Computational Methods in Optimal Control
Lecture 3. More Methods

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July 24, 2018
The error associated with Runge-Kutta scheme is often of the form $O(h^p)$, where $p > 0$ is the order of the method (often $\leq 4$). Range-Kutta methods achieve convergence as the mesh spacing tends to zero, and attaining a given error tolerance could require a very fine mesh. We now examine purely polynomial-based schemes, which can converge much faster when the solution is smooth. In particular, for a polynomial-based method, the error can be $O(1/N^N)$ where $N$ is the degree of the polynomials.

\begin{align*}
\text{minimize} & \quad C(x(1)) \\
\text{subject to} & \quad \dot{x}(t) = f(x(t), u(t)), \quad u(t) \in \mathcal{U}, \quad t \in \Omega, \\
& \quad x(-1) = x_0.
\end{align*}

- $\Omega = [-1, +1]$, $x_0$ given, $x(t) \in \mathbb{R}^n$,  
- $\mathcal{U} \subset \mathbb{R}^m$ closed and convex,  
- $f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$ and $C : \mathbb{R}^n \rightarrow \mathbb{R}$
Discrete Problem: Collocation at Gauss quadrature points

minimize \( C(x(1)) \)

subject to \( \dot{x}(\tau_i) = f(x(\tau_i), u_i), \quad u_i \in \mathcal{U}, \quad 1 \leq i \leq N, \)
\[
x(-1) = x_0, \quad x \in \mathcal{P}_N^n.
\]

- \( \mathcal{P}_N = \) polynomials of degree at most \( N, \)
- \( \mathcal{P}_N^n = n\)-fold product \( \mathcal{P}_N \times \ldots \times \mathcal{P}_N. \)
- Gauss quadrature points:
\[
-1 < \tau_1 < \tau_2 < \ldots < \tau_N < +1.
\]
- Additional points in analysis:
\[
\tau_0 = -1 \quad \text{and} \quad \tau_{N+1} = +1.
\]
The Gauss Points

N = 10 Gauss Points

N = 20 Gauss Points
Lagrange Interpolation and the Differentiation Matrix

- Lagrange interpolating polynomials: For \(0 \leq j \leq N\),

\[
\Phi_i(\tau) = \prod_{\substack{j=0 \atop j \neq i}}^{N} \frac{\tau - \tau_j}{\tau_i - \tau_j}, \quad \Phi_i(\tau_j) = \begin{cases} 1 & \text{for } j = i \\ 0 & \text{otherwise} \end{cases}
\]

- If \(x \in \mathcal{P}_N\), then \(x(\tau) = \sum_{j=0}^{N} x(\tau_j)\Phi_j(\tau)\)

- Differentiation matrix \(D \in \mathbb{R}^{N \times (N+1)}\)

\[
\dot{x}(\tau_i) = \sum_{j=0}^{N} \dot{\Phi}_j(\tau_i)x(\tau_j) = \sum_{j=0}^{N} D_{ij}x(\tau_j), \quad D_{ij} = \dot{\Phi}_j(\tau_i)
\]
The Gauss collocation points $\tau_i$, $1 \leq i \leq N$, are the roots of the Legendre polynomial $P_N$ of degree $N$. The associated Gauss quadrature weights $\omega_i$, $1 \leq i \leq N$, are given by

$$\omega_i = \frac{2}{(1 - \tau_i^2)P_N'(\tau_i)^2}. \tag{1}$$

For any $p \in \mathcal{P}_{2N-1}$, we have

$$\int_{-1}^{1} p(t) \, dt = \sum_{i=1}^{N} \omega_i p(\tau_i). \tag{2}$$

If $x \in \mathcal{P}_N$ and $X_i$ denotes $x(\tau_i)$, $0 \leq i \leq N + 1$, then

$$X_{N+1} = x(1) = x(-1) + \int_{-1}^{1} \dot{x}(t) \, dt = X_0 + \sum_{j=1}^{N} \omega_j \dot{x}(\tau_j).$$
NOTE: If $x \in \mathcal{P}_N^n$ is feasible in the discrete control problem, then
\[
\dot{x}(\tau_i) = f(x(\tau_i), u_i) = f(X_i, U_i);
\]
moreover,
\[
\dot{x}(\tau_i) = \sum_{j=0}^{N} D_{ij} x(\tau_j) = \dot{x}(\tau_i) = \sum_{j=0}^{N} D_{ij} X_j.
\]
Hence, the discrete control problem is equivalent to

**minimize** \( C(X_{N+1}) \)

subject to
\[
\sum_{j=0}^{N} D_{ij} X_j = f(X_i, U_i), \quad U_i \in \mathcal{U}, \quad 1 \leq i \leq N,
\]
\[
X_0 = x_0, \quad X_{N+1} = X_0 + \sum_{j=1}^{N} \omega_j f(X_j, U_j).
\]
Lagrangian and Stationarity

\[ C(X_{N+1}) + \sum_{i=1}^{N} \left\langle \mu_i, f(X_i, U_i) - \sum_{j=0}^{N} D_{ij} X_j \right\rangle + \]
\[ + \left\langle \mu_{N+1}, X_0 - X_{N+1} + \sum_{i=1}^{N} \omega_i f(X_i, U_i) \right\rangle. \]

\[ X_j \Rightarrow \sum_{i=1}^{N} D_{ij} \mu_i = \nabla_x H(X_j, U_j, \mu_j + \omega_j \mu_{N+1}), \quad 1 \leq j \leq N, \]
\[ X_{N+1} \Rightarrow \mu_{N+1} = \nabla C(X_{N+1}), \]
\[ U_i \Rightarrow -\nabla_u H(X_i, U_i, \mu_i + \omega_i \mu_{N+1}) \in N_u(U_i), \quad 1 \leq i \leq N. \]
Theorem. The multipliers $\mathbf{\mu} \in \mathbb{R}^{n(N+1)}$ satisfy the stationarity conditions if and only if the polynomial $\lambda \in \mathcal{P}_N^n$ for which $\lambda(1) = \mu_{N+1}$ and $\lambda(\tau_i) = \mu_{N+1} + \mu_i/\omega_i$, $1 \leq i \leq N$, also satisfies

$$
\dot{\lambda}(\tau_i) = -\nabla_x H(x(\tau_i), u_i, \lambda(\tau_i)), \quad 1 \leq i \leq N,
$$

$$
\lambda(1) = \nabla C(x(1)),
$$

$$
\mathcal{N}_U(u_i) \ni -\nabla_u H(x(\tau_i), u_i, \lambda(\tau_i)), \quad 1 \leq i \leq N.
$$
Let $W = \text{diag}(\omega)$, let $\overline{D} = D_{1:N}$, and let $D^\dagger$ be defined by

$$
\overline{D}^\dagger = -W^{-1}\overline{D}W, \quad D_{N+1}^\dagger = -\overline{D}^\dagger 1.
$$

If $\lambda \in \mathcal{P}_N^n$ is a polynomial that satisfies the conditions $\lambda(\tau_i) = \Lambda_i$ for $1 \leq i \leq N + 1$, then

$$
\sum_{j=1}^{N+1} D_{ij}^\dagger \Lambda_j = \dot{\lambda}(\tau_i), \quad 1 \leq i \leq N.
$$
Proof

Suppose $p$ and $q \in \mathcal{P}_N$ with $p(-1) = q(1) = 0$. We have

\[
\sum_{i=1}^{N} \omega_i \dot{p}_i q_i = \int_{-1}^{1} \dot{p}(\tau) q(\tau) \, d\tau = -\int_{-1}^{1} p(\tau) \dot{q}(\tau) \, d\tau = \sum_{i=1}^{N} \omega_i p_i \dot{q}_i,
\]

where $p_i = p(\tau_i)$, $q_i = q(\tau_i)$, $\dot{p}_i = \dot{p}(\tau_i)$, and $\dot{q}_i = \dot{q}(\tau_i)$. In matrix notation,

\[
(W\overline{D}p)^T q = -(Wp)^T \dot{q} \iff p^T \overline{D}^T Wq = -p^T W\dot{q}.
\]

where $p$, $q$, and $\dot{q}$ are $N$ component vectors. Since this hold for all $p$, it follows that

\[
\overline{D}^T Wq = -W\dot{q} \iff \dot{q} = -W^{-1}\overline{D}^T Wq.
\]
Proof of Theorem

Define $\Lambda_i = \mu_{N+1} + \mu_i/\omega_i$ for $1 \leq i \leq N$, $\Lambda_{N+1} = \mu_{N+1}$; Hence, we have $\mu_i = \omega_i(\Lambda_i - \Lambda_{N+1})$ for $1 \leq i \leq N$. Substitute for $D$ in terms of $D^\dagger$ and for $\mu_i$ to obtain

$$\sum_{j=1}^{N+1} D_{ij}^\dagger \Lambda_j = -\nabla_x H(X_i, U_i, \Lambda_i), \quad 1 \leq i \leq N$$

$$\Lambda_{N+1} = \nabla C(X_{N+1}),$$

$$N_U(U_i) \ni -\nabla_u H(X_i, U_i, \Lambda_i), \quad 1 \leq i \leq N$$

Let $\lambda \in \mathcal{P}^n_N$ be the polynomial that is given by $\lambda(\tau_i) = \Lambda_i$ for $1 \leq i \leq N + 1$. Since $D^\dagger$ is a differentiation matrix, we obtain the theorem.
minimize \( C(x(1)) \)

subject to \( \dot{x}(t) = f(x(t), u(t)), \quad u(t) \in \mathcal{U}, \quad t \in [-1, 1], \)

\( x(0) = x_0 \)

First-order optimality conditions for a local minimizer:

\[
\begin{align*}
\dot{x}(t) &= f(x(t), u(t)), \quad u(t) \in \mathcal{U}, \\
x(0) &= x_0 \\
\dot{\lambda}(t) &= -\nabla_x H(x(t), u(t), \lambda(t)), \\
\lambda(1) &= \nabla C(x(1)) \\
N_{\mathcal{U}}(u(t)) &\ni -\nabla_u H(x(t), u(t), \lambda(t)) \quad \text{for all } t \in [-1, 1]
\end{align*}
\]
minimize $C(x(1))$

subject to $\dot{x}(\tau_i) = f(x(\tau_i), u_i), \quad u_i \in U, \quad 1 \leq i \leq N,$

$x(-1) = x_0, \quad x \in \mathcal{P}_N^n.$

First-order optimality conditions for a local minimizer:

$$\begin{align*}
\dot{x}(\tau_i) &= f(x(\tau_i), u_i), \quad u_i \in U, \quad 1 \leq i \leq N, \\
x(-1) &= x_0, \quad x \in \mathcal{P}_N^n \\
\dot{\lambda}(\tau_i) &= -\nabla_x H(x(\tau_i), u_i, \lambda(\tau_i)), \quad 1 \leq i \leq N, \quad \lambda \in \mathcal{P}_N^n \\
\lambda(1) &= \nabla C(x(1)), \\
N_{\mathcal{U}}(u_i) &\ni -\nabla_u H(x(\tau_i), u_i, \lambda(\tau_i)), \quad 1 \leq i \leq N.
\end{align*}$$
minimize \( C(x_N) \)

subject to \( y_i = x_k + h \sum_{j=1}^{s} a_{ij} f(y_j, u_{kj}), \quad i = 1, \ldots, s \)

\( \dot{x}_k = \sum_{i=1}^{s} b_i f(y_i, u_{ki}), \quad u_{ki} \in \mathcal{U} \)

\[
\begin{array}{c}
\text{\( h = 1/N \)}
\end{array}
\]

\[
\begin{array}{c}
\text{\( t_0 \)} \quad \text{\( t_1 \)} \quad \cdots \quad \text{\( t_k \)} \quad \text{\( t_{k+1} \)} \quad \cdots \quad \text{\( t_N = 1 \)}
\end{array}
\]

\[
\begin{array}{c}
\text{\( x \)}
\end{array}
\]

\[
\begin{array}{c}
\text{\( x_k \)} \quad \text{\( x_{k+1} \)}
\end{array}
\]
Review: \textit{s}-stage Runge-Kutta Discretization

First-order optimality conditions for a local minimizer:

\[
\begin{align*}
y_{ki} &= \ x_k + h \sum_{j=1}^{s} a_{ij} f(y_{kj}, u_{kj}), \\
\dot{x}_k &= \sum_{i=1}^{s} b_i f(y_{ki}, u_{ki}), \quad x_0 \text{ given} \\
\lambda_{ki} &= \psi_k - h \sum_{j=1}^{s} \bar{a}_{ij} \lambda_{kj} \nabla_x f(y_{kj}, u_{kj}), \quad \bar{a}_{ij} = \frac{b_i b_j - b_j a_{ji}}{b_i}, \\
\dot{\psi}_k &= - \sum_{i=1}^{s} b_i \lambda_{ki} \nabla_x f(y_{ki}, u_{ki}), \quad \psi_N = \nabla C(x_N), \\
N_{\mathcal{U}}(u_{ki}) &\ni -\lambda_{ki} \nabla_u f(y_{ki}, u_{ki})
\end{align*}
\]
New Model

minimize \[ \int_0^1 g(x(t), u(t)) \, dt \]
subject to \[ \dot{x}(t) = Ax(t) + Bu(t), \quad u(t) \in \mathcal{U}, \quad t \in [0, 1], \]
\[ x(0) = x_0, \]

where \( A \in \mathbb{R}^{n \times n} \) and \( B \in \mathbb{R}^{n \times m} \). Hamiltonian:

\[ H(x, u, \lambda) = g(x, u) + \lambda(Ax + Bu). \]

First-order optimality conditions for a local minimizer:

\[ \dot{x}(t) = Ax(t) + Bu(t), \quad x(0) = x_0, \quad u(t) \in \mathcal{U}, \]
\[ \dot{\lambda}(t) = -[\lambda(t)A + \nabla_x g(x(t), u(t))], \quad \lambda(1) = 0 \]
\[ N_\mathcal{U}(u(t)) \ni -[\lambda(t)B + \nabla_u g(x(t), u(t))] \quad \text{for all } t \in [0, 1] \]
Second-order Taylor Expansion of Objective

\[ g(x, u) \approx g_k + \mathcal{L}_k(x - x_k, u - u_k) + \frac{1}{2} \mathcal{B}_k(x - x_k, u - u_k) \]

where \( \langle \cdot, \cdot \rangle \) denotes \( L^2 \) inner product and

\[
\begin{align*}
\mathcal{L}_k(x - x_k, u - u_k) &= \langle \nabla_x g_k, x - x_k \rangle + \langle \nabla_u g_k, u - u_k \rangle \\
\mathcal{B}_k(x - x_k, u - u_k) &= \langle Q_k(x - x_k), x - x_k \rangle + 2\langle S_k(x - x_k), u - u_k \rangle + \\
&\quad \langle R_k(u - u_k), u - u_k \rangle
\end{align*}
\]

\[
\begin{align*}
\nabla_x g_k(t) &= \nabla_x g(x_k(t), u_k(t)), \\
\nabla_u g_k(t) &= \nabla_u g(x_k(t), u_k(t)), \\
Q_k(t) &= \nabla_{xx} g(x_k(t), u_k(t)), \\
S_k(t) &= \nabla_{ux} g(x_k(t), u_k(t)) \\
R_k(t) &= \nabla_{uu} g(x_k(t), u_k(t))
\end{align*}
\]
Let \((x_k, u_k)\) denote the current iterate. In the SQP method, the next iterate is obtained by solving the quadratic programming problem

\[
\begin{align*}
\text{minimize} & \quad \mathcal{L}_k(x - x_k, u - u_k) + \frac{1}{2} B_k(x - x_k, u - u_k) \\
\text{subject to} & \quad \dot{x}(t) = Ax(t) + Bu(t), \quad x(0) = x_0, \quad u(t) \in \mathcal{U}, \quad t \in [0, 1].
\end{align*}
\]

At a solution, the first-order optimality conditions hold:

\[
\begin{align*}
\dot{x}(t) &= Ax(t) + Bu(t), \quad x(0) = x_0, \quad u(t) \in \mathcal{U} \\
\dot{\lambda}(t) &= -\left(\lambda(t)A + \nabla_x g_k(t) + (x(t) - x_k(t))^T Q_k(t) + (u(t) - u_k(t))^T S_k(t)\right), \quad \lambda(1) = 0 \\
N_{\mathcal{U}}(u(t)) &\ni -\left(\lambda(t)B + \nabla_u g_k(t) + [S_k(t)(x(t) - x_k(t))]^T + [R_k(t)(u(t) - u_k(t))]^T\right).
\end{align*}
\]
The optimality conditions for the SQP scheme and for the original control problem are identical except that $\nabla g(x(t), u(t))$ in the original first-order optimality conditions is replaced by the first-order Taylor expansion around $(x_k(t), u_k(t))$.

Abstractly, the discretizations and algorithms such as SQP amount to the problem:

$$\text{Find } w \in X \text{ such that } T(w) \in F(w),$$

(D)

where $T : X \to Y$, a normed linear space, and $F : X \to 2^Y$. We are given a solution $w^*$ to the control problem and we wish to bound the distance from $w^*$ to a solution of (D).
Take $w = (x, u, \lambda) \in W^{1,\infty} \times W^{0,\infty} \times W^{1,\infty}$, and

$$T(w) = \begin{pmatrix} \dot{x} - Ax - Bu \\ x(0) - x_0 \\ \dot{\lambda} + \lambda A + \nabla_x g_k + (x - x_k)^T Q_k + (u - u_k)^T S_k \\ 0 \\ 0 \\ 0 \\ 0 \\ \lambda(1) \\ - (\lambda B + \nabla_u g_k + [S_k(x - x_k)]^T + [R_k(u - u_k)]^T) \end{pmatrix}$$

$$\mathcal{F}(w) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \mathcal{N}_U(u) \end{pmatrix}$$
Example: Pseudospectral Method

Take \( w = (x, u, \lambda) \in \mathcal{P}_N^n \times \mathbb{R}^{mN} \times \mathcal{P}_N^n \) and

\[
\mathcal{T}(w) = \begin{pmatrix}
\dot{x}(\tau_i) - f(x(\tau_i), u_i), & 1 \leq i \leq N, \\
x(-1) - x_0 \\
\dot{\lambda}(\tau_i) + \nabla_x H(x(\tau_i), u_i, \lambda(\tau_i)), & 1 \leq i \leq N \\
\lambda(1) - \nabla C(x(1)) \\
-\nabla_u H(x(\tau_i), u_i, \lambda(\tau_i)), & 1 \leq i \leq N
\end{pmatrix}
\]

\[
\mathcal{F}(w) = \begin{pmatrix}
0 \\
0 \\
0 \\
0
\end{pmatrix}
\]

\[
N_U(u_i), \quad 1 \leq i \leq N
\]
Test Point $w^I$ for Pseudospectral Method

Suppose that $(x^*, u^*, \lambda^*)$ satisfies the first-order optimality conditions for the continuous control problem. Let us consider the point $w^I = (x^I, u^I, \lambda^I)$ where $x^I$ and $\lambda^I \in P_N^n$, and $u^I \in \mathbb{R}^{mN}$ satisfy

$$
x^I(\tau_i) = x^*(\tau_i), \quad 0 \leq i \leq N
$$

$$
\lambda^I(\tau_i) = \lambda^*(\tau_i), \quad 1 \leq i \leq N + 1
$$

$$
u_i^I = u(\tau_i), \quad 1 \leq i \leq N
$$

By the first-order optimality conditions for the continuous control problem, we have for $1 \leq i \leq N$:

$$
f(x^I(\tau_i), u_i^I) = f(x^*(\tau_i), u^*(\tau_i)) = \dot{x}^*(\tau_i)
$$

$$
\nabla_x H(x^I(\tau_i), u_i^I, \lambda^I(\tau_i)) = \nabla_x H(x^*(\tau_i), u^*(\tau_i), \lambda^*(\tau_i)) = \dot{\lambda}^*(\tau_i)
$$

$$
\nabla_u H(x^I(\tau_i), u_i^I, \lambda^I(\tau_i)) = \nabla_u H(x^*(\tau_i), u^*(\tau_i), \lambda^*(\tau_i))
$$
Residual for Pseudospectral Method

With these substitutions, we have

\[
\mathcal{T}(w^I) = \begin{pmatrix}
\dot{x}^I(\tau_i) - \dot{x}^*(\tau_i), & 1 \leq i \leq N, \\
0 \\
\dot{\lambda}^I(\tau_i) - \dot{\lambda}^*(\tau_i), & 1 \leq i \leq N \\
\lambda^*(1) - \nabla x^I(1) \\
-\nabla_u H(x^*(\tau_i), u^*(\tau_i), \lambda^*(\tau_i)) & 1 \leq i \leq N
\end{pmatrix}
\]

Hence, \( \mathcal{T}(w^I) + \delta \in \mathcal{F}(w^I) \) where

\[
\delta = \begin{pmatrix}
\dot{x}^*(\tau_i) - \dot{x}^I(\tau_i), & 1 \leq i \leq N, \\
0 \\
\dot{\lambda}^*(\tau_i) - \dot{\lambda}^I(\tau_i), & 1 \leq i \leq N \\
\nabla x^I(1) - \nabla x^*(1) \\
0
\end{pmatrix}
\]
Thus the size of the residual $\delta$ depends on difference between the derivative of a polynomial interpolant of either $x^*$ or $\lambda^*$ and the true derivative of either $x^*$ or $\lambda^*$. 
Residual in SQP

Suppose that \( w^* = (x^*, u^*, \lambda^*) \) satisfies the first-order optimality conditions for the continuous control problem. Observe that components 1, 2, and 4 of \( T(w^*) \) are zero. By the first-order conditions for the continuous problem,

\[
\dot{\lambda}^* = -\nabla_x H(x^*, u^*, \lambda^*) \\
= \nabla_x g(x^*, u^*) + \lambda^* A
\]

Hence, we have

\[
T_3(w^*) = \nabla_x g_k - \nabla_x g_* + (x^* - x_k)^T Q_k + (u^* - u_k)^T S_k,
\]

which implies that \( T_3(w^*) + \delta_3 = 0 \) where

\[
\delta_3 = -\left( \nabla_x g_k - \nabla_x g_* + (x^* - x_k)^T Q_k + (u^* - u_k)^T S_k \right).
\]
Similary, observe that

\[
\mathcal{T}_5(w^*) = - (\lambda^* B + \nabla_{ug^*} + (\nabla_{ug_k} - \nabla_{ug^*}) + [S_k(x^* - x_k)]^T + [R_k(u^* - u_k)]^T
\]

By the first-order optimality conditions for \( w^* \), we have

\[
- [\lambda^*(t)B + \nabla_{ug}(x^*(t), u^*(t))] \in N_U(u^*(t)) \quad \text{for all } t \in [0, 1]
\]

Hence, if the trailing part of \( \mathcal{T}_5(w^*) \) is deleted, we are left with a vector contained in \( N_U(u^*(t)) \). More precisely,

\[
\mathcal{T}_5(w^*) + \delta_5 \in N_U(u^*) \quad \text{where}
\]

\[
\delta_5 = \nabla_{ug_k} - \nabla_{ug^*} + [S_k(x^* - x_k)]^T + [R_k(u^* - u_k)]^T.
\]
IN SUMMARY: $\mathcal{T}(w^*) + \delta \in \mathcal{F}(w^*)$ where

$$
\delta = \begin{pmatrix}
0 \\
0 \\
- (\nabla_x g_k + (x^* - x_k)^T Q_k + (u^* - u_k)^T S_k - \nabla_x g_*) \\
0 \\
\nabla_u g_k + [S_k(x^* - x_k)]^T + [R_k(u^* - u_k)]^T - \nabla_u g_*
\end{pmatrix}
$$

Note that $\nabla_x g_k + (x^* - x_k)^T Q_k + (u^* - u_k)^T S_k$ is the first-order Taylor expansion of $\nabla_x g_*$ around $(x_k, u_k)$.

GOAL: Obtain bounds for the residual and convert these bounds into error estimates and convergence results.