$\begin{array}{c} \text{CHEM-E7225} \\ 2023 \end{array}$

Formulation

Numerics



Continuous-time optimal control: Shooting CHEM-E7225 (was E7195), 2023

Francesco Corona (\neg_\neg)

Chemical and Metallurgical Engineering School of Chemical Engineering

Overview

Formulation Numerics We combined the notions on dynamic systems and simulation with the notions on nonlinear programming, to formulate a general discrete-time optimal control problem

• We understood and treated them as special forms of nonlinear programs

$$\min_{\substack{x_0, x_1, \dots, x_K \\ u_0, u_1, \dots, u_{K-1}}} E(x_K) + \sum_{k=0}^{K-1} L(x_k, u_k)$$
subject to
$$x_{k+1} - f(x_k, u_k | \theta_x) = 0, \quad k = 0, 1, \dots, K-1$$

$$h(x_k, u_k) \le 0, \qquad k = 0, 1, \dots, K-1$$

$$r(x_0, x_K) \le 0$$

In general, the system dynamics are defined in continuous time

→ The control inputs are continuous functions of time

We are interested in the continuous-time formulation

• We discuss more precisely the discretisation

Formulation

Numerics

Formulation

Continuous-time optimal control

Formulation

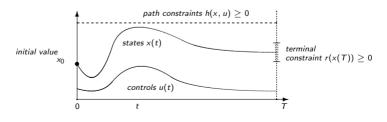
Numerics

Formulation

The simplest form of continuous-time optimal control lets all functions be continuous

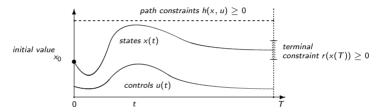
$$\begin{array}{ll} \min\limits_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} & E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) \, dt \\ \\ \text{subject to} & \dot{x}(t) - f\left(x(t), u(t)\right) = 0, \qquad \qquad t \in [0, T] \qquad \text{(Dynamics)} \\ & \quad h\left(x(t), u(t)\right) \leq 0, \qquad \qquad t \in [0, T] \qquad \text{(Path constraints)} \\ & \quad x_0 - x(0) = 0 \qquad \qquad (t = 0) \qquad \text{(Initial value)} \\ & \quad r\left(x(T)\right) \leq 0 \qquad \qquad (t = T) \qquad \text{Terminal constraint} \end{array}$$

That is, the optimisation is over state ad control trajectories, $x(0 \leadsto T)$ and $u(0 \leadsto T)$



Formulation (cont.)

Formulation



The state are a continuous and differentiable function of time over the interval [0, T] Similarly, also the controls are function of time over [0, T]

 \leadsto Though, they can be rough or jumpy fuctions

Formulation (cont.)

Formulation

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} \underbrace{\frac{E\left(x(T)\right)}{\text{Mayer term}} + \int_{0}^{T} L\left(x(t), u(t)\right) dt}_{\text{Lagrange term}}$$

$$\text{Bolza objective function}$$

$$\text{subject to} \quad \frac{\dot{x}(t) - f\left(x(t), u(t)\right) = 0}{\dot{x}(t), u(t)) \leq 0}, \qquad t \in [0, T] \qquad \text{(Dynamics)}$$

$$h\left(x(t), u(t)\right) \leq 0, \qquad t \in [0, T] \qquad \text{(Path constraints)}$$

$$x_0 - x(0) = 0 \qquad (t = 0) \qquad \text{(Initial value)}$$

$$r\left(x(T)\right) \leq 0 \qquad (t = T) \qquad \text{Terminal constraint}$$

We constrain the initial value of the state to be x_0 , by explicitly setting $x(0) = x_0$ Moreover, we constrain the state to satisfy the continuous-time dynamics in [0, T]

$$\dot{x}(t) - f(x(t), u(t)) = 0, \qquad t \in [0, T]$$

When the initial state x(0) is fixed and the trajectory of the controls u(t) are known in [0, T], the dynamic constraint will determine the trajectory of the state x(t) in [0, T]

Formulation (cont.)

Formulation

$$\dot{x}(t) - f(x(t), u(t)) = 0, \qquad t \in [0, T]$$

In discrete-time, we have expressed the dynamic constraint as a vector of constraints

$$\begin{bmatrix} x_{1} - f(x_{0}, u_{0}) \\ x_{2} - f(x_{1}, u_{1}) \\ \vdots \\ x_{k+1} - f(x_{k}, u_{k}) \\ \vdots \\ x_{K-1} - f(x_{K-2}, u_{K-2}) \\ x_{K} - f(x_{K-1}, u_{K-1}) \end{bmatrix}$$

$$K \times N_{x}$$

In continuous-time, the dynamic constraint is understood as an infinitely long vector

Formulation

Numerics

Formulation (cont.)

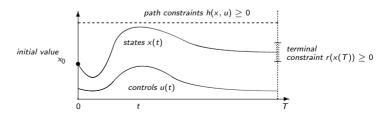
$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} \underbrace{\frac{E\left(x(T)\right)}{\text{Mayer term}}} + \underbrace{\int_{0}^{} L\left(x(t), u(t)\right) dt}_{\text{Lagrange term}}$$

$$\text{Subject to} \quad \dot{x}(t) - f\left(x(t), u(t)\right) = 0, \qquad \qquad t \in [0, T] \qquad \text{(Dynamics)}$$

$$\frac{h\left(x(t), u(t)\right) \le 0}{x_{0} - x(0) = 0} \qquad \qquad (t = 0) \qquad \text{(Initial value)}$$

$$r\left(x(T)\right) \le 0 \qquad \qquad (t = T) \qquad \text{Terminal constraint}$$

We constrain trajectories along the path, by explicitly setting an inequality constraint



Formulation (cont.)

Formulation

$$h(x(t), u(t)) \le 0, \qquad t \in [0, T]$$

In discrete-time, we have expressed the path constraint as a vector of constraints

$$\begin{bmatrix} h(x_0, u_0) \\ h(x_1, u_1) \\ \vdots \\ h(x_k, u_k) \\ \vdots \\ h(x_K, y_K) \end{bmatrix}$$

In continuous-time, the path constraint is understood as an infinitely long vector

Formulation

Formulation (cont.)

r(x(T)) < 0

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} \underbrace{\frac{E\left(x(T)\right)}{\text{Mayer term}}} + \underbrace{\int_{0}^{} L\left(x(t), u(t)\right) dt}_{\text{Lagrange term}}$$

$$\text{Bolza objective function}$$
subject to $\dot{x}(t) - f\left(x(t), u(t)\right) = 0, \qquad t \in [0, T] \qquad \text{(Dynamics)}$

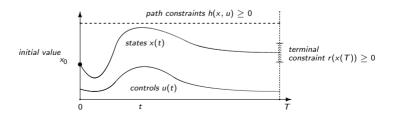
$$h\left(x(t), u(t)\right) \leq 0, \qquad t \in [0, T] \qquad \text{(Path constraints)}$$

$$x_{0} - x(0) = 0 \qquad (t = 0) \qquad \text{(Initial value)}$$

A terminal constraint is expressed as inequality constraint on the terminal state x(T)

(t = T)

Terminal constraint



Formulation

Numerics

Numerics

Continuous-time optimal control



Overview of numerical approaches

Numerics

There exist three main classes of approaches to solve continuous-time optimal control

- State-space methods are based on the Bellman's principle of optimality
 - The Hamilton-Jocobi-Bellman equation, HJB
 - (Continuous-time dynamic programming)
- Indirect methods are based on the Pontryangin's minimum principle
 - First-optimise, then discretise
- Direct methods are based on transcriptions as nonlinear programs
 - First-discretise, then optimise

Formulation Numerics

$$\begin{array}{ll} \displaystyle \min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} & E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) \, dt \\ \\ \text{subject to} & \dot{x}(t) - f\left(x(t), u(t)\right) = 0, \qquad t \in [0, T] \qquad \text{(Dynamics)} \\ & \quad h\left(x(t), u(t)\right) \leq 0, \qquad t \in [0, T] \qquad \text{(Path constraints)} \\ & \quad x_0 - x(0) = 0 \qquad (t = 0) \qquad \text{(Initial value)} \\ & \quad r\left(x(T)\right) \leq 0 \qquad (t = T) \qquad \text{Terminal constraint} \end{array}$$

The general idea of single shooting methods is common to all the shooting methods

- Use an embedded integrator of the differential model
- To eliminate the continuous-time dynamics

Direct methods | Single-shooting

Numerics

$$\begin{aligned} \min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} & E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) \, dt \\ \text{subject to} & \dot{x}(t) - f\left(x(t), u(t)\right) = 0, & t \in [0, T] & \text{(Dynamics)} \\ & h\left(x(t), u(t)\right) \leq 0, & t \in [0, T] & \text{(Path constraints)} \\ & x_0 - x(0) = 0 & (t = 0) & \text{(Initial value)} \\ & & r\left(x(T)\right) \leq 0 & (t = T) & \text{Terminal constraint} \end{aligned}$$



First-discretise, then optimise

• Define a fixed time-grid for [0, T]

$$0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$$

The time-intervals do not need to be necessarily equally spaced, though this is common

2023

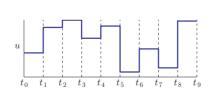
Numerics

Direct methods | Single-shooting (cont.)

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} \quad E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) \, dt$$
 subject to
$$\dot{x}(t) - f\left(x(t), u(t)\right) = 0, \qquad \qquad t \in [0, T] \qquad \text{(Dynamics)}$$

$$h\left(x(t), u(t)\right) \leq 0, \qquad \qquad t \in [0, T] \qquad \text{(Path constraints)}$$

$$x_0 - x(0) = 0 \qquad \qquad (t = 0) \qquad \text{(Initial value)}$$



r(x(T)) < 0

First-discretise, then optimise

(t = T)

• Define a fixed time-grid for [0, T]

$$0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$$

Terminal constraint

• Discretise the controls u(t)

$$u(t \in [t_k, t_{k+1}]) = u_k$$

The control trajectory u(t) is commonly parameterised by piecewise constant functions

• Other parameterisations are possible (other piecewise polynomials)

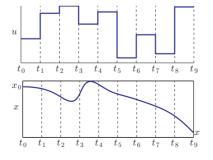
Formulation

Numerics

Direct methods | Single-shooting (cont.)

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) dt$$
subject to $\dot{x}(t) - f\left(x(t), u(t)\right) = 0$, $t \in [0, T]$ (Dynamics)
$$h\left(x(t), u(t)\right) \le 0, \qquad \qquad t \in [0, T] \qquad \text{(Path constraints)}$$

$$x_0 - x(0) = 0 \qquad \qquad (t = 0) \qquad \text{(Initial value)}$$



r(x(T)) < 0

First-discretise, then optimise

(t = T)

• Define a fixed time-grid for [0, T]

$$0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$$

Terminal constraint

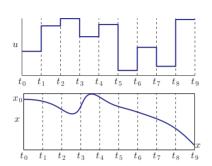
• Discretise the controls u(t)

$$u(t \in [t_k, t_{k+1}]) = u_k$$

• Treat the states x(t) as function of discretised controls $\{u_k\}$ and x_0

Formulation
Numerics

Direct methods | Single-shooting (cont.)



• Define a fixed time-grid for [0, T]

$$0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$$

• Discretise the controls u(t)

$$u(t \in [t_k, t_{k+1}]) = u_k$$

• Treat the states x(t) as function of discretised controls $\{u_k\}$ and x_0

Consider the time $t \in [t_k, t_{k+1}]$, the zero-order hold control active on the interval is u_k We denoted the state trajectory over the short interval $[t_k, t_{k+1}]$ as the solution map

$$\widetilde{x}_k(t|x_k,u_k), \quad t \in [t_k,t_{k+1}]$$

The final value of the short trajectory is the output of the transition function

$$\widetilde{x}_k(t_{k+1}|x_k,u_k) = f_{\Delta t}(x_k,u_k)$$

Formulation

Numerics

Direct methods | Single-shooting (cont.)

$$\min_{\substack{x_0, x_1, \dots, x_K \\ u_0, u_1, \dots, u_{K-1}}} E(x_K) + \sum_{k=0}^{K-1} L_k(x_k, u_k)$$
subject to
$$x_{k+1} - f_{\Delta t}(x_k, u_k | \theta_x) = 0, \quad k = 0, 1, \dots, K-1$$

$$h(x_k, u_k) \le 0, \quad k = 0, 1, \dots, K-1$$

$$r(x_0, x_K) \le 0$$

Discretising the controls transcribes the infinite dimensional problem into a finite one

Single-shooting regards the states x_k as dependent variables obtained by integration

• From the initial state x_0 , under the sequence of controls $\{u_k\}$

$$x_{0} = \underbrace{x_{0}}_{\overline{x}_{0}(x_{0})}$$

$$x_{1} = \underbrace{f_{\Delta t}(x_{0}, u_{0})}_{\overline{x}_{1}(x_{0}, u_{0})}$$

$$x_{2} = f_{\Delta t}(x_{1}, u_{1})$$

$$= \underbrace{f_{\Delta t}(f_{\Delta t}(x_{0}, u_{0}), u_{1})}_{\overline{x}_{2}(x_{0}, u_{0}, u_{1})}$$
...

Direct methods | Single-shooting (cont.)

Numerics

$$\min_{\substack{x_0 \\ u_0, u_1, \dots, u_{K-1}}} E(\overline{x}_K(x_0, u_0, u_1, \dots, u_{K-1})) + \sum_{k=0}^{K-1} L(\overline{x}_k(x_0, u_0, u_1, \dots, u_{K-1}), u_k)$$
subject to
$$h(\overline{x}_k(x_0, u_0, u_1, \dots, u_{K-1}), u_k) \le 0, \quad k = 0, 1, \dots, K-1$$

$$r(x_0, \overline{x}_N(x_0, u_0, u_1, \dots, u_{K-1})) = 0$$

Simulation and optimisation are solved sequentially, the approach is the sequential one

The only decision variable in the nonlinear program is the collection of control vectors

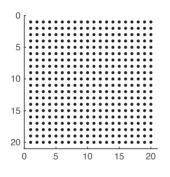
• The decision variable influences all of the problem functions

$$\underbrace{u_0, u_1, \dots, u_{K-1}}_{K \times N_u}$$

Formulation
Numerics

Direct methods | Single-shooting (cont.)

The nonlinear program is dense, any generic solver can be used for the task



The Lagrangian function $\mathcal{L}\left(w,\lambda,\mu\right)$

$$\begin{split} \mathcal{L}\left(w,\lambda,\mu\right) \\ = f\left(w\right) + \lambda^{T}g\left(w\right) + \mu^{T}h\left(w\right) \end{split}$$

The Hessian of the Lagrangian

$$\nabla_{w}^{2} \mathcal{L}\left(w, \lambda, \mu\right)$$

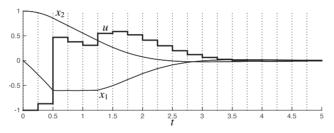
In general, there is no structure in $\nabla_{w}^{2}\mathcal{L}\left(w,\lambda,\mu\right)$

$$\frac{\partial^{2} \mathcal{L}\left(w, \lambda, \mu\right)}{\partial w_{i} \partial w_{k}} \neq 0$$

Direct methods | Single-shooting (cont.)

Formulation Numerics

Single shooting solution using simulation based on a order-4 Runge-Kutta integrator

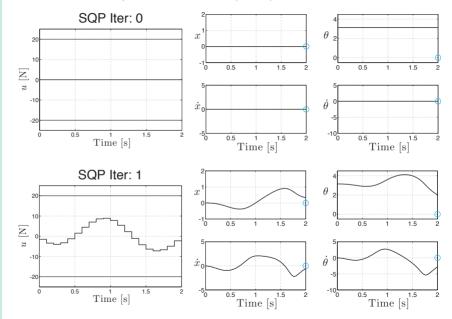


The state trajectory can be computed during the iterations of the optimisation scheme ${\bf r}$

• The model equations are satisfied by definition

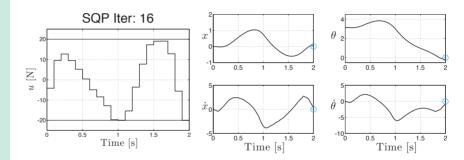
Formulation
Numerics

Direct methods | Single-shooting (cont.)



Direct methods | Single-shooting (cont.)

Formulation
Numerics



Direct methods | Single-shooting (cont.)

Numerics

The forward integrator map of the system dynamics is formally defined as a function

$$\begin{split} f_{\text{int}} : \mathcal{R}^{N_x + (K \times N_u)} \times \mathcal{R} &\to \mathcal{R}^{N_x} \\ : (x_0, u_0, u_1, \dots, u_{K-1}, t) &\mapsto x(t) \end{split}$$

Function $f_{\rm int}$ propagates continuous dynamics, it may get highly nonlinear for large T

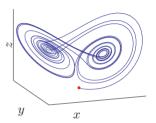
Formulation

Numerics

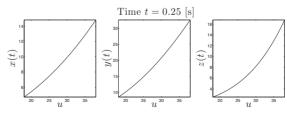
Example

$$\dot{x}(t) = 10 (y(t) - x(t))
\dot{y}(t) = x(t) (u(t) - z(t)) - y(t)
\dot{z}(t) = x(t)y(t) - 3z(t)$$

From some fixed initial condition (x_0, y_0, z_0) and constant control u(t)

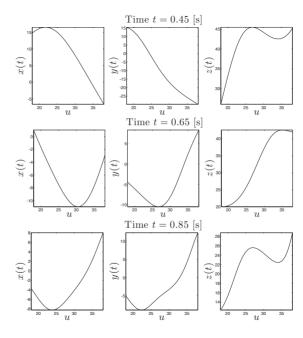


System's states x(t) as a function of the controls u(t) = const, at simulation time t



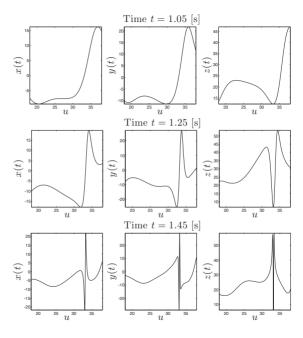
Formulation

Numerics



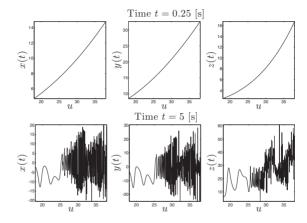
Formulation

Numerics



Direct methods | Single-shooting (cont.)

Numerics



For short integration times, the relationship between states and controls is close to linear and as the becomes highly nonlinear with the duration of the simulation time

L

Direct methods | Multiple-shooting

Formulation Numerics

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) dt$$
 subject to
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$$h\left(x(t), u(t)\right) \leq 0, \qquad t \in [0, T] \qquad \text{(Path constraints)}$$

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The general idea of multiple shooting methods is common to all the shooting methods

- Use an embedded integrator of the differential model
- To eliminate the continuous-time dynamics

Yet, the integration of the dynamics over a long period of time can be counterproductive

→ Restrict the integration to relatively shorter inntervals

Direct methods | Multiple-shooting (cont.)

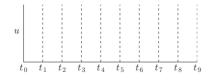
Formulatio
Numerics

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First-discretise, then optimise

• Define a fixed time-grid for [0, T]

$$0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$$

The time-intervals do not need to be necessarily equally spaced, though this is common

Formulation

Numerics

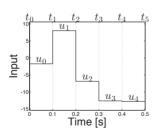
Direct methods | Multiple-shooting (cont.)

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} \quad E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) \, dt$$
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$$x_0 - x(0) = 0 \qquad \qquad (t = 0) \qquad \text{(Initial value)}$$

$$r\left(x(T)\right) \leq 0 \qquad \qquad (t = T) \qquad \text{Terminal constraint}$$



First-discretise, then optimise

• Define a fixed time-grid for [0, T]

$$0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$$

• Discretise the controls u(t)

$$u(t \in [t_k, t_{k+1}]) = u_k$$

The control trajectory u(t) is commonly parameterised by piecewise constant functions

• Other parameterisations are possible (other piecewise polynomials)

Formulation
Numerics

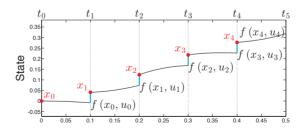
Direct methods | Multiple-shooting (cont.)

$$\min_{\substack{x(0 \leadsto T) \\ u(0 \leadsto T)}} \quad E\left(x(T)\right) + \int_0^T L\left(x(t), u(t)\right) \, dt$$
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$$x_0 - x(0) = 0 \qquad \qquad (t = 0) \qquad \text{(Initial value)}$$

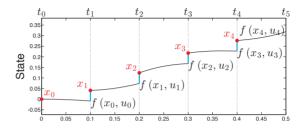
$$r\left(x(T)\right) \leq 0 \qquad \qquad (t = T) \qquad \text{Terminal constraint}$$



Treat the states x(t) as function of discretised controls u_k , starting from a given x_k

Formulation
Numerics

Direct methods | Multiple-shooting (cont.)



The integration of the dynamics is performed over the much sorter interval $[t_k, t_{k+1}]$ • The forward integrator is only mildly nonlinear

$$x_{k+1} = f_{\Delta t} \left(x_k, u_k | \theta_x \right)$$

The states x_k used in the integration become decision variables of the optimisation

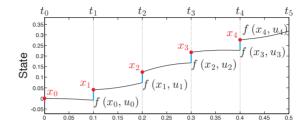
$$\min_{\substack{x_0, x_1, \dots, x_K \\ u_0, u_1, \dots, u_{K-1}}} E(x_K) + \sum_{k=0}^{K-1} L(x_k, u_k)$$
subject to
$$x_{k+1} - f_{\Delta t}(x_k, u_k | \theta_x) = 0, \quad k = 0, 1, \dots, K-1$$

$$h(x_k, u_k) \le 0, \qquad k = 0, 1, \dots, K-1$$

$$r(x_0, x_N) = 0$$

Formulation
Numerics

Direct methods | Multiple-shooting (cont.)



The integration over the interval $[t_k, t_{k+1}]$ is meaningful if the shooting gap is closed

$$x_{k+1} - f_{\Delta t}(x_k, u_k | \theta_x) = 0$$

To ensure continuity, the shooting gaps become equality constraints of the optimisation

$$\min_{\substack{x_0, x_1, \dots, x_K \\ u_0, u_1, \dots, u_{K-1}}} E(x_K) + \sum_{k=0}^{K-1} L(x_k, u_k)$$
subject to
$$x_{k+1} - f_{\Delta t}(x_k, u_k | \theta_x) = 0, \quad k = 0, 1, \dots, K-1$$

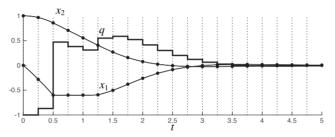
$$h(x_k, u_k) \le 0, \qquad k = 0, 1, \dots, K-1$$

$$r(x_0, x_N) = 0$$

Direct methods | Mutliple-shooting (cont.)

Formulation
Numerics

Multiple shooting solution using simulation based on a order-4 Runge-Kutta integrator



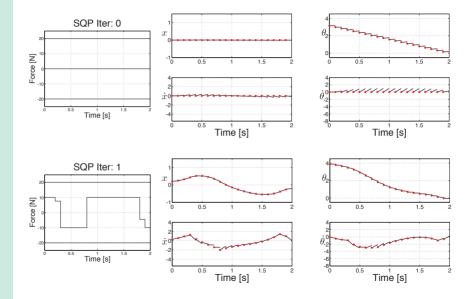
Because the continuity conditions hold, the short-interval simulations join at time nodes

• The model equations satisfied only once the nonlinear program has converged

Formulation

Numerics

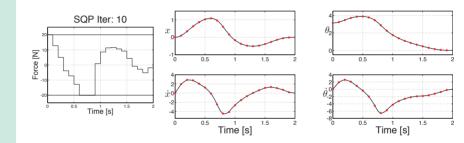
Direct methods | Multiple-shooting (cont.)



Direct methods | Multiple-shooting (cont.)

Formulation

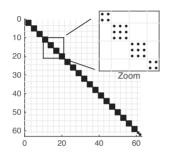
Numerics



Formulation Numerics

Direct methods | Multiple-shooting (cont.)

The nonlinear program is sparse, structure-exploiting solvers should be used



The Lagrangian function $\mathcal{L}\left(w,\lambda,\mu\right)$

$$\begin{split} \mathcal{L}\left(w,\lambda,\mu\right) \\ = f\left(w\right) + \lambda^{T}g\left(w\right) + \mu^{T}h\left(w\right) \end{split}$$

The Hessian of the Lagrangian

$$\nabla_{w}^{2} \mathcal{L}\left(w, \lambda, \mu\right)$$

The Hessian of the Lagrangian is block-diagonal, with small symmetric blocks

• All the other second derivatives are zero

The block-diagonality property of the Hessian is extremely favourable

- \leadsto Hessian approximations
- → QP subproblems