

Optimal Profile Generation for Distributed Parameter Systems: Combining *Flatness* & Semi-Infinite Optimization

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Abstract

One of the most difficult challenges in the chemical industries is the determination of the profiles (e.g., concentration, temperature, etc.) that should be enforced in a process unit in order to maximize a some measure of performance. This optimal profile calculation problem is exacerbated as many of the process units of interest (e.g., fixed-bed reactors) are Distributed Parameter Systems (DPS) and are often modelled using Partial Differential Equations (PDE). The problem of optimal profile generation is most often tackled via one (or a combination) of two routes: either by discretizing the differential equations to a set of algebraic equations and solving the resulting "conventional" optimization problem, or by using the Maximum Principle and solving using Dynamic Programming. Care must be taken in using these conventional approaches due to how the necessary computations scale with problem size and the required accuracy of solution. Further, in these approaches, it is usually quite difficult to ensure that path constraints (i.e., restrictions on the admissible trajectories throughout the time-span that the optimization problem is posed over) are respected at every point in the trajectory, without a very fine discretization and very large computational requirements.

For lumped dynamical systems, a growing number of researchers have recognized that the geometric structure of the system's dynamics can be exploited to convert the dynamic optimization problem into an equivalent algebraic optimization problem. This transformation is facilitated by a judicious choice of coordinate system for expressing the dynamics and a set of basis functions for parameterizing the dynamics. In this paper, we consider the class of nonlinear systems that are equivalent to controllable linear systems under state-space and feedback transformations. This property of a nonlinear dynamical system is called *flatness* and systems belonging to this class are called linearizable or *flat* systems.

For *flat* systems, the resulting Semi-Infinite Optimization (SIO) problem can be solved to determine the values of the coefficients in the parameterization of the optimal trajectory. The extension of *flatness* of system dynamics, and the resulting benefits to controller synthesis and optimization, to DPS has been investigated by a very few

researchers and limited results are available in the literature (e.g., Rouchon and co-workers, and Lynch and Rudolph).

In this paper, we examine various methods to transform PDE models to sets of Ordinary Differential Equations (ODE) (e.g., spatial discretization, the method of characteristics, modal decomposition / Galerkin's method, etc.). When the resulting ODEs are flat, a conversion to an algebraically constrained SIO problem is possible and the optimization problem can be solved to yield a profile "surface" that describes how the optimal operating profile should evolve in time. The paper begins with a very brief discussion of the pre-processing steps required for conversion of various forms of PDE models to systems of ODEs, and a discussion of the transformation of ODE constrained dynamic optimization problems to algebraically constrained optimization problems via *flatness*, (including a brief summary of the differential geometric framework necessary for understanding the approach). Then, the solution of the resulting SIO problem is discussed in terms path constraints, solution requirements, and scaling with problem size. Finally, the ideas presented in the paper are demonstrated with some problems taken from the literature.

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