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Multi-objective optimal control of chemical processes using ACADO toolkit

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ABSTRACT

Many practical chemical engineering problems involve the determination of optimal trajectories given multiple and conflicting objectives. These conflicting objectives typically give rise to a set of Pareto optimal solutions. To enhance real-time decision making efficient approaches are required for determining the Pareto set in a fast and accurate way. Hereto, the current paper illustrates the use of the freely available toolkit ACADO Multi-Objective (www.acadotoolkit.org) on several chemical examples. The rationale behind ACADO Multi-Objective is the integration of direct optimal control methods with scalarisation-based multi-objective methods enabling the exploitation of fast deterministic gradient-based optimisation routines.

1. Introduction

In practical chemical optimal control problems, multiple and conflicting objectives are often present. This gives rise to a set of Pareto optimal solutions instead of one single solution (Miettinen, 1999). The most often exploited approaches to generate this Pareto set are (i) the Weighted Sum (WS) of the individual objectives or (ii) stochastic genetic algorithms (Deb, 2001). In the former case, a number of single-objective optimal control problems are solved for a grid of different weights using deterministic optimisation routines. In the latter case, a population of candidate solutions is updated based on repeated cost computations such that this population gradually evolves to the Pareto frontier. Unfortunately, both approaches exhibit certain restrictions. For the Weighted Sum it is known that (i) an equal distribution of weights does not necessarily lead to an even spread along the Pareto front, and that (ii) points in a non-convex part of the Pareto front cannot be obtained (Das & Dennis, 1997). Stochastic approaches, although quite successful over the years (see, e.g., Bhaskar, Gupta, & Ray, 2000; Mitra, Majumdar, & Raha, 2004; Silva & Biscaia, 2003 and the references therein), (i) may become time consuming due to the repeated model simulations required, (ii) are less suited to incorporate constraints exactly, and (iii) are limited to rather low dimensional search spaces. This last aspect restricts the control discretisations to coarse approximations.

To mitigate these drawbacks, several novel scalarisation-based multi-objective techniques, i.e., Normal Boundary Intersection (NBI) (Das & Dennis, 1998), Normalised Normal Constraint (NNC) (Messac, Ismail-Yahaya, & Mattson, 2003; Messac & Mattson, 2004) and Enhanced Normalised Normal Constraint (ENNC) have been integrated with direct optimal control techniques (Abo-Ghander et al. 2010; Logist, Van Erdeghem, & Van Impe, 2009). In addition, these techniques have been implemented in the freely available ACADO Multi-Objective toolkit (Logist, Houska, Diehl, & Van Impe, 2010). The rationale is that this integration overcomes the disadvantages of the Weighted Sum, while still allowing the exploitation of fast deterministic solvers. Hence, the aim of this paper is to illustrate the usefulness of ACACO Multi-Objective as a tool to facilitate real-time decision making for dynamic chemical processes. To this end, several case-studies are presented, starting from a conceptual problem and adding gradually more complexity. Moreover, to the best of the authors' knowledge, ACADO Multi-Objective is one of the first optimal control packages that provides systematic multi-objective optimisation features.

2. Problem formulation

In general, a multiple objective optimal control problem can be formulated as follows.

$$\min_{\mathbf{x}(\xi),\mathbf{u}(\xi),\mathbf{p},\xi_f} \{J_1, \ldots, J_m\} \tag{1}$$

subject to:

$$\frac{d\mathbf{x}}{d\xi} = \mathbf{f}(\mathbf{x}(\xi), \mathbf{u}(\xi), \mathbf{p}, \xi) \quad \xi \in [0, \xi_f], \tag{2}$$

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$$\mathbf{0} = \mathbf{b}_c(\mathbf{x}(0), \mathbf{x}(\xi_f), \mathbf{p}), \tag{3}$$

$$\mathbf{0} \geq \mathbf{c}_p(\mathbf{x}(\xi), \mathbf{u}(\xi), \mathbf{p}, \xi), \tag{4}$$

$$\mathbf{0} \geq \mathbf{c}_t(\mathbf{x}(\xi_f), \mathbf{u}(\xi_f), \mathbf{p}, \xi_f). \tag{5}$$

Here, $\mathbf{x}$ are the state variables. $\mathbf{u}$ are the control variables and $\mathbf{p}$ denote the parameters to be optimised. The vector $\mathbf{f}$ represents the dynamic system equations (on the interval $\xi \in [0, \xi_f]$) with initial and terminal boundary conditions given by the vector $\mathbf{b}_c$. The vectors $\mathbf{c}_p$ and $\mathbf{c}_t$ indicate respectively path and terminal inequality constraints on the states and controls. Each individual objective function can consist of both Mayer and Lagrange terms.

$$J_i = h_i(\mathbf{x}(\xi_f), \mathbf{p}, \xi_f) + \int_0^{\xi_f} g_i(\mathbf{x}(\xi), \mathbf{u}(\xi), \mathbf{p}, \xi) d\xi. \tag{6}$$

The admissible set $\mathcal{S}$ is defined to be the set of feasible points $\mathbf{y} = (\mathbf{x}(\cdot), \mathbf{u}(\cdot), \mathbf{p}, \xi_f)$ that satisfy the dynamic equation as well as the boundary, path and terminal constraints in the above multi-objective optimal control problem.

In multi-objective optimisation, typically no single optimal solution exists, but a set of Pareto optimal solutions must be obtained.

A point $\mathbf{y}_a \in \mathcal{S}$ is Pareto optimal if and only if there is no other point $\mathbf{y}_b \in \mathcal{S}$ with $J_i(\mathbf{y}_b) \leq J_i(\mathbf{y}_a)$ for all $i \in \{1, \ldots, m\}$ and $J_j(\mathbf{y}_b) < J_j(\mathbf{y}_a)$ for at least one $j \in \{1, \ldots, m\}$.

Broadly speaking, a solution is called Pareto optimal if there exists no other feasible solution that improves one objective function without worsening another.

3. ACADO Multi-Objective

ACADO Multi-Objective extends the ACADO toolkit for automatic control and dynamic optimisation (Houska, Ferreau, & Diehl, 2011) with several multi-objective approaches. Due to the self-contained object-oriented, C++implementation, the toolkit (i) is easy-to-use, (ii) does not require third-party software, and (iii) allows a flexible control over algorithmic settings.

The idea behind ACADO Multi-Objective is the integration of efficient multi-objective scalarisation techniques with fast deterministic direct optimal control approaches (Logist, Houska, et al., 2010). Scalarisation methods convert the original multi-objective optimisation problem into a (series of) parametric single-objective optimisation problem whose solution each time yields one point of the Pareto set. By consistently varying the method's parameter(s) (often referred to as *weights*) an approximation of the Pareto set is obtained. Despite its intrinsic drawbacks, combining the different objectives into a convex Weighted Sum (WS) is still one of the most popular scalarisation methods. NBI and NNC are alternative approaches that mitigate the WS drawbacks. Direct optimal control approaches transform the original infinite dimensional optimal control problem via discretisation into a finite dimensional Non-Linear Program (NLP). Sequential strategies (e.g., Single Shooting (SiS)) discretise only the controls, leading to small but dense NLPs. In contrast, simultaneous approaches (e.g., Multiple Shooting (MuS) and Orthogonal Collocation) discretise both the controls and states, resulting in large but structured NLPs. The NLPs can be solved efficiently by deterministic optimisation routines, which exploit the sparsity.

A number of optimal control packages exist, e.g., (i) commercial software as gPROMS (Process System Enterprise Limited, 2010) and PROPT (Tomlab Optimization Inc, 2010) and (ii) non-commercial codes as DynoPC (Lang & Biegler, 2007), MUSCOD-II (Leineweber, Bauer, Bock, & Schlöder, 2003; Leineweber, Schäfer, Bock, & Schlöder, 2003), DyOS (Schlegel, Stockmann, Binder, & Marquardt, 2005) and DOTcvpSB (Hirmajer, Balsa-Canto, & Banga, 2009). However, it should be noted that none of these packages offer systematic and advanced multi-objective features. Fig. 1 shows the structure of ACADO Multi-Objective. Its features are the following.

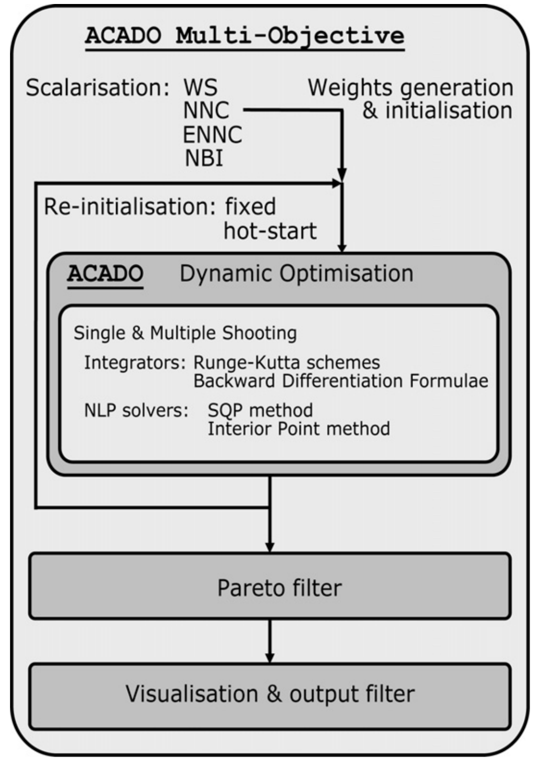

Fig. 1. Schematic overview of ACADO Multi-Objective.

- **Multiple objective optimisation methods.** Four scalarisation methods have been implemented: Weighted Sum, Normal Boundary Intersection, Normalised Normal Constraint and Enhanced Normalised Normal Constraint. The implementation is generic such that, in principle, problems with any number of objectives can be tackled.
  - **Weighted Sum (WS).** The convex Weighted Sum of the individual objectives is still most often used in practice:

$$\min_{\mathbf{y} \in \mathcal{S}} J_{WS} = \sum_{i=1}^{m} w_i J_i(\mathbf{y}), \tag{7}$$

  with a *scalarisation parameter* or *weight vector* $\mathbf{w} = [w_1, w_2, \ldots, w_m]^\top \in \mathbb{R}_+^m$ (with $\sum_{i=1}^m w_i = 1$). However, it exhibits as drawbacks that (i) the returned solutions strongly depend on the scale and scaling of the objectives, (ii) a uniform variation of the weights does not necessarily result in an even spread on the Pareto set and (iii) points in non-convex regions of the Pareto set cannot be obtained (Das & Dennis, 1997).
  - **Normal Boundary Intersection (NBI).** NBI (Das & Dennis, 1998) has been developed based on geometrically intuitive arguments in order to overcome the deficiencies of the WS. The multi-objective optimisation problem is reformulated as follows:

$$\max_{\mathbf{y} \in \mathcal{S}, l \in \mathbb{R}} l \tag{8}$$

$$\text{s.t.}: \quad \mathbf{J}^* + \boldsymbol{\Phi}\mathbf{w} - l\boldsymbol{\Phi}\mathbf{e} = \mathbf{J}(\mathbf{y}), \tag{9}$$

  with $\mathbf{J}^* = [J_1^*, J_2^*, \ldots, J_m^*]^\top$ the *utopia point* which contains the minima of the individual objective functions $J_i(\mathbf{y}_i^*)$, and $\boldsymbol{\Phi}$ the *pay-off* matrix. In this matrix the ith column contains the vector $\mathbf{J}(\mathbf{y}_i^*) - \mathbf{J}^*$. Similar to the WS, the vector $\mathbf{w}$ represents the scalarisation parameters. The rationale behind NBI is to maximise