Towards slow manifold based model reduction in optimal control of multiple time scale ODE

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Outline

1. Optimal Control
2. Singular Perturbed Problems
3. Model Reduction in Optimal Control

Optimal Control Problem (OCP)

$$\begin{aligned} \min_{z,u} \quad & E\left(z(T)\right) + \int_0^T L(z(t), u(t))\,\mathrm{d}t \\ \text{subject to} \quad & \dot{z}(t) = \tilde{f}(z(t), u(t)) \\ & 0 \leq s(z(t), u(t)) \\ & 0 \leq r(z(0), z(T)) \end{aligned}$$

where

- $z \in \mathbb{R}^{n_z}$ state variables
- $u \in \mathbb{R}^{n_u}$ control variables
- problem is often high-dimensional and stiff $\rightsquigarrow$ Model Reduction

Outline

Singular Perturbed Problem (SPP)

variables evolve on different time scales. Instead of $\dot{z}(t) = \tilde{f}\big(t, z(t)\big)$, consider

SPP

$$\dot{x}(t) = f\big(x(t), y(t), u(t)\big) \tag{2a}$$

$$\varepsilon \dot{y}(t) = g\big(x(t), y(t), u(t)\big) \tag{2b}$$

with fixed $0 < \varepsilon \ll 1$.

Decomposition of variables:

- $z = (x, y)$ where x is a slow variable (also called reaction progress variable) and y is a fast variable.
- ε measure for time scale separation

Singular Perturbed Problem (SPP)

What happens in the limit $\varepsilon \to 0$?

SPP for $\varepsilon = 0$

$$\dot{x}(t) = f\big(x(t), y(t), u(t)\big) \tag{3a}$$

$$0 = g\big(x(t), y(t), u(t)\big) \tag{3b}$$

- $\Rightarrow$ We get a system of differential algebraic equations (DAEs)! Can be seen as system of ODEs on manifold $M = \{g\big(x(t), y(t), u(t)\big) = 0\}$
- If partial derivative g_y is non-singular, use implicit function theorem: $\exists$ function h such that $y = h(x, u)$. System becomes

$$\dot{x}(t) = f\big(x(t), h(x(t), u(t)), u(t)\big)$$

Manifold also for $\varepsilon > 0$?

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Geometrically: Bundling of trajectories onto manifolds

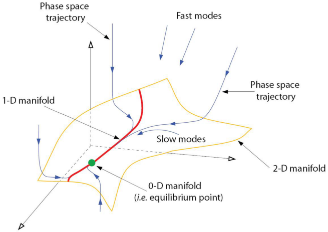
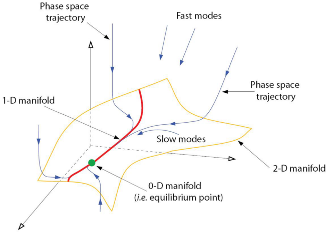


Figure : Courtesy of A.N. Al-Khateeb, J.M. Powers, S. Paloucci

Manifold also for $\varepsilon > 0$?

Geometrically: Bundling of trajectories onto manifolds



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Analytically, under some assumptions it holds

Theorem (Fenichel)

$\exists\ \varepsilon_0 > 0\ \ \forall\ 0 < \varepsilon \leq \varepsilon_0$ there is a function $h(\cdot;\varepsilon) : K \subset \mathbb{R}^{n_x+n_u} \to \mathbb{R}^{n_y}$ such that

$$\mathcal{M}_\varepsilon := \{(x,y,u) : y = h(x,u;\varepsilon), (x,u) \in K\}$$

is locally invariant under the flow of (3).

Boundary Value Problem by Lebiedz and Unger for calculation of $h(x^*, \varepsilon)$:

$$\min_{z(\cdot)=\big(x(\cdot),y(\cdot)\big)} \quad \left\|\ddot{z}(t_0)\right\|_2^2 \tag{4a}$$

$$\text{s.t.} \quad \dot{z}(t) = \tilde{f}\big(t, z(t)\big), \quad t \in [t_0, t_f] \tag{4b}$$

$$0 = c(z(t)) \tag{4c}$$

$$x(t_f) = x^* \tag{4d}$$

where

- funktion c includes conservation of mass etc. (in case of chemical reactions)
- $\tilde{f} = (f, \frac{1}{\varepsilon} g)$
- $0 < t_f - t_0 \ll 1$

Outline

OCP for singular perturbed systems

$$
\begin{aligned}
\min_{x,y,u} \quad & E\left(x(T),\ y(T)\right) + \int_0^T L\big(x(t), y(t), u(t)\big)\, \mathrm{d}t \\
\text{subject to} \quad & \dot{x}(t) = f\left(t, x(t), y(t), u(t)\right) \\
& \varepsilon \dot{y}(t) = g\left(t, x(t), y(t), u(t)\right) \\
& 0 \leq s\big(x(t), y(t), u(t)\big) \\
& 0 \leq r\big(x(0), y(0), x(T), y(T)\big)
\end{aligned}
$$

with stiff dynamics (time scale separation)

reduced OCP

$$\begin{aligned}
\min_{x,u} \quad & E\left(x(T),\ h(x(T),u(T),\varepsilon)\right) + \int_0^T L\big(x(t), h(x,u,\varepsilon), u(t)\big)\,\mathrm{d}t \\
\text{subject to} \quad & \dot{x}(t) = f\left(t, x(t), h(x,u,\varepsilon), u(t)\right) \\
& 0 \leq s\big(x(t), h(x,u,\varepsilon), u(t)\big) \\
& 0 \leq r\big(x(0), h(x(0),u(0),\varepsilon), x(T), h(x(T),u(T),\varepsilon)\big)
\end{aligned}$$

where

- reduced model order: $n_x + n_y \rightsquigarrow n_x$ state variables
- resulting ODE is less stiff

But still some issues

- strong dependence on efficient calculation of derivatives $\frac{\partial}{\partial x,u} h(x, u; \varepsilon)$ for solving the reduced OCP
- efficient coupling of calculation of the manifold and the OCP
- predecessor used two different tools:
  - DOT: tool for solving OCPs with multiple shooting approach arround IPOPT
  - MoRe: tool for efficient calculation of manifold

Calculation of derivatives of h

Boundary value problem is transformed into NLP (with collocation or shooting method) with parameter $p \in \mathbb{R}^q$ (values for $x^\star, u$)

$$(P(p)) \qquad \begin{array}{ll} \min\limits_{x} & f(x,p) \\ \text{s.t.} & g_i(x,p) \leq 0 \ \ (i = 1, \dots, m) \\ & g_i(x,p) = 0 \ \ (i = m+1, \dots, k) \end{array}$$

Sensitivity Theorem

Let $\bar{x}$ be a local minimum of $P(p_0)$ satisfying LICQ and the second order sufficient conditions (SOSC) of the NLP $P(p_0)$ with strict complementarity and Lagrangian multpliers $\bar{\lambda}_i$. Then $\exists P_0 \subset \mathbb{R}^q$ open and $\exists$ continuously differentiable functions $x : P_0 \to \mathbb{R}^n,\ \lambda_i : P_0 \to \mathbb{R}$ such that

(i) $x(p_0) = \bar{x},\ \lambda_i(p_0) = \bar{\lambda}_i$

(ii) $x(p), \lambda_i(p)$ satisfy SOSC for $P(p)$ for all $p \in P_0$.

Calculation of derivatives of h (2)

Corollary

Denote the Lagrangian of $P(p)$ by $L(x, \lambda, p)$. Define $J(x) = \{1 \leq i \leq k \ : \ g_i(x, p) = 0\}$ and $G(x, p) := (g_i(x, p))_{i \in J(\bar{x})}$. Then it holds

$$\begin{pmatrix} x'(p_0) \\ \lambda'(p_0) \end{pmatrix} = \begin{pmatrix} \frac{\mathrm{d}^2}{\mathrm{d}x^2} L(\bar{x}, \bar{\lambda}, p_0) & \frac{\mathrm{d}}{\mathrm{d}x} G(\bar{x}, p_0)^T \\ \frac{\mathrm{d}}{\mathrm{d}x} G(\bar{x}, p_0) & 0 \end{pmatrix}^{-1} \cdot \begin{pmatrix} \frac{\mathrm{d}^2}{\mathrm{d}x\,\mathrm{d}p} L(\bar{x}, \bar{\lambda}, p_0) \\ \frac{\mathrm{d}}{\mathrm{d}p} G(\bar{x}, p_0) \end{pmatrix}$$

$\Rightarrow$ derivatives can be calculated with low extra costs.

results of my predecessor

Example (enzyme kinetics - Michaelis-Menten)

$$S + E \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P + E$$

used for optimal control with artificial objective function:

$$\begin{aligned} \min_{x,y,u} \quad & \int_0^5 -50y + u^2 \, \mathrm{d}t \\ \text{s.t.} \quad \dot{x} &= -x + (x + 0.5)y + u \\ \varepsilon\dot{y} &= \quad x - (x+1)y \\ x(0) &= 1,\ y(0) = \eta \end{aligned}$$

results of my predecessor (2)

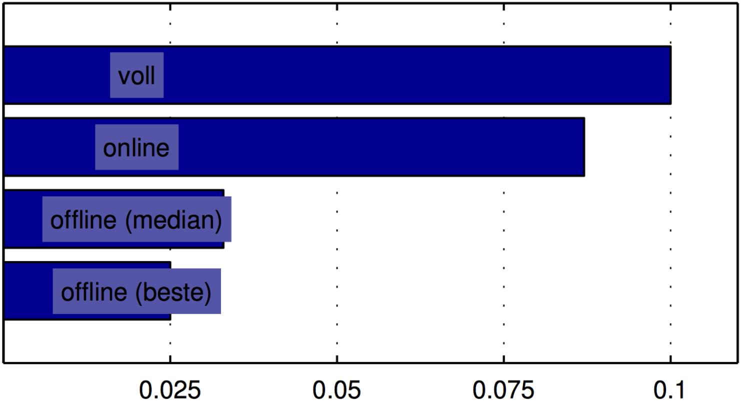

Figure : time in seconds for each iteration of the resulting NLP