symmetric methods. It is easy to construct methods to be symplectic and symmetric at the same time by combining Theorem 4.3 with Theorem 4.6. Besides, the following theorem (as a corollary of Theorem 4.6) in conjunction with Theorem 3.4 makes the construction of “high-order” symmetric methods much easier \([41, 44, 49]\) owing to the pretty Legendre polynomial expansion technique.

Theorem 4.7. \([44]\) The csRK method with \( B_{\tau} = 1 \) and \( C_{\tau} = \tau \) is symmetric if \( A_{\tau,\sigma} \) has the following form in terms of Legendre polynomials

\[
A_{\tau,\sigma} = \frac{1}{2} + \sum_{\substack{i+j \text{ odd} \,\, 0 \leq i,j \in \mathbb{Z}}} \alpha_{(i,j)} L_i(\tau) L_j(\sigma), \quad \alpha_{(i,j)} \in \mathbb{R},
\]

\((4.19)\)

where \( \alpha_{(i,j)} \) can be any real parameters for odd \( i+j \).

4.3. Energy-preserving methods

Energy-preserving methods for Hamiltonian systems (even Poisson systems) have been developed within the framework of continuous-stage methods (or at least closely related to csRK methods) in recent years. For more information, please refer to \([4, 3, 11, 13, 22, 28, 30, 31, 41, 44, 49]\) and references therein. Energy-preserving methods based on weighted orthogonal polynomials may be considered in our future work, but we do not plan to pursue this subject here.

5. Conclusions

This paper investigates the construction of RK-type methods within the framework of RK methods with continuous stage. The most highlighted advantage of developing such special class of RK methods is that we do not need to consider and study the tedious solution of nonlinear algebraic equations associated with order conditions. In recent years, Tang et al \([41, 44, 46, 48, 49]\) developed several continuous-stage methods and explored their applications in geometric numerical
integration. However, these previous studies are limited upon the use of one type of orthogonal polynomials, i.e., Legendre polynomials. To get over such limitation, we lead weight functions into the formulation of csRK methods and develop new constructive theory of RK-type methods. By doing this, a lot of weighted orthogonal polynomials can be directly utilized. Recognizing that orthogonal polynomials play an all-pervasive role in modern mathematics and engineering fields, but their applications in numerical ordinary differential equations seems relatively fewer, or at least not fully explored. Based on these considerations, we try to enlarge their applications in this paper and hopefully it may further greatly enhance the RK approximation theory in numerical analysis.

As is well known, Gauss-Legendre RK methods (can be explained as collocation methods [21]) must be the only existing standard RK methods with the optimal superconvergence order [5], which are based on the famous Gauss quadrature rules. Recognizing that there are infinitely many Gauss-Christoffel’s quadrature rules (see Theorem [2.5]) and they possess the same highest order as Gauss quadrature rules, a natural question comes out: Can we construct other RK methods sharing the same stage and order with Gauss-Legendre RK methods for solving a general ODEs? Unfortunately, this aim turns out to be too ambitious. From Theorem [2.4], we can deduce that it is impossible to realize it at least within our approach, because when we use a quadrature rule (even with the highest order), the order of the resulting methods is always limited by the degrees of those Butcher coefficients, which will hinder us from making it. Legendre polynomials are deemed to be the optimal choice in such sense.

Based on our newly-developed theories of csRK methods, we have constructed some new geometric integrators including symplectic methods for Hamiltonian systems and symmetric methods for time-reversible systems. Although these methods are described mainly in terms of Jacobi polynomials, they are not essentially dependent upon this special type of orthogonal polynomials. Other symplectic or symmetric methods could be constructed with the similar techniques by virtue of any weighted orthogonal polynomials you can imagine. Besides, it is possible to get other types of geometric integrators in the context of csRK methods, e.g., energy-preserving methods, conjugate-symplectic methods, first-integral-preserving methods, Lyapunov-function-preserving methods etc.

At last but not the least, we have observed that orthogonal polynomials are of great and clear significance in study of spectral methods. The discovery of spectral accuracy and super-geometric convergent rate of a spectral algorithm is very attractive [17, 18, 52, 51]. On account of this, the relationship between csRK methods and spectral methods as well as the efficient implementability of csRK methods will be investigated elsewhere.

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