203a Analysis and Formulation of a Class of Complex Dynamic Optimization Problems

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Dynamic process optimization aims at providing an optimal operational strategy using rigorous mathematical optimization techniques. Dynamic process systems are frequently modeled using Differential Algebraic Equations (DAEs), and from a mathematical viewpoint, optimization of such a system is an optimal control problem. In this talk we will analyze some open questions that are associated with Nonlinear Programming (NLP) based methods for solving optimal control problems.

Although a lot of research has gone into areas such as numerical algorithms for optimal control problems, choice of discretization schemes and meshing; there are a number of open questions that need to be addressed. With respect to direct transcription (simultaneous approach) of optimal control problems, some of the fundamental questions that need to be addressed are: "Does the solution of the discretized NLP converge to true solution of the original optimal control problem as the discretization size (step size h) is made smaller and smaller? If so for what classes of problems, and under what set of assumptions? What are the rates of convergence as a function of discretization size? Can the NLP multipliers be used to construct approximate adjoint profiles?" We will try to address some of these issues in this talk.

For unconstrained optimal control problems (ODEs + objective function), and for optimal control problems with final-time equality constraints (ODEs + objective function + final-time equality constraints) we analyze the direct transcription problem discretized using collocation at Radau points. Radau collocation offers the highest precision after Gauss quadrature, but it has the added advantage that the end point of a mesh is a collocation point. This allows one to set constraints easily at the end point of an element. Also Radau collocation is well suited for stiff ODEs (L-stable), initial value DAEs, and is algebraically stable. We analyze convergence from a Nonlinear Programming (NLP)/matrix algebra perspective. This enables us to predict the norms of various constituents of a matrix that is ``close" to the KKT matrix of the discretized problem. We will present the convergence rates for the various components, for a sufficiently small discretization size, as functions of the discretization size and the number of collocation points. We will illustrate this using several test examples. As an outcome we also have an adjoint estimation procedure given the Lagrange multipliers for the large scale NLP, which finds applications in a number of areas such as error analysis, mesh refinement, and real time optimization using the method of neighboring extrema. The result can also be extended to problems with final-time equality constraints, and the analysis can be linked to the concept of controllability in a very systematic manner.

The above analysis requires that the resulting NLPs satisfy Linear Independence Constraint Qualification (LICQ) and Sufficient Second-Order Conditions (SSOC). SSOC requires the reduced Hessian to be positive definite. The conditioning of the problem requires the reduced Hessian to satisfy certain order properties. We will then treat two cases where these assumptions fail to hold – totally singular optimal control problems and path constrained optimal control problems. We will present some numerical experiments on the conditioning of the reduced Hessian for totally singular control problems. We will also present some simple observations that can be used to solve totally singular problems using the indirect approach (Pontryagin's maximum principle) using collocation based methods. This avoids the need to differentiate the high-index constraints that arise in such systems. We will also present some preliminary results on constraint qualifications for discretized path constrained problems.

The addition of convergence results, an adjoint estimation procedure, and further analysis on singular and path constrained optimal control problems; makes NLP based methods more reliable and a preferred choice for solving dynamic optimization problems.