Solution of Dynamic Optimization Problems by Successive Quadratic Programming and Orthogonal Collocation

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Abstract

Optimal control and estimation problems are currently solved by embedding a differential equation solv
nto the optimization strategy. The optimization algorithm chooses the control profile, or paramet
stimates, and requires the differential equation routine to solve the equations and evaluate the objective ar
onstraint functionals at each step. Two popular methods for optimal control that follow this strategy a
Control Vector Iteration (CVI) and Control Vector Parameterization (CVP). CVI requires solution of th
Euler-Lagrange equations and minimization of the Hamiltonian while CVP involves repeated differenti
quation solutions driven by direct search optimization [1].

Both methods can be prohibitively expensive even for small problems because they tend to converge slow
nd require solution of differential equations at each iteration. We introduce a method that avoids th
equirement by simultaneously converging to the optimum while solving the differential equations. To c
his, we apply orthogonal collocation to the system of differential equations and convert them into algebra
nes. We then apply an optimization strategy that does not require satisfaction of equality constraints at eac
teration. Here the method is applied to a small initial value optimal control problem, although we are by n
neans restricted to problems of this type.

I. Method Development

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

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

vhere

a_i - unknown coefficients

P_{i-1} - (i-1) order Legendrc polynomial.

[Tie coefficients a_i in (1) can be found by substituting $y_n(t)$ into the initial value problem: -$ =f(yj)\ y(Q)= >0 and solving: -^——/(>VO = 0. at discrete points /,- which arc the roots of $P_n(t) = 0$. This system can b ;olved by Gaussian elimination if $f(t,y)$ is linear or by Newton's method if $f(t,y)$ is nonlinear. In either cas< he system of ODF/s is converted into algebraic equations.

Recently, optimization techniques have been developed [3, 4] that solve algebraic equality constrainc)roblems without requiring satisfaction of the equations at each iteration. Among the most promising c hese is the Successive Quadratic Programming (SQP) [4] algorithm. Loosely speaking, this method linearize nequality and equality constraints and constructs a convex quadratic objective function from gradients of th)bjectivc and constraint functions. The resulting quadratic program (QP) can be solved using any standan Inite-step QP algorithm [5, 6]. Solution of the QP determines the search direction while a one-dimension; ninimization along this direction locates the next point. Here, only the linearized sets of equality constrain ire solved by the QP. As SQP converges to the optimum, the solution of the linearized sets converges to th •olution of the equality constraints. If no degrees of freedom are present for optimization, the SQP algorithi educes to Newton's method.

Because we no longer need to solve the collocation equations at each iteration, this Simultaneoi

$$\underset{\{u(t),q\}}{Min} \quad F[y(t_f), u(t_f), q, t_f] \tag{2}$$

$$\text{s.t.} \quad \frac{dy}{dt} = f(y, u, q, t)$$

$$h(y, u, q, t) = 0$$

$$g(y, u, q, t) \leq 0$$

where

u(t) - continuous control variables

y(t) - state variables

q - constant control parameters

h - algebraic equality constraints

g - algebraic inequality constraints

F - objective functional

t_f - fixed final time

We can substitute polynomial approximations $y_n = y_o + t \sum_{i=1}^{N} a_i P_{i-1}$ for y(t) and include the coefficients 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, thus no apriori estimated ranges. To remedy this, an equivalent formulation is found by writing the approximation as a Lagrange interpolation polynomial:

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

Here $t_o = 0$ 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

This formulation easily accomodates algebraic inequality and equality constraints, g and h, which are ofte lifficult to handle with control vector iteration [7].

Having defined the set of decision variables x = [y^ u^ q], we write the ODFs as algebraic equalities at allocation points. If additional constraints g, h at other points in time t_p are present, these arc included in th lonlinear program also. By substituting equations (3) and (4) into (2), the approximated problem no^ >ecomes:

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

$$\text{s.t.} \quad r_t = dy_n(tj)/di - j\backslash y_b\ u_b\ t_b\ q) = 0 \qquad /= 1, n$$

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

$$g(t_p, y_n(t_p) l u_n(t_p l q) <= 0$$

$$y_l \leq y_i \leq y_u$$

(5

>requivalently:

$$\min \quad F(x)$$

$$\text{s.t.} \quad r(jc) = 0$$

$$h(x) = 0$$

$$g(x) \leq 0$$

$$x_j \leq x \leq x_u$$

(6

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

$$\min_{\{d\}} \quad \nabla F(x^k)^T d + \backslash d^T B^k d$$

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

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

2. Example

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

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

(8

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 temperature below 282°F. Therefore, control problem is:

$$Max \quad B(1{\cdot}0)$$

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

$$\frac{dB}{dt} = k_1 A$$

$$A(0) = A_o$$

$$Max \quad y_2(1.0)$$

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

$$\dot{y}_2 = u y_1$$

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

$$0 \leq u \leq 5 \qquad (1$$

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

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

$$H = -\lambda_1(u + u^2/2)y_1 + \lambda_2 u y_1 \qquad (1$$

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

.utivvigvu IAJ wpuiiiai i^uiiito. IIIV jvyv^v/Lvi^ invuiuuo wv.iv mutu la^ivi anu UJV.II iiia/vuiia, ao J* iu

ipproach the optimum obtained with CVI from above. Note that the 5 point SOCOLL solution is withi).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 sma lumber of decision variables and the ease in solving the equations with DGKAR. It should also b ncntioncd that three additional runs of the CVP method were needed in order to establish judicious bounc br values of *bj*. 'ITiese arc not shown in Table 1. Often, these methods can be prohibitive because direi search methods are slow to converge, especially for large problems, and the bounds on *bj* cannot be specified priori. The CVP optimum is 0.8% lower than the CVI maximum even though CVP solved the differenti; equations as CVI did. Moreover, the CVP objective can never reach the CVI optimum because the function; ;hoice for u(t) is incomplete. Since the SOCOLL approximation approaches the true optimum as n increase ts results arc not as restrictive as CVFs.

Table 2 compares values of the optimal control profile for CVI, CVP and 5 point SOCOLL at th allocation points. Here the agreement between CVI and SOCOLL is much better than with CVI and CVI ^igure 1 shows the optimal control profiles for the methods compared above. Here we observe a limitation (SOCOLL. As with other collocation methods, SOCOLL cannot approximate steep gradients well unle: ligher order terms or collocation on finite elements are used. Also, constraints on the control trajectory ca easily be applied and satisfied at collocation points but may not be satisfied elsewhere (e.g., between 0.95 an L0). Again, collocation on finite elements embedded in SOCOLL can handle this limitation. For th example, however, we can obtain a better solution through some insight into the control trajectory. We not hat the value of u_i is 5.0 at the last collocation point. Since the trajectory defined by the Lagrang nterpolation polynomial violates the upper bound on u_n between the last collocation point and 1.0, we merel '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 withoi effecting the collocation constraints or continuity and differentiability (wrt x) of the objective function. W applied the following clipping procedure:

if $M_{fl}(1.0) \geq 5.0$, find /^c **[0.953,1.0]** where ^ = 5.

Set w(/)= 5 for /e[/$_c$,1]; the variables $y(t)$ and ^(/), /€ [/$_c$,1] are calculated by:

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

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

,incc the differential equations arc linear once u is constant. The clipped SOCOLL optimum is within'0.1')f the CVI optimum. Agreement with CV1 at collocation points is not as good as with the unclippc JOCOLL method, but its control trajectory is bounded between 0 and 5 and agrees reasonably well with CV tnd Figure 1.

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

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

3. Conclusions

A simple method has been described for efficiently solving dynamic optimization problems. For a sma)ptimal control problem, very good approximate optima can be found with relatively little computation; effort. The formulation presented above can easily be extended to handle collocation on finite elements (fc itiff systems of ODE's) as well as two point and other boundary value problems. A key point observed in th ;olution of this small problem is that the system of differential equations is never solved explicitly. Insteac he optimization algorithm converges simultaneously to solve the set of ODE's and find the optim<

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 CVl and CVP present no problem within this framework.

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

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Figure 1: COMPARISON OF OPTIMAL PROFILES

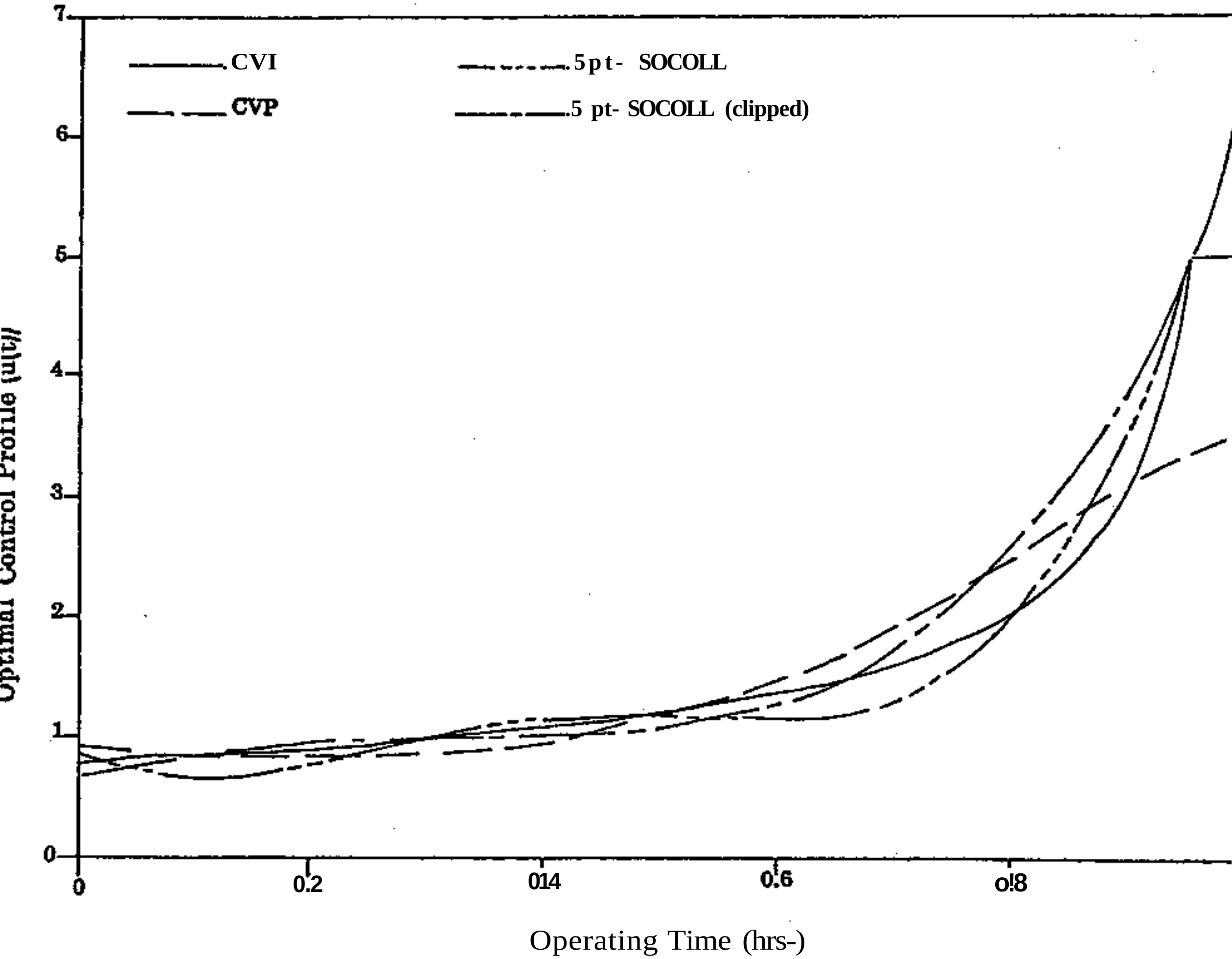

Table 1: COMPARISON OF METHODS

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	45.12	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

Table 2: OPTIMAL PROFILE AT COLLOCATION POINTS

t	CVI	5ptSOCOLL	5ptSOCOLL (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