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SHORT NOTE

SOLUTION OF DYNAMIC OPTIMIZATION PROBLEMS BY SUCCESSIVE QUADRATIC PROGRAMMING AND ORTHOGONAL COLLOCATION

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Abstract—Current strategies for optimization of dynamic systems usually require repeated solution of the differential equation model and may therefore be inefficient. This note explores the use of orthogonal collocation to reduce the dynamic optimization problem to an equality constrained nonlinear program (NLP). The NLP is then solved using a strategy that simultaneously converges and optimizes the algebraic model. Using a small example for comparison, significant reductions in computational effort are observed.

INTRODUCTION

Optimal control and estimation problems are currently solved by embedding a differential equation solver into the optimization strategy. The optimization algorithm chooses the control profile or parameter estimates and requires the differential equation routine to solve the equations and evaluate the objective and constraint functionals at each step. Two popular methods for optimal control that follow this strategy are Control Vector Iteration (CVI) and Control Vector Parameterization (CVP). CVI requires solution of the Euler–Lagrange equations and minimization of the Hamiltonian while CVP involves repeated differential equation solutions driven by direct search optimization[1].

Both methods can be prohibitively expensive even for small problems because they tend to converge slowly and require solution of differential equations at each iteration. In this note we introduce a method that avoids this requirement by simultaneously converging to the optimum while solving the differential equations. To do this we apply orthogonal collocation to the system of differential equations and convert them into algebraic ones. We then apply an optimization strategy that does not require satisfaction of equality constraints at each iteration. Here the method is applied to a small initial value, optimal control problem, although we are by no means restricted to problems of this type.

METHOD DEVELOPMENT

Unlike finite difference ODE solvers, orthogonal collocation applies a polynomial approximation to the differential equation and requires satisfaction of the equation at discrete collocation points, the zeros of orthogonal polynomials[2]. The polynomial solution is thus a continuous function of t that is often as accurate as a finite difference solution using many more points. For example, the polynomial approximation for initial value problems defined over a finite interval is:

$$y_n = y_0 + t \sum_{i=1}^{n} a_i P_{i-1}(t) \tag{1}$$

were a_i are the unknown coefficients and P_{i-1} is the $(i-1)$ order Legendre polynomial.

The coefficients a_i in (1) can be found by substituting $y_n(t)$ into the initial value problem: $(\mathrm{d}y/\mathrm{d}t) = f(y, t)$; $y(0) = y_0$ and solving: $(\mathrm{d}y_n/\mathrm{d}t) - f(y_n, t) = 0$, at discrete points t_i which are the roots of $P_n(t) = 0$. This system can be solved by Gaussian elimination if $f(t, y)$ is linear or by Newton's method if $f(t, y)$ is nonlinear. In either case, the system of ODE's is converted into algebraic equations.

Recently, optimization techniques have been developed[3, 4] that solve algebraic equality constrained problems without requiring satisfaction of the equations at each iteration. Among the most promising of these is the Successive Quadratic Programming (SQP) [4] algorithm. Loosely speaking, this method linearizes inequality and equality constraints and constructs a convex quadratic objective function from gradients of the objective and constraint functions. The resulting quadratic program (QP) can be solved using any standard, finite-step QP algorithm (e.g. [5, 6]). Solution of the QP determines the search direction while a one-dimensional mimimization along this direction locates the next point. Here, only the linearized sets of equality constraints are solved by the QP. As SQP converges to the optimum, the solution of the linearized sets converges to the solution of the equality constraints. In fact, if no degrees of freedom are present for optimization, the SQP algorithm reduces to Newton's method.

Because we no longer need to solve the collocation equations at each iteration, this Simultaneous Optimization and COLLocation (SOCOLL) method can prove to be very powerful for optimization problems described by differential equations.

Consider the following initial value optimization (Mayer optimal control) problem:

$$\min_{\{u(t),\, q\}} F[y(t_f), u(t_f), q, t_f]$$

$$\begin{aligned} \text{s.t.}\quad & \mathrm{d}y/\mathrm{d}t = f(y, u, q, t) \\ & h(y, u, q, t) = 0 \\ & g(y, u, q, t) \le 0 \end{aligned} \tag{2}$$

where $u(t)$ are the continuous control variables, $y(t)$ are the state variables, q are the constant control parameters, h are the algebraic equality constraints, g are the algebraic inequality constraints, F is the objective functional and t_f is fixed final time.

We can substitute polynomial approximations: $y_n = y_0 + t\sum_{i=1}^{N} a_i P_{i-1}$ for $y(t)$ and include the coefficients a_i as decision variables in the optimization problem. However, it is difficult to provide bounds and starting points for these coefficients because they have no physical significance and thus no *a priori* estimated ranges. To remedy this, an equivalent formulation is found by writing the approximation as a Lagrange interpolation polynomial:

$$y_n(t) = \sum_{i=0}^{n} y_i l_i(t) \quad \text{where } l_i(t) = \prod_{\substack{j=0\\ j\neq i}}^{n} (t-t_j)/(t_i - t_j). \quad (3)$$

Here $t_0 = 0$ and t_i, $i = 1, n$, are zeros of an nth order Legendre polynomial defined from 0 to t_f. Choosing $y_i \equiv y_n(t_i)$ as decision variables for the optimization problem, it is now much easier to supply meaningful bounds and starting points from physical insight about the problem. Other decision variables are the constant parameters, q (if present) and coefficients u_i of the polynomial approximation to the control profiles. The control profiles may be approximated by:

$$u_n = \sum_{i=1}^{n} u_i \bar{l}_i(t) \text{ where } \bar{l}_i(t) = \prod_{\substack{j=1\\ j\neq i}}^{n} (t-t_j)/(t_i-t_j) \quad (4)$$

although we are not limited to this form.

This formulation easily accommodates algebraic inequality and equality constraints, g and h, which are often difficult to handle with control vector iteration [7].

Having defined the set of decision variables $x = [y_i, u_i, q]$, we write the ODE's as algebraic equalities at n collocation points. If additional constraints, g, h, at other points in time t_p, are present, these are included in the nonlinear program also. By substituting Eqs. (3) and (4) into (2), the approximated problem now becomes:

$$\min_{\{y_i, u_i, q\}} F(y_n(t_f), u_n(t_f), t_f, q)$$

$$\text{s.t.} \quad r_i = \mathrm{d}y_n(t_i)/\mathrm{d}t - f(y_i, u_i, t_i, q) = 0, \quad i = 1, n \quad (5)$$

$$h(t_p, y_n(t_p), u_n(t_p), q) = 0$$

$$g(t_p, y_n(t_p), u_n(t_p), q) \leq 0$$

$$y_l \leq y_i \leq y_u$$

$$u_l \leq u_i \leq u_u$$

or equivalently:

$$\min_{\{x\}} F(x) \quad (6)$$

$$\text{s.t.} \quad r(x) = 0$$
$$h(x) = 0$$
$$g(x) \leq 0$$
$$x_l \leq x \leq x_u.$$

We now simply apply the SQP method to (6). At each iteration, k, SQP sets up and solves the QP:

$$\min_{\{d\}} \nabla F(x^k)^T d + \frac{1}{2} d^T B^k d$$

$$\text{s.t.} \quad r(x^k) + \nabla r(x^k)^T d = 0$$

$$h(x^k) + \nabla h(x^k)^T d = 0$$

$$g(x^k) + \nabla g(x^k)^T d \leq 0$$

$$x_l \leq x^k + d \leq x_u$$

to determine the search direction, d, for the next iterate x^{k+1}. Here the B^k matrix is constructed from gradient information at previous iterations.

This approach yields an implicit othogonal collocation solution to the ODE's, is easy to apply and converges to the optimum superlinearly. To illustrate performance of this method, consider the following optimal control problem [1].

EXAMPLE

A batch reactor operating over a one hour period produces two products according to the parallel reaction mechanism: $A \rightarrow B$, $A \rightarrow C$. Both reactions are irreversible and first order in A and have rate constants given by:

$$k_i = k_{io} \exp\{-E_i/RT\} \qquad i = 1,2$$

where

$$k_{10} = 10^6/s$$

$$k_{20} = 5.10^{11}/s$$

$$E_1 = 10000 \text{ cal/gmol}$$

$$E_2 = 20000 \text{ cal/gmol}.$$

The objective is to find the temperature-time profile that maximizes the yield of B for operating temperatures below 282°F. The optimal control problem is therefore:

$$\text{Max} \quad B(1.0)$$

$$\text{s.t.} \quad \frac{\mathrm{d}A}{\mathrm{d}t} = -(k_1 + k_2)A$$

$$\frac{\mathrm{d}B}{\mathrm{d}t} = k_1 A$$

$$A(0) = A_0$$

$$B(0) = 0$$

$$T \leq 282°F.$$

Introducing the following transformations:

$$y_1 = \frac{A}{A_0} \; y_2 = \frac{B}{A_0} \; u = k_1, \frac{u^2}{2} = k_2$$

simplifies the optimization problem to:

$$\text{Max} \quad y_2(1.0)$$

$$\dot{y}_1 = -(u + u^2/2)y_1$$

$$\dot{y}_2 = uy_1$$

$$y_1(0) = 1, \; y_2(0) = 0$$

$$0 \leq u \leq 5.$$

Note that the control variable $u(t)$ is the rate constant k_1 and directly corresponds to temperature. This insight eliminates the exponential terms and simplifies the structure of the problem.

The simultaneous optimization and collocation (SOCOLL) method was compared to the two traditional methods for solving optimal control problems: control vector iteration (CVI) and control vector parameterization (CVP). With CVI, the Hamiltonian:

$$H = -\lambda_1(u + u^2/2)y_1 + \lambda_2 u y_1$$

is maximized with respect to $u(t)$. Given an initially guessed control profile, the algorithm first integrates the state equations forward in time to get y, then the adjoint equations ($\dot{\underline{\lambda}} = -\partial H/\partial \underline{y}$) backward in time to obtain $\underline{\lambda}$. The control profile, $\underline{u}(t)$, is then undated using $\partial H/\partial u$. Here we apply the conjugate gradient algorithm of Lasdon *et al.*[8], with the method of Pagurek & Woodside[9] used to handle control bounds. The CVP method was much more straightforward; the control profile was defined by feedback terms in y_1, that is $u = b_0 + b_1 y_1 + b_2 y_1^2$. Optimal values for b_i were found by applying the Complex method of Box[10] to the optimization problem. Both CVI and CVP used the DGEAR subroutine[11], a version of Gear's method for stiff initial value problems, to solve the ODE's. For this problem the converged solution to CVI can be made arbitrarily accurate by specifying tolerances for the ODE solver and the optimality conditions. (All tolerances in this study were set to 10^{-6}.) With CVP, the final control profile is optimal only with respect to a linear combination of basis functions and can never be better than with CVI.

Using the SOCOLL method, the problem was first approximated by Lagrange interpolation polynomials for n ranging from 1 to 5. Because the control profile is only specified at n collocation points, its approximating polynomial (4) is of one order less than the polynomial for y. To provide a fair comparison between CVI, CVP and SOCOLL, the starting points for y_1 and y_2 were set to values of the initial feasible simulation at the collocation points. The three methods were compared for two initially guessed constant profiles: $u(t) = 1.0$ and $u(t) = 5.0$. These correspond to operation at temperatures of 196 and 282°F, respectively, for the entire reaction time.

The results are presented in Table 1. Starting from either profile, the CVI and SOCOLL methods converged to optimal points. The SOCOLL methods were much faster and their maxima, as n increases, approach the optimum obtained with CVI from above. Note that the 5 point SOCOLL solution is within 0.5% of the CVI optimum, although CVI required from 2.5 to 8.7 times as much computational effort.

Surprisingly, the CVP method did not require excessive computational effort. This is due to the small number of decision variables and the ease in solving the equations with DGEAR. It should also be mentioned that three additional runs of the CVP method were needed in order to establish judicious bounds for values of b_i. These are not shown in Table 1. Often, these methods can be prohibitive because direct search methods are slow to converge, especially for large problems, and, of course, because the bounds on b_i cannot be specified *a priori*. The CVP optimum is 0.8%

Table 1. Comparison of methods

Starting Profile u(t) = 1.

Method	CPU Secs.*	Optimum	No. Iterations
1 pt. SOCOLL	0.84	0.66667	9
2 pt. SOCOLL	1.44	0.59438	11
3 pt. SOCOLL	5.64	0.59308	30
4 pt. SOCOLL	11.83	0.57858	41
5 pt. SOCOLL	17.92	0.57661	44
5 pt. SOCOLL (clipped)	14.12	0.57263	30
CVI	45.16	0.57349	20**
CVP	30.07	0.56910	377***

Starting Profile u(t) = 5.

Method	CPU Secs.*	Optimum	No. Iterations
1 pt. SOCOLL	1.38	0.66667	21
2 pt. SOCOLL	2.41	0.59438	20
3 pt. SOCOLL	9.69	0.59308	52
4 pt. SOCOLL	14.92	0.57858	53
5 pt. SOCOLL	26.06	0.57661	62
5 pt. SOCOLL (clipped)	32.60	0.57275	66
CVI	226.35	0.57322	58**
CVP	18.61	0.56910	213***

* Execution Times, DEC-20 Computer, Carnegie-Mellon Computation Center

** Number of CVI Profile Updates

*** Number of Objective Function Calls

lower than the CVI maximum even though CVP solved the differential equations as accurately as CVI did. Moreover, the CVP objective can never reach the CVI optimum because the functional choice for $u(t)$ is incomplete. Since the SOCOLL approximation approaches the true optimum as n increases, its results are not as restrictive as CVP's.

Table 2 compares values of the optimal control profile for CVI, CVP and 5 point SOCOLL at the collocation points. Here the agreement between CVI and SOCOLL is much better than with CVI and CVP. Figure 1 shows the optimal control profiles for the methods compared above. Here we observe a limitation of SOCOLL. As with other collocation methods, SOCOLL cannot approximate steep gradients well unless higher order terms or collocation on finite elements are used. Also, constraints on the control trajectory can easily be applied and satisfied at collocation points but may not be satisfied elsewhere (e.g. between 0.95 and 1.0). Again, collocation on finite elements embedded in SOCOLL can handle this limitation. For this example, however, we can obtain a better solution through some insight into the control trajectory. We note that the value of u_i is 5.0 at the last collocation point. Since the trajectory defined by the Lagrange interpolation polynomial violates the upper bound on u_n between the last collocation point and 1.0, we merely "clip" $u(t)$ by defining it as:

$$u(t) = \min(5.0, u_n(t)).$$

Since $u_n \geq 5.0$ only after the last collocation point (0.953), the control profile can be clipped without affecting the collocation constraints or continuity and differentiability (wrt x) of the objective function. We applied the following clipping procedure:

If $u_n(1.0) \geq 5.0$, find $t_c \in [0.953, 1.0]$ where $u_n = 5$. Set $u(t) = 5$ for $t \in [t_c, 1]$; the variables $y_1(t)$ and $y_2(t)$, $t \in [t_c, 1]$ are calculated by:

$$y_1(t) = y_1(t_c)\exp[-17.5(t - t_c)]$$

$$y_2(t) = y_2(t_c) + (-5/17.5)y_1(t_c) \times [\exp\{-17.5(t - t_c)\} - 1]$$

since the differential equations are linear once u is constant. The clipped SOCOLL optimum is within 0.1% of the CVI optimum. Agreement with CVI at collocation points is not as good as with the unclipped SOCOLL method but its control trajectory is bounded between 0 and 5 and agrees reasonably well with CVI and Fig. 1.

These results are indicative of applications to other initial value optimal control problems. The accuracy of the solution is limited only by the error introduced by the collocation procedure. Once a problem formulation has been chosen that insures that collocation can be applied accurately, then the accuracy of the solution to the optimal control problem is subject only to the tolerance on the optimality conditions.

Table 2. Optimal profile at collocation points

t	CVI	5 pt SOCOLL	5 pt SOCOLL (clipped)	CVP
0.0469	0.76702	0.76074	0.78692	0.83969
0.2308	0.87847	0.84027	0.97820	0.77699
0.5000	1.15798	1.16616	1.04957	1.11780
0.7692	1.85941	1.66126	2.30851	2.27606
0.9531	5.00000	5.00000	4.99738	3.34930

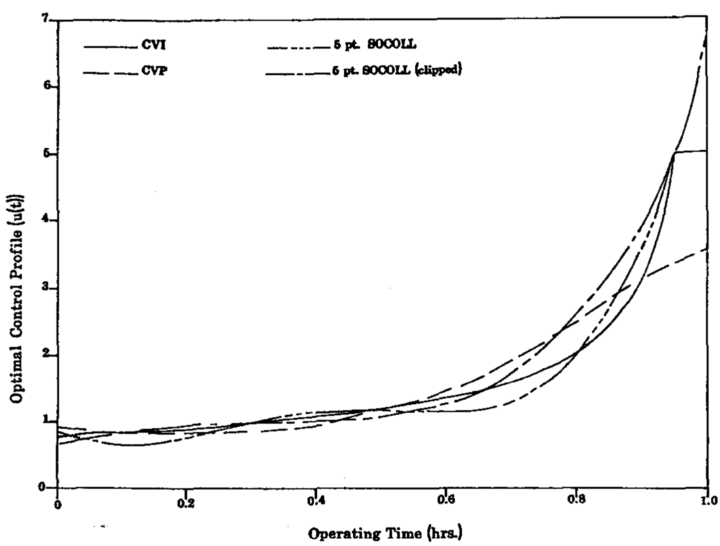

Fig. 1. Comparison of optimal profiles —— CVI; — ---— 5pt. SOCOLL— — CVP— -— 5 pt SOCOLL (clipped).

The implementation of the SQP algorithm used here also has local superlinear and global convergence properties. It operates in a much smaller space than the CVI algorithm and will generally be more accurate than the CVP algorithm because it is not as limited by the basis functions for the optimal control profile.

CONCLUSIONS

A simple method has been described for efficiently solving dynamic optimization problems. For a small optimal control problem we show that very good approximate optima can be found with relatively little computational effort. The formulation presented above can easily be extended to handle collocation on finite elements (for stiff systems of ODE's) as well as two point and other boundary value problems. A key point observed in the solution of this small problem is that the system of differential equations is never solved explicitly. Instead the optimization algorithm converges simultaneously to solve the set of ODE's and find the optimal trajectory. Thus, the often considerable computational effort of solving a set of ODE's at each iteration is saved.

To conclude we note the following points:

(1) The SOCOLL strategy handles stiff ordinary differential equations without difficulty since it yields an implicit collocation solution.

(2) The solution of this method is only limited by the accuracy of the collocation procedure.

(3) The optimization procedure solves the collocation equations only once. It converges to the optimum and the equation solutions simultaneously.

(4) The optimal control problem is thus transformed to a nonlinear program. Multiple boundary conditions and point constraints that cannot be handled easily with CVI and CVP present no problem within this framework.

Therefore, we can expect the SOCOLL method to be an efficient and effective tool for solving a wide variety of dynamic optimization problems. The results given here can be generalized to larger, more complicated problems by applying finite element collocation.

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