Brief paper

A unified framework for the numerical solution of optimal control problems using pseudospectral methods☆

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ABSTRACT

A unified framework is presented for the numerical solution of optimal control problems using collocation at Legendre–Gauss (LG), Legendre–Gauss–Radau (LGR), and Legendre–Gauss–Lobatto (LGL) points. It is shown that the LG and LGR differentiation matrices are rectangular and full rank whereas the LGL differentiation matrix is square and singular. Consequently, the LG and LGR schemes can be expressed equivalently in either differential or integral form, while the LGL differential and integral forms are not equivalent. Transformations are developed that relate the Lagrange multipliers of the discrete nonlinear programming problem to the costates of the continuous optimal control problem. The LG and LGR discrete costate systems are full rank while the LGL discrete costate system is rank-deficient. The LGL costate approximation is found to have an error that oscillates about the true solution and this error is shown by example to be due to the null space in the LGL discrete costate system. An example is considered to assess the accuracy and features of each collocation scheme.

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1. Introduction

In recent years, pseudospectral methods have become increasingly popular in the numerical solution of optimal control problems (Benson, Huntington, Thorvaldsen, & Rao, 2006; Elnagar, Kazemi, & Razzaghi, 1995; Fahroo & Ross, 2001, 2008b; Garg et al., 2009; Kameswaran & Biegler, 2008; Rao et al., 2010; Vlassenbroeck & Doreen, 1988). Pseudospectral methods are a class of *direct collocation* where the optimal control problem is transcribed to a nonlinear programming problem (NLP) by parameterizing the state and control using global polynomials and collocating the differential–algebraic equations using nodes obtained from a Gaussian quadrature. The use of global polynomials together with Gaussian quadrature collocation points is known to provide accurate approximations that converge exponentially for problems whose solutions are smooth. For problems where the solutions

are nonsmooth or not well approximated by global polynomials of a reasonably low degree, it is preferable to use a finite-element approach (see Kameswaran and Biegler (2008)) where the time interval [−1, 1] is partitioned into subintervals and a different polynomial is used over each subinterval. In this paper we examine the properties of global pseudospectral methods for the numerical solution of optimal control problems using Gaussian quadrature collocation points.

The three most commonly used sets of collocation points are *Legendre–Gauss* (LG), *Legendre–Gauss–Radau* (LGR), and *Legendre–Gauss–Lobatto* (LGL) points. These three sets of points are obtained from the roots of a Legendre polynomial and/or linear combinations of a Legendre polynomial and its derivatives. In recent years, the most well documented pseudospectral methods using these sets of collocation points are the *Legendre–Gauss–Lobatto pseudospectral method* (Elnagar et al., 1995; Fahroo & Ross, 2001), the *Legendre–Gauss pseudospectral method* (Benson et al., 2006; Rao et al., 2010), and the *Legendre–Gauss–Radau pseudospectral method* (Garg et al., 2009).

Upon cursory examination it may appear as if LG, LGR, and LGL points are essentially similar, with only minor differences due to the fact that each set of nodes is a different form of Gaussian quadrature. As we will show in this paper, however, the differences between these three pseudospectral methods are not merely cosmetic. Instead, the use of either LG or LGR points leads

to a distinctly different mathematical form as compared with that of using LGL points. As a result, the LG and LGR methods have different convergence properties from the LGL method.

The contributions of this research are as follows. First, we show that the differentiation matrices of the LG and LGR schemes are rectangular and full rank, whereas the LGL differentiation matrix is square and singular. As a result, the LG and LGR methods can be written equivalently in either differential or implicit integral form, while the LGL method does not have an equivalent implicit integral form. Second, we show that the LG and LGR transformed adjoint systems (analogous to the definition in Hager (2000)) are full rank while the LGL transformed adjoint system is rank-deficient. Consequently, the LG and LGR costate approximations converge exponentially while the LGL costate is potentially nonconvergent. Third, it is identified that the error in the LGL costate is oscillatory due to the oscillatory nature of the null space of the LGL transformed adjoint system. Finally, by studying a representative example, we demonstrate that the LG and LGR state and control converge at a significantly faster rate as compared with the LGL method. The numerical example substantiates the aforementioned nonconvergence of the LGL costate. This paper provides the first rigorous analysis that identifies the key mathematical properties of pseudospectral methods using collocation at Gaussian quadrature points, enabling a researcher or end-user to see clearly the accuracy and convergence (or nonconvergence) that can be expected when applying a particular pseudospectral method on a problem of interest.

2. LG, LGR, and LGL collocation points

The LG, LGR, and LGL collocation points lie on the open interval $\tau \in (-1, 1)$, the half open interval $\tau \in [-1, 1)$ or $\tau \in (-1, 1]$, and the closed interval $\tau \in [-1, 1]$, respectively. Let N be the number of collocation points and $P_N(\tau)$ be the Nth-degree Legendre polynomial. The LG points are the roots of $P_N(\tau)$ (Abramowitz & Stegun, 1965), the LGR points are the roots of $P_{N-1}(\tau) + P_N(\tau)$ (Abramowitz & Stegun, 1965), the flipped LGR points are the negative of the LGR points, and the LGL points are the roots of $\dot{P}_{N-1}(\tau)$ together with the points -1 and 1 (Abramowitz & Stegun, 1965). In this paper we use the flipped LGR points, while Garg et al. (2009) uses the standard set of LGR points. The LG, LGR, and LGL points have the property that

$$\int_{-1}^{+1} p(\tau)\mathrm{d}\tau = \sum_{i=1}^{N} w_i p(\tau_i)$$

is exact, respectively, for polynomials of degree at most $2N - 1$ (LG), $2N - 2$ (LGR), and $2N - 3$ (LGL), where w_i, $1 \leq i \leq N$ are, respectively, the LG, LGR, and LGL quadrature weights.

3. Conventions and notation

For each method derived in this paper, $(\tau_1, \ldots, \tau_N)$ denote the LG, LGR, or LGL quadrature (collocation) points. Furthermore, for the LG method we introduce the noncollocated points $(\tau_0, \tau_{N+1}) = (-1, +1)$ while for the LGR method we introduce the noncollocated point $\tau_0 = -1$. For each method, the state is approximated using a basis of Lagrange polynomials,

$$L_i(\tau) = \prod_{\substack{j=K \\ j \neq i}}^{N} \frac{\tau - \tau_j}{\tau_i - \tau_j}, \quad K \leq i \leq N, \tag{1}$$

where $K = 1$ if the initial point is collocated and $K = 0$ otherwise.

Next, all vector functions of time are *row* vectors; that is, $\mathbf{x}(\tau) = [x_1(\tau), \ldots, x_n(\tau)] \in \mathbb{R}^n$, and we define the approximation of the state and the control at $\tau = \tau_i$ as $\mathbf{X}_i$ and $\mathbf{U}_i$, respectively.

Furthermore, when referring to the state approximations at the N collocation points, we use $N \times n$ matrices $\mathbf{X}^{\text{LG}}$, $\mathbf{X}^{\text{LGR}}$, or $\mathbf{X}^{\text{LGL}}$, where each row contains $\mathbf{X}_i$. Similarly, for the LG and LGR methods the notation $\mathbf{X}$ refers to the $(N+1) \times n$ matrix formed by $\mathbf{X}_0$ plus either $\mathbf{X}^{\text{LG}}$ or $\mathbf{X}^{\text{LGR}}$. Using a notation similar to that for the state, we define the $N \times n$ matrices $\mathbf{U}$ and $\boldsymbol{\Lambda}$ that correspond to the control and Lagrange multipliers, respectively. Finally, the notation $\mathbf{X}_{i:j}$ will be used to denote *rows i through j* of $\mathbf{X}$ while the notation $\mathbf{D}_{i:j}$ attached to a differentiation matrix $\mathbf{D}$ denotes *columns i through j* of the matrix $\mathbf{D}$. In addition, the boldface symbol $\mathbf{1}$ will be used to denote a column vector of all ones.

We let $\mathbf{B}^{\mathsf{T}}$ denote the transpose of a matrix $\mathbf{B}$. Given vectors $\mathbf{a}$ and $\mathbf{b} \in \mathbb{R}^n$, the notation $\langle \mathbf{a}, \mathbf{b} \rangle$ is used to denote the dot product between $\mathbf{a}$ and $\mathbf{b}$. If $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$, then $\nabla\mathbf{f}$ is the m by n Jacobian matrix whose i-th row is ∇f_i. In particular, the gradient of a scalar-valued function is a row vector. If $\phi : \mathbb{R}^{m \times n} \to \mathbb{R}$ and $\mathbf{X}$ is an m by n matrix, then $\nabla\phi$ denotes the m by n matrix whose (i, j) element is $(\nabla\phi(\mathbf{X}))_{ij} = \partial\phi(\mathbf{X})/\partial X_{ij}$.

Expository approach

To simplify the exposition, we focus on the following unconstrained optimal control problem on the time interval $\tau \in [-1, +1]$.

$$\begin{aligned} \text{minimize} \quad & \Phi(\mathbf{x}(1)), \\ \text{subject to} \quad & \dot{\mathbf{x}}(\tau) = \mathbf{f}(\mathbf{x}(\tau), \mathbf{u}(\tau)), \qquad \mathbf{x}(-1) = \mathbf{x}_0, \end{aligned} \tag{2}$$

where $\mathbf{f} : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$, and $\mathbf{x}_0$ is the initial condition, which we assume is given. Note that the time interval can be transformed from $[-1, 1]$ to the time interval $[t_0, t_f]$ via the affine transformation $t = (t_f - t_0)\tau/2 + (t_f + t_0)/2$. By the Pontryagin minimum principle, the first-order optimality conditions of the continuous-time optimal control problem of (2) are given as

$$\boldsymbol{\lambda}(1) = \nabla\Phi(\mathbf{x}(1)), \tag{3}$$

$$\dot{\boldsymbol{\lambda}}(\tau) = -\nabla_x \langle \boldsymbol{\lambda}(\tau), \mathbf{f}(\mathbf{x}(\tau), \mathbf{u}(\tau)) \rangle, \tag{4}$$

$$\mathbf{0} = \nabla_u \langle \boldsymbol{\lambda}(\tau), \mathbf{f}(\mathbf{x}(\tau), \mathbf{u}(\tau)) \rangle. \tag{5}$$

4. Collocation at LG, LGR and LGL points

In this section we develop our framework for the numerical solution of optimal control problems using collocation at Legendre–Gauss (LG), Legendre–Gauss–Radau (LGR), and Legendre–Gauss–Lobatto (LGL) points. It is important to note that, although both the LG and LGR schemes have noncollocated endpoint(s), *we still approximate the state at these endpoints as explained below.*

4.1. Collocation at LG points

Consider collocation at the N LG points and let $\tau_0 = -1$ and $\tau_{N+1} = +1$ be noncollocated points. Setting $K = 0$ in (1), the state is approximated by a polynomial of degree at most N as

$$\mathbf{x}^N(\tau) = \sum_{i=0}^{N} \mathbf{X}_i L_i(\tau). \tag{6}$$

It is important to observe that the series (6) includes the Lagrange polynomial associated with the *noncollocated* point $\tau_0 = -1$. Differentiating (6) and evaluating the result at the kth collocation point, τ_k, gives

$$\dot{\mathbf{x}}^N(\tau_k) = \sum_{i=0}^{N} \mathbf{X}_i \dot{L}_i(\tau_k) = \sum_{i=0}^{N} D_{ki}\mathbf{X}_i, \quad D_{ki} = \dot{L}_i(\tau_k). \tag{7}$$

The $N \times (N + 1)$ *non-square* matrix $\mathbf{D}$ is called the *Gauss pseudospectral differentiation matrix*, where we note that the extra column of $\mathbf{D}$ is due to the Lagrange polynomial $L_0(\tau)$ associated with the noncollocated point $\tau_0 = -1$. Suppose now that we let

$\mathbf{D} = [\mathbf{D}_0 \ \mathbf{D}_{1:N}]$ where $\mathbf{D}_0$ is the first column of $\mathbf{D}$ and $\mathbf{D}_{1:N}$ are the remaining N columns. We now prove the following properties of $\mathbf{D}$: (a) $\mathbf{D}_{1:N}$ is nonsingular and (b) $\mathbf{D}_0 = -\mathbf{D}_{1:N}\mathbf{1}$; equivalently, $-\mathbf{D}_{1:N}^{-1}\mathbf{D}_0 = \mathbf{1}$.

Proposition 1. *The matrix* $\mathbf{D}_{1:N}$ *obtained by deleting the first column of the Gauss pseudospectral differentiation matrix* $\mathbf{D}$ *is invertible.*

Proof of Proposition 1. Suppose that for some nonzero $\mathbf{p} \in \mathbb{R}^{N+1}$ with $p_0 = 0$, we have $\mathbf{Dp} = \mathbf{0}$. Let p be the unique polynomial of degree at most N which satisfies $p(\tau_i) = p_i, 0 \le i \le N$. Since the components of $\mathbf{Dp}$ are the derivatives of p evaluated at the collocation points, we have

$$0 = (\mathbf{Dp})_i = \dot{p}(\tau_i), \quad 1 \le i \le N.$$

Since $\dot{p}$ is a polynomial of degree at most $N - 1$, it must be identically zero since it vanishes at N points. Hence, p is constant. Since $p(-1) = 0$ and p is constant, it follows that p is identically 0. This shows that $p_i = p(\tau_i) = 0$ for each i. Since the equation $\mathbf{Dp} = \mathbf{0}$ with $p_0 = 0$ has no nonzero solution, $\mathbf{D}_{1:N}$ is nonsingular. $\quad\square$

Proposition 2. $\mathbf{D}_0 = -\mathbf{D}_{1:N}\mathbf{1}$; *equivalently,* $-\mathbf{D}_{1:N}^{-1}\mathbf{D}_0 = \mathbf{1}$.

Proof of Proposition 2. The components of the vector $\mathbf{D1}$ are the derivatives at the collocation points of the constant polynomial $p(\tau) = 1$. Therefore, $\mathbf{D1} = \mathbf{0}$, which implies that $\mathbf{D1} = \mathbf{D}_0 + \mathbf{D}_{1:N}\mathbf{1} = \mathbf{0}$. Rearranging, we obtain

$$\mathbf{D}_0 = -\mathbf{D}_{1:N}\mathbf{1}. \tag{8}$$

Multiplying by $\mathbf{D}_{1:N}^{-1}$ gives $-\mathbf{D}_{1:N}^{-1}\mathbf{D}_0 = \mathbf{1}$. $\quad\square$

Using the matrix $\mathbf{D}$, the dynamics are collocated at the N LG points as

$$\mathbf{DX} = \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) \Longleftrightarrow \mathbf{D}_{1:N}\mathbf{X}^{\text{LG}} = \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) - \mathbf{D}_0\mathbf{X}_0. \tag{9}$$

Next, let $\mathbf{X}_{N+1}$ be the approximation of the state at $\tau_{N+1} = +1$. Because $\dot{\mathbf{x}}^N$ is a polynomial of degree at most $N - 1$, we have from the LG quadrature rule that

$$\mathbf{X}_{N+1} = \mathbf{X}_0 + \mathbf{w}^{\mathsf{T}}\mathbf{DX} = \mathbf{X}_0 + \mathbf{w}^{\mathsf{T}}\mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}). \tag{10}$$

The finite-dimensional nonlinear programming problem (NLP) arising from the LG discretization is then given as

minimize $\quad \Phi(\mathbf{X}_{N+1})$

$$\text{subject to} \quad \begin{cases} \mathbf{DX} = \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}), \\ \mathbf{X}_{N+1} = \mathbf{X}_0 + \mathbf{w}^{\mathsf{T}}\mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}), \\ \mathbf{X}_0 = \mathbf{x}_0, \end{cases} \tag{11}$$

where the NLP variables are $(\mathbf{X}_0, \dots, \mathbf{X}_{N+1})$ and $(\mathbf{U}_1, \dots, \mathbf{U}_N)$. The Lagrangian of the NLP (11) is

$$\mathcal{L} = \Phi(\mathbf{X}_{N+1}) + \langle \mathbf{\Lambda}^{\text{LG}}, \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) - \mathbf{DX} \rangle$$
$$+ \langle \mathbf{\Lambda}_{N+1}, \mathbf{w}^{\mathsf{T}}\mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) + \mathbf{X}_0 - \mathbf{X}_{N+1} \rangle,$$

where $\mathbf{\Lambda}$ is a Lagrange multiplier and $\mathbf{X}_0 = \mathbf{x}_0$ is the fixed initial condition. The Karush–Kuhn–Tucker (KKT) optimality conditions for the NLP of (11) are then given as

$$\mathbf{D}_{1:N}^{\mathsf{T}}\mathbf{\Lambda}^{\text{LG}} = \nabla_X \langle \mathbf{\Lambda}^{\text{LG}} + \mathbf{W1}\mathbf{\Lambda}_{N+1}, \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) \rangle, \tag{12}$$

$$\mathbf{\Lambda}_{N+1} = \nabla_X \Phi(\mathbf{X}_{N+1}), \tag{13}$$

$$\mathbf{0} = \nabla_U \langle \mathbf{W}^{-1}\mathbf{\Lambda}^{\text{LG}} + \mathbf{1}\mathbf{\Lambda}_{N+1}, \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) \rangle, \tag{14}$$

where $\mathbf{W}$ is an $N \times N$ diagonal matrix of LG weights.

4.1.1. LG transformed adjoint system

Analogous to Hager (2000), we now reformulate the KKT conditions of the NLP given in (11) so that they become a discretization of the first-order optimality conditions for the continuous control problem (2). First, let

$$\lambda = \mathbf{W}^{-1}\mathbf{\Lambda}^{\text{LG}} + \mathbf{1}\Lambda_{N+1}$$
$$\lambda_{N+1} = \Lambda_{N+1}. \tag{15}$$

Let $\mathbf{D}^\dagger$ be the $N \times (N + 1)$ matrix given by

$$D_{ij}^\dagger = -\frac{w_j}{w_i}D_{ji}, \quad (i, j) = 1, \dots, N, \tag{16}$$

$$D_{i,N+1}^\dagger = -\sum_{j=1}^{N} D_{ij}^\dagger, \quad i = 1, \dots, N. \tag{17}$$

Substituting (15) into (12)–(14) and simplifying, we obtain

$$\lambda_{N+1} = \nabla_X \Phi(\mathbf{X}_{N+1}), \tag{18}$$

$$-(\mathbf{D}_{1:N}^\dagger \lambda + \mathbf{D}_{N+1}^\dagger \lambda_{N+1}) = \nabla_X \langle \lambda, \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) \rangle, \tag{19}$$

$$\nabla_U \langle \lambda, \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}) \rangle = \mathbf{0}. \tag{20}$$

Comparing (18)–(20) to the continuous-time first-order optimality conditions (3)–(5), we observe that the transformed variable λ_{N+1} satisfies exactly the same conditions as the continuous costate $\lambda(t)$ evaluated at the endpoint. Also, the discrete and continuous necessary condition for the control has exactly the same structure. Below we show that the system (19) is a pseudospectral scheme for the costate equation. First, though, we note that the expression $\lambda_0 = \Lambda_{N+1} - \mathbf{D}_0^{\mathsf{T}}\mathbf{\Lambda}^{\text{LG}}$ provides an approximation to the continuous costate evaluated at $\tau = -1$. Then, applying (8), (15), (16) and (19), we have

$$\lambda_0 = \lambda_{N+1} + \sum_{j=1}^{N} w_j \nabla_X \langle \lambda_j, \mathbf{f}(\mathbf{X}_j, \mathbf{U}_j) \rangle. \tag{21}$$

Hence, λ_0 amounts to a quadrature approximation to the integral over $[-1, 1]$ of the adjoint equation. We now show that $\mathbf{D}^\dagger$ is a differentiation matrix and hence, the system (19) is a pseudospectral scheme for the costate equation.

Theorem 1. *The matrix* $\mathbf{D}^\dagger$ *defined in* (16) *and* (17) *is a differentiation matrix for the space of polynomials of degree N. More precisely, if q is a polynomial of degree at most N and* $\mathbf{q} \in \mathbb{R}^{N+1}$ *is the vector with ith component* $q_i = q(\tau_i), 1 \le i \le N + 1$, *then*

$$(\mathbf{D}^\dagger\mathbf{q})_i = \dot{q}(\tau_i), \quad 1 \le i \le N \ (q \text{ of degree } \le N).$$

Proof of Theorem 1. Let $\mathbf{E}$ denote the differentiation matrix defined in the statement of the theorem. That is, $\mathbf{E}$ is an $N \times (N+1)$ matrix with the property that for all $\mathbf{q} \in \mathbb{R}^{N+1}$, we have

$$(\mathbf{Eq})_i = \dot{q}(\tau_i), \quad 1 \le i \le N,$$

where q is the polynomial of degree at most N which satisfies $q_j = q(\tau_j), 1 \le j \le N + 1$. If p and q are smooth, real-valued functions with $q(1) = p(-1) = 0$, then integration by parts gives

$$\int_{-1}^{1} \dot{p}(\tau)q(\tau)d\tau = -\int_{-1}^{1} p(\tau)\dot{q}(\tau)d\tau. \tag{22}$$

Suppose p and q are polynomials of degree at most N, with $N \ge 1$; in this case, $\dot{p}q$ and $p\dot{q}$ are polynomials of degree at most $2N - 1$. Since Gauss quadrature is exact for polynomials of degree at most $2N - 1$, the integrals in (22) can be replaced by their quadrature equivalents to obtain

$$\sum_{j=1}^{N} w_j \dot{p}_j q_j = -\sum_{j=1}^{N} w_j p_j \dot{q}_j, \tag{23}$$

where $p_j = p(\tau_j)$ and $\dot{p}_j = \dot{p}(\tau_j), 1 \le i \le N$, p is any polynomial of degree at most N which vanishes at -1, and q is any polynomial

of degree at most N which vanishes at $+1$. A polynomial of degree N is uniquely defined by its value at $N + 1$ points. Let p be the polynomial of degree at most N which satisfies $p(-1) = 0$ and $p_j = p(\tau_j)$, $1 \le j \le N$. Let q be the polynomial of degree at most N which satisfies $q(+1) = 0$ and $q_j = q(\tau_j)$, $1 \le j \le N$. Substituting $\dot{\mathbf{p}} = \mathbf{Dp}$ and $\dot{\mathbf{q}} = \mathbf{Eq}$ in (23) gives

$$(\mathbf{WDp})^{\mathsf{T}}\mathbf{q}_{1:N} = -(\mathbf{Wp}_{1:N})^{\mathsf{T}}\mathbf{Eq},$$

where $\mathbf{W}$ is the diagonal matrix of quadrature weights. Since the first component of $\mathbf{p}$ and the last component of $\mathbf{q}$ vanish, this reduces to

$$\mathbf{p}_{1:N}^{\mathsf{T}}(\mathbf{D}_{1:N}^{\mathsf{T}}\mathbf{W} + \mathbf{WE}_{1:N})\mathbf{q}_{1:N} = 0.$$

Since $\mathbf{p}_{1:N}$ and $\mathbf{q}_{1:N}$ are arbitrary, we deduce that

$$\mathbf{D}_{1:N}^{\mathsf{T}}\mathbf{W} + \mathbf{WE}_{1:N} = \mathbf{0},$$

which implies that

$$E_{ij} = -\frac{w_j}{w_i}D_{ji}, \quad (i, j) = 1, \dots, N. \tag{24}$$

Since $\mathbf{E}$ is a differentiation matrix, $\mathbf{E1} = \mathbf{0}$, which yields

$$E_{i,N+1} = -\sum_{j=1}^{N} E_{ij}, \quad 1 \le i \le N. \tag{25}$$

Comparing (16) with (24) and (17) with (25), we see that $\mathbf{D}^{\dagger} = \mathbf{E}$. □

Thus we have shown that the transformed KKT conditions are related to a pseudospectral discretization of the continuous costate equation. Furthermore, the differentiation matrices of the state and costate discretizations are based on the derivatives of polynomials of degree N. Note that either $\mathbf{D}$ or $\mathbf{D}^{\dagger}$ operate on polynomial values to give the derivative at the collocation points. However, $\mathbf{D}$ operates on the polynomial values $p(\tau_i)$, $0 \le i \le N$, while $\mathbf{D}^{\dagger}$ operates on the polynomial values $p(\tau_i)$, $1 \le i \le N + 1$.

4.1.2. Integral formulation using LG collocation

We will now show that the LG pseudospectral discretization of the state equation has an equivalent integrated formulation. Let p be any polynomial of degree at most N. By the construction of the $N \times (N + 1)$ matrix $\mathbf{D}$, we have $\mathbf{Dp} = \dot{\mathbf{p}}$ where

$$\begin{aligned} p_i &= p(\tau_i), \quad 0 \le i \le N, \\ \dot{p}_i &= \dot{p}(\tau_i), \quad 1 \le i \le N. \end{aligned} \tag{26}$$

Multiplying the identity $\dot{\mathbf{p}} = \mathbf{Dp} = \mathbf{D}_0 p_0 + \mathbf{D}_{1:N}\mathbf{p}_{1:N}$ by $\mathbf{D}_{1:N}^{-1}$ and utilizing Proposition 2 gives

$$p_i = p_0 + \left(\mathbf{D}_{1:N}^{-1}\dot{\mathbf{p}}\right)_i, \quad 1 \le i \le N. \tag{27}$$

Next, we obtain a different expression for $p_i - p_0$ based on the integration of the interpolant of the derivative. First, set $K = 1$ in (1) and let $L_j^{\dagger}(\tau)$ be the resulting Lagrange polynomial basis. Notice that the Lagrange polynomials L_j defined in (6) are degree N while the Lagrange polynomials $L_j^{\dagger}$ are degree $N - 1$. Then because $\dot{p}$ is a polynomial of degree at most $N - 1$, it can be interpolated exactly by the Lagrange polynomials $L_j^{\dagger}$:

$$\dot{p} = \sum_{j=1}^{N} \dot{p}_j L_j^{\dagger}(\tau). \tag{28}$$

Integrating $\dot{p}$ from -1 to τ_i, we obtain

$$\begin{aligned} p(\tau_i) &= p(-1) + \sum_{j=1}^{N} \dot{p}_j A_{ij}, \\ A_{ij} &= \int_{-1}^{\tau_i} L_j^{\dagger}(\tau)\mathrm{d}\tau, \quad 1 \le i \le N. \end{aligned} \tag{29}$$

Utilizing the notation (26), we have

$$p_i = p_0 + (\mathbf{A}\dot{\mathbf{p}})_i, \quad 1 \le i \le N. \tag{30}$$

The relations (27) and (30) are satisfied for any polynomial of degree at most N. We equate (27) and (30) to obtain

$$\mathbf{A}\dot{\mathbf{p}} = \mathbf{D}_{1:N}^{-1}\dot{\mathbf{p}}.$$

Choose $\dot{\mathbf{p}}$ from the columns of the identity matrix to deduce that $\mathbf{A} = \mathbf{D}_{1:N}^{-1}$. Multiply (9) by $\mathbf{A} = \mathbf{D}_{1:N}^{-1}$ and utilize Proposition 2 to obtain

$$\mathbf{X}_i = \mathbf{X}_0 + \mathbf{A}_i\mathbf{F}(\mathbf{X}^{\mathrm{LG}}, \mathbf{U}^{\mathrm{LG}}), \quad 1 \le i \le N + 1, \tag{31}$$

where $\mathbf{A}_i$ is the ith row of $\mathbf{A} = \mathbf{D}_{1:N}^{-1}$, $1 \le i \le N$, and $\mathbf{A}_{N+1} = \mathbf{w}^{\mathsf{T}}$. Hence, the differential form of the state equation $\mathbf{DX} = \mathbf{F}(\mathbf{X}^{\mathrm{LG}}, \mathbf{U}^{\mathrm{LG}})$ and the integral form of (31) are *equivalent*; the elements of $\mathbf{A}$ are the integrals of the Lagrange basis $L_j^{\dagger}$, while the elements of $\mathbf{D}$ in the differential form are the derivatives of the Lagrange basis L_i defined in (7). Note that the integral form of LG collocation provides an approximation to the state at each of the LG points *plus* the terminal point. We call the differential form of LG collocation derived in this paper the *Gauss pseudospectral method*.

Similar to the derivation of (31), we can also formulate an integrated version of the discrete costate dynamics:

$$\lambda_i = \lambda_{N+1} - \mathbf{B}_i\nabla_X\langle\lambda, \mathbf{F}(\mathbf{X}, \mathbf{U})\rangle, \quad 0 \le i \le N, \tag{32}$$

where $\mathbf{B}_0 = -\mathbf{w}^{\mathsf{T}}$, $\mathbf{B}_i$ for $1 \le i \le N$ is the ith row of $\mathbf{B} = (\mathbf{D}_{1:N}^{\dagger})^{-1}$, and

$$B_{ij} = \int_{+1}^{\tau_i} L_j^{\dagger}(\tau)\mathrm{d}\tau.$$

A compact representation of the LG pseudospectrally discretized first-order optimality conditions are given by (18), (20), (31) and (32), which we collect below:

$$\mathbf{X}_i = \mathbf{X}_0 + \mathbf{A}_i\mathbf{F}(\mathbf{X}, \mathbf{U}), \quad 1 \le i \le N + 1,$$
$$\lambda_i = \lambda_{N+1} - \mathbf{B}_i\nabla_X\langle\lambda, \mathbf{F}(\mathbf{X}, \mathbf{U})\rangle, \quad 0 \le i \le N,$$
$$\lambda_{N+1} = \nabla_X\Phi(\mathbf{X}_{N+1}),$$
$$\mathbf{0} = \nabla_U\langle\lambda, \mathbf{F}(\mathbf{X}, \mathbf{U})\rangle.$$

Thus, we have shown that the differential and integral forms of the state and costate dynamics in the Gauss pseudospectral method are *equivalent*.

4.2. Collocation at LGR points

Consider collocation at the N *flipped* LGR points $(\tau_1, \dots, \tau_N)$ (where $\tau_N = +1$) on $[-1, +1]$ and let $\tau_0 = -1$ be a noncollocated initial point. Setting $K = 0$ in (1), the state is approximated by a polynomial of degree at most N as

$$\mathbf{x}^N(\tau) = \sum_{i=0}^{N} \mathbf{X}_i L_i(\tau). \tag{33}$$

It is important to observe that the series (33) includes the Lagrange polynomial associated with the *noncollocated* point $\tau_0 = -1$. Differentiating (33) and evaluating the result at the kth collocation point, τ_k, gives

$$\dot{\mathbf{x}}^N(\tau_k) = \sum_{i=0}^{N} \mathbf{X}_i\dot{L}_i(\tau_k) = \sum_{i=0}^{N} D_{ki}\mathbf{X}_i, \quad D_{ki} = \dot{L}_i(\tau_k). \tag{34}$$

The $N \times (N + 1)$ *non-square* matrix $\mathbf{D}$ is called the *Radau pseudospectral differentiation matrix*. Similar to the result for LG collocation, the matrix $\mathbf{D}$ has one more column than row due to the Lagrange polynomial $L_0(\tau)$ associated with the noncollocated point $\tau_0 = -1$. In a manner similar to that given in Garg et al. (2009), the following properties can be shown for the Radau differentiation matrix: (a) $\mathbf{D}_{1:N}$ is nonsingular and (b) $\mathbf{D}_0 = -\mathbf{D}_{1:N}\mathbf{1}$ or equivalently, $-\mathbf{D}_{1:N}^{-1}\mathbf{D}_0 = \mathbf{1}$. Collocating the dynamics at the N

flipped LGR points, we have

$$\mathbf{DX} = \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}). \tag{35}$$

The finite-dimensional nonlinear programming problem (NLP) associated with the LGR method is then given as

minimize $\quad \Phi(\mathbf{X}_N)$

subject to $\quad \mathbf{DX} = \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}), \qquad \mathbf{X}_0 = \mathbf{x}_0. \tag{36}$

The Lagrangian of the NLP (36) is then given as

$$\mathcal{L} = \Phi(\mathbf{X}_N) + \langle \mathbf{\Lambda}^{\text{LGR}}, \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) - \mathbf{DX} \rangle + \langle \mathbf{\mu}, \mathbf{x}_0 - \mathbf{X}_0 \rangle,$$

where $\mathbf{\Lambda}$ and $\mathbf{\mu}$ are Lagrange multipliers. Unlike the LG scheme, we introduce the multiplier $\mathbf{\mu}$ corresponding to the initial condition– if we were to treat $\mathbf{X}_0$ as fixed in the Radau Lagrangian, then there would be an asymmetry since $\mathbf{U}_0$, the control corresponding to the $\tau = -1$, appears in the Radau discretization. The KKT optimality conditions for the NLP of (36) are then given as

$$\mathbf{\mu} = -\mathbf{D}_0^\mathsf{T} \mathbf{\Lambda}^{\text{LGR}}, \tag{37}$$

$$\nabla_X \langle \mathbf{\Lambda}^{\text{LGR}}, \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) \rangle = \mathbf{D}_{1:N}^\mathsf{T} \mathbf{\Lambda}^{\text{LGR}}, \tag{38}$$

$$\nabla(\Phi(\mathbf{X}_N)) + \langle \mathbf{\Lambda}_N, \mathbf{f}(\mathbf{X}_N, \mathbf{U}_N) \rangle = \mathbf{D}_N^\mathsf{T} \mathbf{\Lambda}^{\text{LGR}}, \tag{39}$$

$$\nabla_U \langle \mathbf{\Lambda}^{\text{LGR}}, \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) \rangle = \mathbf{0}. \tag{40}$$

The system dynamics in (36) can be rewritten

$$\mathbf{D}_{1:N} \mathbf{X}_{1:N} = \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) - \mathbf{D}_0 \mathbf{x}_0. \tag{41}$$

Similarly, the costate equations (38) and (39) can be rewritten

$$\mathbf{D}_{1:N}^\mathsf{T} \mathbf{\Lambda}^{\text{LGR}} = \nabla_X \langle \mathbf{\Lambda}^{\text{LGR}}, \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) \rangle + \mathbf{e}_N \nabla \Phi(\mathbf{X}_N), \tag{42}$$

where $\mathbf{e}_N$ is the last column of the identity matrix. Finally, as shown in Garg et al. (2009), the $N \times N$ matrix $\mathbf{D}_{1:N}$ appearing on the left-hand side of (41) and (42) is *invertible* (see Garg et al. (2009) for the proof).

4.2.1. LGR transformed adjoint system

Analogous to Garg et al. (2009), the transformed adjoint variables corresponding to Radau collocation can be expressed in terms of the $N \times n$ matrix $\mathbf{\lambda}$ and the row vector $\mathbf{\lambda}_0$,

$$\mathbf{\lambda} = \mathbf{W}^{-1} \mathbf{\Lambda}^{\text{LGR}}, \tag{43}$$

$$\mathbf{\lambda}_0 = -\mathbf{D}_0^\mathsf{T} \mathbf{\Lambda}^{\text{LGR}} \tag{44}$$

where $\mathbf{W}$ is a diagonal matrix of LGR weights. Let $\mathbf{D}^\dagger$ be an $N \times N$ matrix defined as follows:

$$D_{NN}^\dagger = -D_{NN} + \frac{1}{w_N} \quad \text{and} \quad D_{ij}^\dagger = -\frac{w_j}{w_i} D_{ji} \quad \text{otherwise}. \tag{45}$$

Using the transformations of (43) and (44), together with $\mathbf{D}^\dagger$, we obtain the following transformed KKT conditions for the flipped LGR discretization (see Garg et al. (2009) for details):

$$\mathbf{\lambda}_0 = \mathbf{\mu}, \tag{46}$$

$$\nabla \Phi(\mathbf{X}_N) = \mathbf{\lambda}_0 - \sum_{i=1}^{N} w_i \nabla_X \langle \mathbf{\lambda}_i, \mathbf{f}(\mathbf{X}_i, \mathbf{U}_i) \rangle, \tag{47}$$

$$\mathbf{D}^\dagger \mathbf{\lambda} = -\nabla_X \langle \mathbf{\lambda}, \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) \rangle + \frac{\mathbf{e}_N}{w_N} (\mathbf{\lambda}_N - \nabla \Phi(\mathbf{X}_N)), \tag{48}$$

$$\mathbf{0} = \nabla_U \langle \mathbf{\lambda}, \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}) \rangle. \tag{49}$$

Observe that the discrete and continuous necessary condition for the control [compare (5) and (49)] have exactly the same structure. Moreover, the transformed variable $\mathbf{\lambda}_0$ in (46), corresponding to the continuous costate $\mathbf{\lambda}(-1)$, is free, exactly as in the continuous optimality conditions (3)–(5). The summation in (47) approximates the integral of $\dot{\mathbf{\lambda}}$ over the interval $[-1, 1]$. Hence, the right

side of (47) approximates $\mathbf{\lambda}(1)$, which corresponds to $\mathbf{\lambda}_N$, and the condition (47) is a subtle way of enforcing the equality $\nabla \Phi(\mathbf{X}_N) = \mathbf{\lambda}_N$, in an approximate sense. Moreover, when $\nabla \Phi(\mathbf{X}_N) = \mathbf{\lambda}_N$, then the last term in the discrete dynamics (48) vanishes. Finally, as has been shown in Garg et al. (2009), the system (48), with the last term dropped, is a pseudospectral scheme for the costate equation. More precisely, if p is a polynomial of degree at most $N - 1$ and $p_j = p(\tau_j)$, $1 \le j \le N$, then

$$(\mathbf{D}^\dagger \mathbf{p})_i = \dot{p}(\tau_i), \quad 1 \le i \le N \ (p \text{ of degree } \le N - 1). $$

Thus we have shown that the transformed KKT conditions are related to a pseudospectral discretization of the continuous costate equation. However, the differentiation matrix $\mathbf{D}^\dagger$ in the costate discretization is connected with the derivatives of polynomials of degree at most $N - 1$, while the differentiation matrix in the state discretization is based on the derivatives of polynomials of degree N.

4.2.2. Integral formulation using LGR collocation

In Garg et al. (2009) it was shown that the pseudospectral method using the standard LGR points has an equivalent integrated formulation. The flipped LGR points possess the same integral/differential property given as follows.

Suppose now that p is any polynomial of degree at most N. Then, by the construction of the $N \times (N + 1)$ differentiation matrix $\mathbf{D}$, we have $\mathbf{Dp} = \dot{\mathbf{p}}$ where

$$p_i = p(\tau_i), \quad 0 \le i \le N, \qquad \dot{p}_i = \dot{p}(\tau_i), \quad 1 \le i \le N. \tag{50}$$

Multiplying the identity $\dot{\mathbf{p}} = \mathbf{Dp} = \mathbf{D}_0 p_0 + \mathbf{D}_{1:N} \mathbf{p}_{1:N}$ by $\mathbf{D}_{1:N}^{-1}$ and utilizing the fact that $\mathbf{D}_0 = -\mathbf{D}_{1:N} \mathbf{1}$, we obtain

$$p_i = p_0 + (\mathbf{D}_{1:N}^{-1} \dot{\mathbf{p}})_i, \quad 1 \le i \le N. \tag{51}$$

Next, set $K = 1$ in (1) and let $L_i^\dagger(\tau)$ be the resulting Lagrange polynomial basis. Then $\dot{p}$ can be interpolated exactly as

$$\dot{p}(\tau) = \sum_{j=1}^{N} \dot{p}_j L_j^\dagger(\tau). $$

Integrating from -1 to τ_i, we obtain

$$p_i = p_0 + (\mathbf{A}\dot{\mathbf{p}})_i, \quad 1 \le i \le N, \tag{52}$$

$$A_{ij} = \int_{-1}^{\tau_i} L_j^\dagger(\tau) \, d\tau, \quad 1 \le i, j \le N. \tag{53}$$

By (51) and (52), we have $\mathbf{A} = \mathbf{D}_{1:N}^{-1}$. Furthermore, by (41) and the fact that $\mathbf{D}_{1:N}^{-1} \mathbf{D}_0 = -\mathbf{1}$,

$$\mathbf{X}_i = \mathbf{X}_0 + \mathbf{A}_i \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}), \quad 1 \le i \le N, \tag{54}$$

where $\mathbf{A}_i$ is the ith row of $\mathbf{A}$. Hence, the differential form of the state equation $\mathbf{DX} = \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}})$ is equivalent to the integrated form (54), where the elements of $\mathbf{A}$ are integrals of the Lagrange basis functions $L_j^\dagger$ defined in (53) while the elements of $\mathbf{D}$ in the differential form are the derivatives of the Lagrange basis function L_i defined in (34). We call the differential form of LGR collocation derived in this paper the *Radau pseudospectral method*.

4.3. Collocation at LGL points

Consider now collocation using the N LGL collocation points. Unlike either Gauss or Radau collocation, where additional nodes were introduced at the endpoints, there is no need for additional nodes with LGL since the endpoint -1 and $+1$ are collocation points. Hence, the state at the endpoints naturally appear in the discrete problem. Setting $K = 1$ in (1), the state is approximated

by a polynomial of degree at most $N - 1$ as (Elnagar et al., 1995; Fahroo & Ross, 2001)

$$\mathbf{x}^N(\tau) = \sum_{i=1}^{N} \mathbf{X}_i L_i(\tau). \tag{55}$$

Differentiating the series and evaluating at the collocation point τ_k gives (Elnagar et al., 1995; Fahroo & Ross, 2001)

$$\dot{\mathbf{x}}^N(\tau_k) = \sum_{i=1}^{N} \mathbf{X}_i \dot{L}_i(\tau_k) = \sum_{i=1}^{N} D_{ki} \mathbf{X}_i, \quad D_{ki} = \dot{L}_i(\tau_k). \tag{56}$$

The $N \times N$ *square* matrix $\mathbf{D}$ is called the *Lobatto pseudospectral differentiation matrix*. In the LGL case the matrix $\mathbf{D}$ is square because the collocation points are the same as the approximation points (that is, the endpoints are also collocation points). Note that the Lobatto differentiation matrix is *singular* since $\mathbf{D1} = \mathbf{0}$.

The finite-dimensional NLP corresponding to the LGL pseudospectral method is then given as

$$\text{minimize} \quad \Phi(\mathbf{X}_N)$$
$$\text{subject to} \quad \mathbf{DX}^{\text{LGL}} = \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}), \quad \mathbf{X}_1 = \mathbf{x}_0. \tag{57}$$

The Lagrangian associated with (57) is

$$\mathcal{L} = \Phi(\mathbf{X}_N) + \langle \mathbf{\Lambda}^{\text{LGL}}, \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}) - \mathbf{DX}^{\text{LGL}} \rangle + \langle \mathbf{\mu}, \mathbf{x}_0 - \mathbf{X}_1 \rangle.$$

The KKT optimality conditions for the NLP of (57) are then given as (Fahroo & Ross, 2001)

$$\nabla \langle \mathbf{\Lambda}_1, \mathbf{f}(\mathbf{X}_1, \mathbf{U}_1) \rangle - \mathbf{D}_1^{\mathsf{T}} \mathbf{\Lambda}^{\text{LGL}} = \mathbf{\mu}, \tag{58}$$

$$\mathbf{D}_N^{\mathsf{T}} \mathbf{\Lambda}^{\text{LGL}} - \nabla_X \langle \mathbf{\Lambda}_N, \mathbf{f}(\mathbf{X}_N, \mathbf{U}_N) \rangle = \nabla_X \Phi(\mathbf{X}_N) \tag{59}$$

$$\nabla_X \langle \mathbf{\Lambda}_{2:N-1}, \mathbf{F}(\mathbf{X}_{2:N-1}, \mathbf{U}_{2:N-1}) \rangle = \mathbf{D}_{2:N-1}^{\mathsf{T}} \mathbf{\Lambda}_{2:N-1}, \tag{60}$$

$$\nabla_U \langle \mathbf{\Lambda}^{\text{LGL}}, \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}) \rangle = \mathbf{0}. \tag{61}$$

4.3.1. LGL transformed adjoint system

Using an approach nearly identical to that used for LGR collocation, the KKT conditions of the NLP are now reformulated so that they become a discretization of the first-order optimality conditions for the continuous control problem (2). Let w_i, $1 \le i \le N$, be the LGL quadrature weights; the transformed adjoint is the $N \times n$ matrix $\mathbf{\lambda}$ defined by Fahroo and Ross (2001)

$$\lambda_i = \mathbf{\Lambda}_i / w_i, \quad 1 \le i \le N. \tag{62}$$

Let $\mathbf{D}^{\dagger}$ be the $N \times N$ matrix defined as follows:

$$D_{ii}^{\dagger} = D_{ii}, \quad 2 \le i \le N - 1$$
$$D_{11}^{\dagger} = -D_{11} - \frac{1}{w_1}$$
$$D_{NN}^{\dagger} = -D_{NN} + \frac{1}{w_N} \tag{63}$$
$$D_{ij}^{\dagger} = -\frac{w_j}{w_i} D_{ji}, \quad 1 \le i, j \le N, \ i \ne j.$$

The substitutions (62) and (63) in (59)–(60) lead to the following transformed costate equation:

$$\mathbf{D}^{\dagger} \mathbf{\lambda} = -\nabla_X \langle \mathbf{\lambda}, \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}) \rangle + \frac{\mathbf{e}_1}{w_1}(\mathbf{\mu} - \mathbf{\lambda}_1)$$
$$+ \frac{\mathbf{e}_N}{w_N}(\mathbf{\lambda}_N - \nabla_X \Phi(\mathbf{X}_N)), \tag{64}$$

where $\mathbf{e}_1$ and $\mathbf{e}_N$ are the first and last columns of the $N \times N$ identity matrix. Finally, (61) implies that

$$\nabla_U \langle \mathbf{\lambda}, \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}) \rangle = \mathbf{0}. \tag{65}$$

Observe that the continuous and discrete control necessary conditions (5) and (65) again have the same structure. The discrete and continuous adjoint of (4) and (64), however, are quite different from one another because the continuous endpoint condition (3)

is not present in the discrete system (64). Finally, it has been shown in Fahroo and Ross (2006) that $\mathbf{D}^{\dagger} = \mathbf{D}$ for LGL collocation, thus making $\mathbf{D}^{\dagger}$ a differentiation matrix connected with the LGL quadrature points.

4.3.2. Integral formulation using LGL collocation

An integral analog of LGL collocation can be developed as follows: Given a polynomial p of degree at most $N - 1$, its derivative $\dot{p}$ is a polynomial of degree at most $N - 2$. Set $K = 1$ in (1) and let $L_j^{\dagger}(\tau)$ be the Lagrange polynomial basis used to interpolate $\dot{p}$. Then $\dot{p}$ can be interpolated exactly using $L_j^{\dagger}(\tau)$ as

$$\dot{p}(\tau) = \sum_{j=1}^{N} \dot{p}_j L_j^{\dagger}(\tau), \quad \dot{p}_j = \dot{p}(\tau_j).$$

Again, we integrate from -1 to τ_i to obtain the relation

$$p(\tau_i) = p(-1) + \sum_{j=1}^{N} \dot{p}_j A_{ij},$$
$$A_{ij} = \int_{-1}^{\tau_i} L_j^{\dagger}(\tau) \, d\tau, \quad 2 \le i \le N. \tag{66}$$

If this is applied to each component of the state variable, then we have

$$\mathbf{X}_i = \mathbf{X}_0 + \mathbf{A}_i \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}), \quad 2 \le i \le N, \tag{67}$$

where $\mathbf{A}_i$ is the ith row of $\mathbf{A}$. Note, though, that the integrated scheme (67) is not equivalent to the original LGL collocation system, it is an altogether different scheme. In fact, the original LGL discrete system contains N equations, one equation for each collocation point while (67) represents $N - 1$ equations because the first row of the matrix $\mathbf{A}$ is zero. It is noted that the Lobatto integration matrix given (67) is the same as that found in Axelsson (1964).

5. Unified view of pseudospectral methods

5.1. State endpoint approximation

With each of the collocation schemes, the state at the final time is approximated by a quadrature rule associated with the collocation points. For LG collocation, this quadrature rule is contained in the constraint (10):

$$\mathbf{X}_{N+1} = \mathbf{X}_0 + \mathbf{w}_{\text{LG}}^{\mathsf{T}} \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}}). \tag{68}$$

Here $\mathbf{X}_0$ and $\mathbf{X}_{N+1}$ are the approximations to the state at $\tau = -1$ and $\tau = +1$ respectively, and $\mathbf{w}_{\text{LG}}^{\mathsf{T}} \mathbf{F}(\mathbf{X}^{\text{LG}}, \mathbf{U}^{\text{LG}})$ is a quadrature approximation to the integral $\int_{-1}^{+1} \dot{\mathbf{x}}(t) \, dt$.

Now consider the Lobatto differentiation matrix $\mathbf{D}^{\text{LGL}}$ and the corresponding quadrature weight $\mathbf{w}_{\text{LGL}}$. By the exactness of the LGL quadrature rule, we have

$$(\mathbf{w}_{\text{LGL}}^{\mathsf{T}} \mathbf{D}^{\text{LGL}})_j = \int_{-1}^{+1} \dot{L}_j^{\dagger}(t) \, dt = \begin{cases} -1, & j = 1, \\ 0, & 2 \le j \le N - 1, \\ +1, & j = N \end{cases}$$

where j corresponds to the jth element in the row vector $\mathbf{wD}$. Hence, multiplying each side of the LGL state equation $\mathbf{DX}^{\text{LGL}} = \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}})$ by $\mathbf{w}_{\text{LGL}}^{\mathsf{T}}$ yields the identity

$$\mathbf{X}_N = \mathbf{X}_1 + \mathbf{w}_{\text{LGL}}^{\mathsf{T}} \mathbf{F}(\mathbf{X}^{\text{LGL}}, \mathbf{U}^{\text{LGL}}). \tag{69}$$

For Lobatto collocation, $\mathbf{X}_1$ and $\mathbf{X}_N$ correspond to the state at $\tau = -1$ and $\tau = +1$ respectively. Hence, the Lobatto identity (69) is analogous to the Gauss identity (68).

Finally, let us consider the LGR collocation scheme. Since the Lagrange polynomials in (33) start from $i = 0$, it follows that for the Radau differentiation matrix $\mathbf{D}^{\text{LGR}}$ and the corresponding

quadrature weights $\mathbf{w}_{\text{LGR}}$, we have

$$(\mathbf{w}_{\text{LGR}}^{\mathsf{T}}\mathbf{D}^{\text{LGR}})_j = \int_{-1}^{+1} \dot{L}_j(t)\,\mathrm{d}t = \begin{cases} -1, & j = 0, \\ 0, & 1 \le j \le N-1, \\ +1, & j = N. \end{cases}$$

As a result, multiplying each side of the LGR state equation $\mathbf{D}\mathbf{X}^{\text{LGR}} = \mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}})$ by $\mathbf{w}_{\text{LGR}}^{\mathsf{T}}$ yields the identity

$$\mathbf{X}_N = \mathbf{X}_0 + \mathbf{w}_{\text{LGR}}^{\mathsf{T}}\mathbf{F}(\mathbf{X}^{\text{LGR}}, \mathbf{U}^{\text{LGR}}). \tag{70}$$

For Radau collocation, $\mathbf{X}_0$ and $\mathbf{X}_N$ correspond to the state at $\tau = -1$ and $\tau = +1$ respectively. Hence, each collocation scheme ultimately leads to a state approximation at the terminal time based on the scheme's quadrature rule [see (68)–(70)].

With each of the schemes, the initial state is introduced in the discretization through interpolation. In particular, for either LG or LGR collocation, the initial value of the state variable appears as the coefficient of L_0 in the expansion (6). Here L_0 is the Lagrange basis function associated with the noncollocated point $\tau_0 = -1$. For LGL collocation, the initial value of the state appears as the coefficient of $L_1^{\dagger}$ in (55). In this case, $L_1^{\dagger}$ is the Lagrange basis function associated with the collocated Lobatto point $\tau_1 = -1$.

5.2. Map from control to state

Another interesting feature of the three pseudospectral schemes concerns the discrete mapping from the control to the state. Consider the continuous-time dynamics

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{u}), \tag{71}$$

where $\mathbf{x}(\tau) \in \mathbb{R}^n$ is the state and $\mathbf{u}(\tau) \in \mathbb{R}^m$ is the control. When either the LG or LGR method is used to discretize the continuous dynamics, we obtain a system of the form $\mathbf{D}\mathbf{X} = \mathbf{D}_0\mathbf{X}_0 + \mathbf{D}_{1:N}\mathbf{X}_{1:N} = \mathbf{F}(\mathbf{U})$, where $\mathbf{D}$ is the Gauss/Radau differentiation matrix and $\mathbf{D}_0$ is the first column of $\mathbf{D}$. We have already shown that $\mathbf{D}_{1:N}$ is invertible and that $\mathbf{D}_{1:N}^{-1}\mathbf{D}_0 = -\mathbf{1}$. Consequently, we have

$$\mathbf{X}_{1:N} = \mathbf{1}\mathbf{X}_0 + \mathbf{D}_{1:N}^{-1}\mathbf{F}(\mathbf{U}). \tag{72}$$

If the initial condition is given, then (72) yields a unique discrete state $\mathbf{X}_{1:N}$ for each choice of the control $\mathbf{U}$, analogous to the differential equation (71). For the Lobatto scheme, the dynamics of (71) are approximated as

$$\mathbf{D}^{\text{LPM}}\mathbf{X}_{1:N} = \mathbf{F}(\mathbf{U}), \tag{73}$$

where we recall that the matrix $\mathbf{D}^{\text{LPM}}$ is square and *singular*. Consequently, (73) will only have a solution if $\mathbf{F}(\mathbf{U})$ lies in the column space of $\mathbf{D}^{\text{LPM}}$. And if $\mathbf{F}(\mathbf{U})$ lies in the column space of $\mathbf{D}^{\text{LPM}}$, there are an infinite family of states satisfying (73) corresponding to the null space of $\mathbf{D}^{\text{LPM}}$. Hence, the correspondence between control and state with Lobatto is much more complex than with either Gauss or Radau due to the singularity of the Lobatto differentiation matrix.

5.3. Costate dynamics

The three pseudospectral schemes treat the costate endpoint conditions quite differently. For LG collocation, the endpoint condition appears explicitly in the transformed adjoint condition (18). For LGR collocation, the initial condition appears explicitly in (46) while the terminal condition appears in the approximate form (47). For LGL collocation, the boundary conditions are embedded inside the costate dynamics (64).

There is a fundamental difference between the LGL costate dynamics and the costate dynamics for LGR and LG. The discrete costate dynamics form a linear system of equations in $\boldsymbol{\lambda}$; for LG and LGR, the equations are typically invertible, while for LGL, the matrix in the equations has a null space. In particular, for LG the discrete costate dynamics are defined by Eqs. (18)–(19), which represent $N + 2$ equations in the $N + 2$ unknowns $\boldsymbol{\lambda}_0, \ldots, \boldsymbol{\lambda}_{N+1}$. For LGR

the costate dynamics are defined by (47)–(48), which represent $N + 1$ equations in the $N + 1$ unknowns $\boldsymbol{\lambda}_0, \ldots, \boldsymbol{\lambda}_N$. The LGL costate dynamics is given by (64), which represents N equations in $N + 1$ unknowns $\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_N, \boldsymbol{\mu}$. Hence, the matrix of the linear system has a null space and there exists an infinite number of solutions to the LGL costate dynamics. The dimension of the null space is at least n since $\boldsymbol{\lambda}_i \in \mathbb{R}^n$.

Despite the null space in the LGL costate dynamics, a wealth of numerical examples, including the two that follow in Section 6, have been published in the literature (Fahroo & Ross, 2001, 2006, 2008a,b; Gong, Ross, Kang, & Fahroo, 2008; Ross & Fahroo, 2008). These examples demonstrate that the LGL scheme leads to convergent approximations to the state and control variable. However, due to the null space in the discrete costate dynamics, the concept of convergence for the costate is open to interpretation. Gong et al. (2008), show in their "Covector Mapping Theorem" that any solution to the first-order optimality conditions (3)–(5) for the continuous control problem, approximately satisfies the first-order optimality conditions for the discrete LGL problem (57), and the error tends to zero as $N \to \infty$. This shows that among the infinite set of solutions associated with the discrete costate dynamics, there exists a good approximation to the continuous costate. Moreover, in Gong et al. (2008) the authors propose a *closure condition* for selecting a good approximation to the continuous costate from among the infinite set of solutions to the costate dynamics. In the context of our control problem (2), the closure condition amounts to choosing a solution to the discrete costate Eq. (64) which satisfies the conditions $\|\boldsymbol{\lambda}_1 - \boldsymbol{\mu}\| \le \delta$ and $\|\boldsymbol{\lambda}_N - \nabla_X \Phi(\mathbf{X}_N)\| \le \delta$, where δ is some given error tolerance. In Theorem 4 of Gong et al. (2008) it is shown that an asymptotically valid choice for δ is of the form $\delta = N^{(1.5-m)}$, where $m \ge 4$, independent of N, depends on the number of derivatives of smoothness of an optimal solution. In practice, the null space for the LGL costate dynamics is often observed to be highly oscillatory. As a result, page 276 of Fahroo and Ross (2001) suggested that the computed costate can be post-processed using a filter to obtain a good approximation to the continuous costate.

6. Example

In order to demonstrate the key characteristics of the Gauss, Radau, and Lobatto pseudospectral methods, consider the following optimal control problem: minimize $J = -y(2)$ subject to the dynamic constraint $\dot{y} = \frac{5}{2}(-y + yu - u^2)$ and the initial condition $y(0) = 1$. The solution to this optimal control problem is $y^*(t) = 4/a(t)$, $u^*(t) = y^*(t)/2$, and $\lambda_y^*(t) = -\exp(2\ln(a(t)) - 5t/2)/b$, where $a(t) = 1 + 3\exp(5t/2)$ and $b = \exp(-5) + 6 + 9\exp(5)$.

The example was solved using the Gauss, Radau, and Lobatto pseudospectral methods using the NLP solver SNOPT with optimality and feasibility tolerances of 10^{-15} and 2×10^{-15}, respectively. For each method, the initial guess was the exact solution to the continuous optimal control problem. Figs. 1–3 show the base 10 logarithm of the L_∞-norm errors for the state, control, and costate, respectively. Fig. 1 shows that the state error using either the Gauss or Radau pseudospectral methods is approximately two to four orders of magnitude smaller than the state for the Lobatto pseudospectral method for $N \le 15$. In Fig. 2, it is seen that the Gauss and Radau control is between two and seven orders of magnitude more accurate than the corresponding Lobatto controls for $N \le 15$. For $N > 15$, the Gauss and Radau state and control errors drop to machine precision (approximately 10^{-16}), while the Lobatto errors achieve machine precision at $N = 30$.

In Fig. 3 it is seen that the Gauss and Radau costate errors decrease to near the optimizer tolerances (approximately 10^{-15}) while the Lobatto costate error remains above 10^{-2}. Fig. 4 shows an enlarged plot of the exact costate and the approximations generated by all three methods for $N = 30$. It is seen that
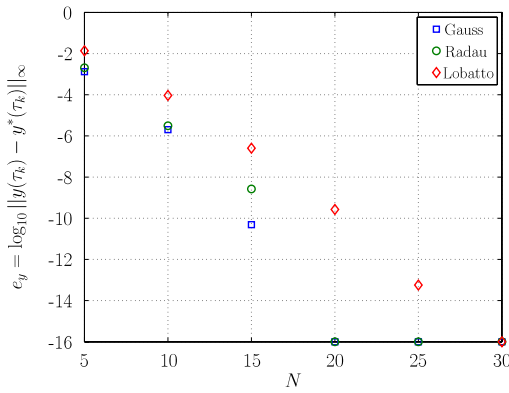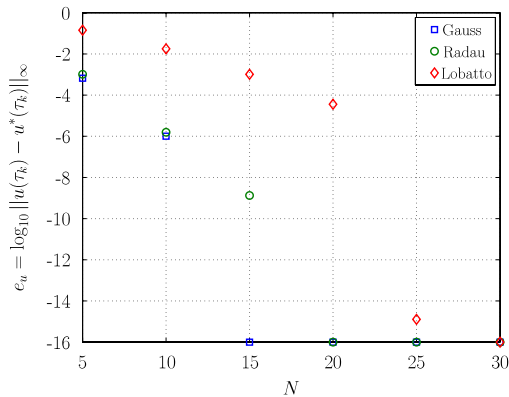
Fig. 1. State errors for example.
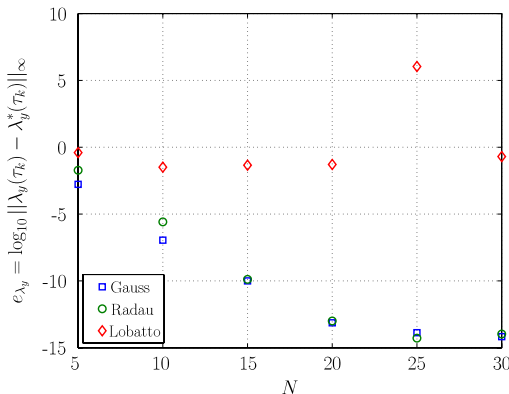

Fig. 2. Control errors for example.
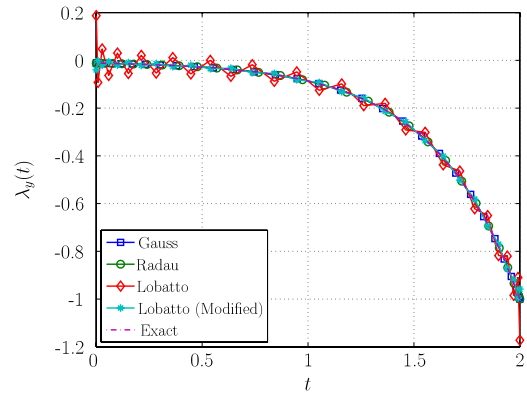

Fig. 3. Costate errors for example.

Fig. 4. Enlargement of costate for example.
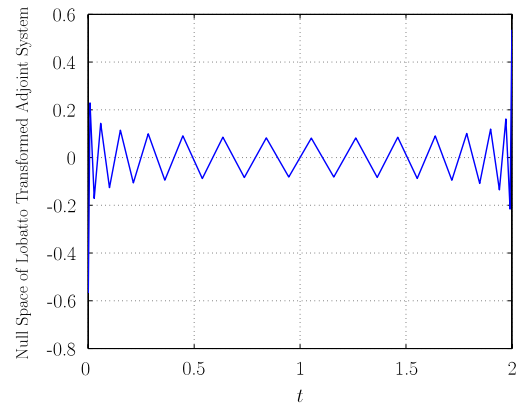
Fig. 5. Null space of Lobatto transformed adjoint system.

the Lobatto costate oscillates about the exact solution while the Gauss and Radau costates are indistinguishable from the optimal solution. The oscillation of the Lobatto costate is due to the null space in the Lobatto costate dynamics discussed in Section 5. Since $n = 1$ in this problem, the dimension of the null space is 1. In Fig. 5 we plot a vector in the null space. Comparing Figs. 4 to 5, we see that the oscillations in the Lobatto costate around the correct costate are essentially due to the addition of vector in the null space. Fig. 4 shows a modified Lobatto costate obtained by adding 0.4 times the null space vector given in Fig. 5 to the costate estimate obtained from the NLP solver; it is seen that the modified costate is quite close to the continuous costate.

7. Conclusions

A unified framework has been presented for the numerical solution of optimal control problems using collocation at Legendre–Gauss (LG), Legendre–Gauss–Radau (LGR), and Legendre–Gauss–Lobatto (LGL) points. It was shown that the LG and LGR differentiation matrices are rectangular and full rank whereas the LGL differentiation matrix is square and singular. This fact leads to the property that the LG and LGR schemes can be expressed equivalently in either differential or integral form, while the differential and integral forms of the LGL method are not equivalent. It was found that LG and LGR transformed adjoint systems are full rank whereas the LGL transformed adjoint system is rank-deficient. The rank-deficiency in the LGL discrete costate leads to the property that the LGL costate oscillates about the true solution. A numerical example was studied, where it was observed that the error in the state and control approximations tend to zero at an exponential rate for all 3 methods, but that the Gauss and Radau state and control converge at a faster rate than that of Lobatto. It was found, however, that the Lobatto costate did not converge for the example, while the Gauss and Radau costates converged at a rate similar to that for the state and control.

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