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Bi-objective optimization of dynamic systems by continuation methods

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ABSTRACT

As a proof of concept the properties of path-following methods are studied for multi-objective optimization problems involving dynamic systems (also called multi-objective dynamic optimization or multi-objective optimal control problems), which have never been presented before. Two case studies with two objectives are considered to cover convex, as well as non-convex trade-off curves or Pareto sets. In order for the method to be applicable, the infinite dimensional dynamic problems have to be discretized and scalarization parameters have to be introduced, which leads to large-scale parametric nonlinear optimization problems. For both the chemical tubular reactor and the fed-batch bioreactor case study it is found that a path-following continuation approach is able to compute the Pareto fronts accurately and efficiently. A branch switching technique is required whenever a constraint switches from active to inactive or vice versa. When dealing with non-convex problems, a technique for detecting inflection points is required. Simple switching techniques are suggested and have been tested successfully.

1. Introduction

Multi-objective or multi-criterion optimization deals with problems of the form:

$$\begin{aligned} \min_x \quad & \left(J_1(x), \ldots, J_q(x)\right), \\ \text{s.t.}\ h_i(x) &= 0, \quad i = 1, \ldots, n, \\ g_j(x) &\le 0, \quad j = 1, \ldots, m, \end{aligned} \tag{1}$$

in which x are the optimization variables, J_k the objective functions, h_i the equality constraints and g_j the inequality constraints. Most decisions of everyday life can be regarded as multi-objective optimization problems, because in most cases our decisions are trade-offs between two or more possibilities. These possibilities, or objectives, can very well be contradictory (Collette and Siarry, 2003). Solutions of these problems are always trade-offs between the objectives. When comparing the solutions, improvement of one objective is only possible at the cost of deterioration of another objective. Such solutions are called *Pareto optimal*. The main difference between single-objective and multi-objective optimization is, that there is not only one optimal solution, but a set of optimal solutions (Deb, 2014). This set is called *Pareto front*. In practice, however, the user or decision maker can only use one of these solutions. The user's choice depends on other, higher level information (Deb, 2014). Therefore it is the main goal of multi-objective optimization to generate many solutions, in order to give the user an accurate overview about what can be chosen from (Deb, 2014). To achieve this goal, Pareto fronts are usually calculated by (i) turning the multi-objective optimization problem into a sequence of single-objective optimization problems or (ii) exploiting evolutionary methods in which a set of candidate solutions gradually evolves to the Pareto set (Miettinen, 1999; Deb, 2002). For methods from the former class, various scalarization techniques, for example weighted sum method, hyperboxing scheme and normalized normal constraint, are known in literature (Marler and Arora, 2004; Logist et al., 2009; Bortz et al., 2014). Typical challenges these methods face, are ensuring a homogeneous distribution of the computed points on the Pareto front, as well as capturing non-convex Pareto fronts. An alternative approach are path-following methods resulting from numerical continuation theory, which have been suggested in literature (Rakowska et al., 1991; Lundberg and Poore, 1993; Seferlis and Hrymak, 1996; Hillermeier, 2001; Gudat et al., 2007; Harada et al., 2007; Potschka et al., 2011; Ringkamp et al., 2012) but so far hardly have been applied to large-scale

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Nomenclature

Theoretical sections

β_0	Fritz–John parameter
ε	tolerance
$\varepsilon_1, \varepsilon_2$	disturbance
Γ	curve length parameter
$\mathcal{L}$	Lagrangian
λ, φ	Lagrange multipliers
ν	Fritz–John state
ω	continuation parameter
Φ	adaptation parameter
Ψ	line through solution space
τ	tangent vector
$\tilde{x}$	augmented state vector
Υ	step size
$\varkappa$	arc-length
ξ	number of iteration steps
ζ	slope of line through solution space
e	unit vector
F	vector of system equations
g	inequality constraint
h	equality constraint
J	cost functional
p	auxiliary scalar equation
s	slack variable
w	weighting factor
w^*	branch switching point
x	state vector
y	solution of algebraic system

Case study 1

α	dimensionless reacton constant
β	dimensionless heat transfer parameter
γ	dimensionless activation energy
δ	dimensionless heat of reaction
c	reactant concentration, mol/l
c_f	feed concentration, mol/l
K	scaling factor
L	length of reactor, m
N	number of grid points
T_f	feed temperature, K
T_W	jacket temperature, K
T_{max}	maximum reactor temperature, K
T_{min}	minimum reactor temperature, K
$T_{W,\max}$	maximum jacket temperature, K
$T_{W,\min}$	minimum jacket temperature, K
v	flow velocity, m/s
x_1	dimensionless reactant concentration
x_2	dimensionless reactor temperature
z	dimensionless spatial coordinate

Case study 2

μ	growth rate, 1/h
π	production rate, g/g h
σ	substrate consumption rate, g/g h
c_s	substrate concentration, g/l
$c_{s,F}$	feed substrate concentration, g/l
N	number of grid points
t	time coordinate, h
t_e	terminal time, h
u	volumetric rate of the feed stream, l/h
x_1	biomass, g
x_2	substrate, g
x_3	product (lysine), g
x_4	fermenter volume, l

optimization problems resulting from the multi-objective optimization of dynamic systems. Path-following methods are able to easily calculate non-convex Pareto fronts. Further, they can be combined with established predictor corrector continuation methods from bifurcation analysis to solve bi-criterial optimization problems with a large number of optimization variables (Thompson Hale, 2005; Pérez, 2014). One of the major challenges of this approach is the occurrence of bifurcations due to constraints (Rao and Papalambros, 1989a,b; Guddat et al., 1990), which has been tackled recently (Martin et al., 2016), but not yet solved for large-scale problems.

The idea discussed in the following is an extension of the predictor corrector continuation algorithm reported in the conference paper (Keßler et al., 2016). It is used as a path-following method for large-scale bi-criterial optimization problems. The application to dynamic models illustrates the feasibility of the method for multi-objective optimization problems with differential equations as constraints, i.e. multi-objective dynamic optimization or multi-objective optimal control problems. Normally such problems are solved using (i) direct optimal control approaches using gradient based methods such as the sequential approach/single shooting and simultaneous approach/multiple shooting (Abo-Ghander et al., 2010; Logist et al., 2012) and (ii) stochastic approaches (Bhaskar et al., 2000; Mitra et al., 2004; Patel and Padhiyar, 2016).

2. Theoretical background

This section introduces the theoretical background of the methods used to produce the results of this work. We will explain the weighted sum scalarization method for solving multi-objective optimization problems and outline its drawbacks and we will show how predictor corrector continuation algorithms work and how they can be used to overcome these drawbacks.

2.1. Weighted sum method

A traditional approach in multi-objective optimization is the weighted sum method (Marler and Arora, 2004). In this approach, the multi-objective optimization problem is reformulated, such that the objectives are combined in a weighted sum, which then gets minimized, to find a Pareto optimal solution (Marler and Arora, 2004)

$$\begin{aligned} &\min_x J(x) = \sum_{i=1}^{q} w_k \cdot J_k(x), \\ &\text{s.t. } h_i(x) = 0, \quad i = 1, \ldots, n \\ &g_j(x) \le 0, \quad j = 1, \ldots, m, \end{aligned} \tag{2}$$

with w_k being the weight or scalarization parameter of the kth objective (Deb, 2014; Das and Dennis, 1997).

2.2. Optimality conditions

The numerical continuation algorithm outlined in Section 2.3 is able to solve algebraic systems. In order for this method to be applicable to optimization problems, we need to transform the optimization problem into an algebraic problem. To do this, we make use of optimality conditions.

The most commonly used necessary conditions for an optimum of a constrained optimization problem are called Karush–Kuhn–Tucker (KKT) conditions.

Inequality constraints can be transformed into equality constraints, by introducing so called *slack variables* s_j (Boyd and Vandenberghe, 2004). That is possible, because $g_j(x) \le 0$ only holds, if there is a $s_j \in \Re$, such that $g_j(x) + s_j^2 = 0$. If the inequality