Singular Optimal Control Computation

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A quadratic functional version of the linear quadratic optimal control problem is employed to develop insights into the computation and theory of singular optimal controls. It is shown that sufficiency, existence, and uniqueness conditions and convergence conditions for gradient-type algorithms require the same basic assumption, namely a positivity assumption on the second-variation operator and an inclusion requirement with regard to the range space of the second variation operator. The theory is interpreted for both the nonsingular and singular problems to show the inherent differences between the two problems. It is shown that the gradient, conjugate gradient, and Davidon-Fletcher-Powell (DFP) algorithms converge if the existence conditions for the optimal control are satisfied, and that the rate of convergence is superlinear for the DFP method applied to nonsingular problems. Operational aspects for improving the rate of convergence on singular problems are discussed along with an informative comparison of the behavior of gradient and accelerated gradient methods on singular problems.

I. Introduction

SINGULAR optimal control problems occur in numerous aerospace applications (e.g., intermediate thrust arcs, aircraft climb performance, steering angle rate constrained problems, etc.) and they typically have been treated as special cases in both theory and computation. It has only been in the last decade that a full set of necessary and sufficient conditions have been developed for the totally singular problem.[1-5] These conditions are similar but different from the associated nonsingular conditions. The computation of singular optimal control subarcs has a reputation for being difficult, although function space conjugate direction methods[6-8] have been shown recently to give relatively good performance in computing singular subarcs.

In computing optimal singular controls, a number of approaches are available: 1) parameterization of the control function, which results in a parameter optimization problem; 2) approximation by a sequence of nonsingular problems[9,10] which can then be attacked by any method; 3) shooting methods (or initial Lagrange multiplier guessing schemes)[10]; and 4) function-space gradient-type techniques.[6,7] Techniques 1 and 3 require a priori knowledge of the sequencing of singular and nonsingular subarcs, whereas the techniques of 4 do not. Thus, emphasis in this research has involved gradient-type methods since singular problems usually consist of multiple subarcs.

Simulations in Refs. 7 and 8 indicate that the function-space Davidon-Fletcher-Powell (DFP) method, an accelerated gradient method, works very well on singular problems. Thus, a theoretical study of the convergence properties of gradient-type methods was undertaken to determine the problem dependence of the convergence properties. The resultant analysis proved to be useful not only in understanding the algorithms, but also in developing a deeper understanding of the singular problem itself.

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In Sec. II the linear quadratic optimal control problem (which is the basis for sufficient conditions and convergence analyses) will be transformed into an unconstrained quadratic functional minimization problem. Properties of the resultant quadratic operator (i.e., the second-variation operator) for both the singular nonsingular cases will be observed. In Sec. III, the nonsingular case will be discussed with respect to both existence of optimal controls and convergence of algorithms. In Sec. IV, the singular case will be presented, and it will be shown that a number of operational problems with singular computation can be explained from this viewpoint. Observations from the theory result in guidelines for the computation of optimal controls when singular subarcs are presented, and these are summarized in Sec. V.

II. Quadratic Functional Aspects of the LQP

Both sufficient conditions for optimal control and convergence studies of algorithms involve expansions in the neighborhood of the optimal solution, resulting in a linear quadratic problem (LQP). Thus, consider:

Minimize

$$J = \tfrac{1}{2}\int_{t_0}^{t_f} [x^T P(t) x + R(t) u^2]\,dt \tag{1}$$

subject to

$$\dot{x} = F(t)x + G(t)u \qquad x(t_0) = x_0 \tag{2}$$

where t_0, t_f are given, $x \equiv n$ vector, $u \equiv$ scalar.

Since the goal of this analysis is to develop insight into the singular problem and its computation, the control will be assumed to be a scalar although all results can be extended easily to the vector control case.

In Ref. 11, an analysis of the performance of the gradient method on the singular problem is presented. Insight into the problem is developed by transforming Eqs. (1) and (2) into an equivalent unconstrained quadratic functional minimization problem. Furthermore, the generalization of the DFP method to optimal control problems (or function space) was accomplished in Ref. 12 only after transforming Eqs. (1) and (2) into a quadratic functional, to which linear operator theory could be applied. The analysis of this paper also requires such a transformation.

Since Eq. (2) is linear, it may be written as

$$x(t) = \phi(t,t_0)x_0 + \int_{t_0}^{t} \phi(t,\tau)G(\tau)u(\tau)\mathrm{d}\tau \equiv Sx_0 + Tu \quad (3)$$

where

$$S: R^n \to L_2^n[t_0,t_f], T: L_2[t_0,t_f] \to L_2^n[t_0,t_f]$$

are linear operators, and

$$L_2^l[t_0,t_f] \equiv \left\{ z(\cdot) \mid \int_{t_0}^{t_f} z(t)^T z(t)\mathrm{d}t < \infty, z(t) \in R^l \right\}$$

Consider the usual inner product on $L_2^l[t_0,t_f]$, i.e.,

$$\langle a(t), b(t) \rangle \equiv \int_{t_0}^{t_f} a(t)^T b(t)\mathrm{d}t \quad a(t), b(t) \in L_2^l[t_0,t_f] \quad (4)$$

Upon substitution of Eq. (3) into Eq. (1), the performance index may be written as

$$J[u] = \tfrac{1}{2}\langle u, Au\rangle + \langle u, w\rangle + J_0 \quad (5)$$

where

$$A \equiv T^*PT + R \quad (6)$$

$$w \equiv T^*PSx_0 \quad (7)$$

$$J_0 \equiv \tfrac{1}{2}\langle Sx_0, PSx_0\rangle \quad (8)$$

The linear operator T^* is the adjoint operator[13] defined by

$$\langle a(t), Tb(t)\rangle = \langle T^*a(t), b(t)\rangle \quad (9)$$

where

$$a \in L_2^n[t_0,t_f] \qquad b \in L_2[t_0,t_f]$$

$$T^*: L_2^n[t_0,t_f] \to L_2[t_0,t_f] \quad (10)$$

The operator A is easily shown to be a self-adjoint operator, i.e., $A^* = A$, by Eq. (9). Thus, the minimization of Eq. (5) (an unconstrained quadratic functional of the control u) is equivalent to the constrained LQP of Eqs. (1) and (2). A major advantage of Eq. (5) with regard to insight is that all existence, sufficient, and convergence conditions involve only characterizations of the linear operators A and w, thus showing the unity of such analyses.

The operator A is called the "second-variation operator" in a sufficient condition analysis, and the "Hessian operator" in a computational algorithm convergence analysis. In both cases the positivity properties of A play a major role.

Definition 1: Let A be a linear, self-adjoint operator defined on $L_2[t_0,t_f]$. Then,

1) A is *positive semidefinite* (denoted $A \geq 0$) if

$$\langle u, Au\rangle \geq 0 \text{ for all } u \in L_2[t_0,t_f] \quad (11)$$

2) A is *positive* (denoted $A > 0$) if

$$\langle u, Au\rangle > 0 \text{ for all } u \neq 0 \qquad u \in L_2[t_0,t_f] \quad (12)$$

3) A is *strongly positive* if there exists an $m > 0$ such that

$$m\langle u,u\rangle \leq \langle u, Au\rangle \text{ for all } u \neq 0 \qquad u \in L_2[t_0,t_f] \quad (13)$$

In finite-dimensional space, positive and strongly positive are equivalent. However, in $L_2[t_0,t_f]$ the difference between positive and strongly positive is the essential difference between a singular and a nonsingular optimal control problem, respectively. Another property of A, assuming that $P(t)$ and $R(t)$ are continuous on $[t_0,t_f]$, is that it is "bounded," i.e., there exists $M < \infty$ such that

$$\langle u, Au\rangle \leq M\langle u,u\rangle \equiv M\|u\|^2 \quad (14)$$

Probably the most important property of a strongly positive operator is that the inverse operator exists and is bounded.

Theorem 1: Suppose A is strongly positive and bounded. Then, A^{-1} exists and is strongly positive and bounded.

For the proof, see Ref. 13, Sec. 104. If an operator A is positive, but not strongly positive, then the inverse operator, A^{-1}, is unbounded. Because of this, the gradient equation for Eq. (5) (i.e., $Au + w = 0$) does not always possess a solution. The existence of a minimizing solution for Eq. (5) is characterized completely as follows.

Theorem 2: The quadratic functional $J[u]$ of Eq. (5) has a minimum solution $\bar{u}$ if and only if: 1) A is positive semidefinite, and 2) w belongs to the range of the operator A (denoted by $w \in R(A)$).

Proof: Since J is twice differentiable, if $\bar{u}$ is a minimum element, then

$$g(\bar{u}) = A\bar{u} + w = 0$$

and

$$\left\langle u, \frac{\mathrm{d}^2 J(\bar{u})}{\mathrm{d}u^2} u \right\rangle \geq 0 \text{ for all } u \in L_2[t_0,t_f]$$

But $A\bar{u} \in R(A)$ implies that $w = -A\bar{u} \in R(A)$. Also, since $\mathrm{d}^2J/\mathrm{d}u^2 = A$, it follows that A is positive semidefinite. Now, suppose $w \in R(A)$. There exists an element $\bar{u}$ such that $A\bar{u} + w = 0$ and

$$J(\bar{u}) = \tfrac{1}{2}\langle \bar{u}, w\rangle + J_0$$

Let u be any element in $L_2[t_0,t_f]$. Then $u = \bar{u} + y$, where $y = u - \bar{u} \in L_2[t_0,t_f]$. After some calculations

$$J(u) = J(\bar{u}) + \tfrac{1}{2}\langle y, Ay\rangle$$

or

$$J(u) - J(\bar{u}) = \tfrac{1}{2}\langle y, Ay\rangle$$

Since A is positive semidefinite, it follows that

$$J(u) \geq J(\bar{u}) \text{ for all } u \in L_2[t_0,t_f]$$

i.e., $\bar{u}$ is a minimum solution for Eq. (5).

It is instructive at this point to consider a simple optimal control example for which $w \notin R(A)$ since properties of the range of the operator are very important in singular problems.

Example 1:

Minimize

$$J_1 = \tfrac{1}{2}\int_0^1 x^2 \mathrm{d}t \quad (15)$$

subject to

$$\dot{x} = u, x(t_0) = x_0 \quad (16)$$

This is the simplest singular problem, and it typically has the additional constraint $|u| \leq 1$. As will be shown, a minimum solution (in the class of continuous functions $x(t)$) does not exist without the $|u| \leq 1$ constraint, except for a single initial condition value. By Eqs. (6) and (7):

$$A = T^*T \text{ where } Tu = \int_0^t u(\tau)\mathrm{d}\tau \quad T^*x = \int_t^1 x(\tau)\mathrm{d}\tau \quad (17)$$

$$w = T^* x_0 \tag{18}$$

Condition 1 of Theorem 2 follows easily from the definition, i.e., for each $u \in L_2[t_0,t_f]$

$$\langle u,Au \rangle = \langle u,T^* Tu \rangle = \langle Tu,Tu \rangle \equiv \| Tu \|^2 \geq 0 \tag{19}$$

and thus A is (at least) a positive semidefinite operator. Thus, existence of an optimal singular control is determined strictly by condition (2), and in particular the initial condition because of the strong dependence of w on x_0. (In more complicated problems this is a typical characteristic of singular subarcs, i.e., the strong dependence upon initial conditions for their existence.) For w to be in $R(A)$, there must exist a control $\tilde{u}$ such that $A\tilde{u} = w$, i.e.,

$$\int_t^l \left[\int_0^s \tilde{u}(\tau) \mathrm{d}\tau \right] \mathrm{d}s = \int_t^l x_0 \mathrm{d}s \tag{20}$$

or

$$\int_t^l \left[\int_0^s \tilde{u}(\tau) \mathrm{d}\tau - x_0 \right] \mathrm{d}s = 0 \tag{21}$$

Since the null space of an integral operator is $\{0\}$, i.e., the zero element, it follows that $w \in R(A)$ only if $x_0 = 0$, as expected. Finally, note that the A-operator for this example is positive (i.e., $\langle u,Au \rangle = \| Tu \|^2 > 0$ for $u \neq 0$ by Eq. (19)), but it is not strongly positive (e.g., consider the control

$$u = \begin{cases} \epsilon^{-1/2} & t \in [0,\epsilon) \\ 0 & t \in (\epsilon,1] \end{cases} \tag{22}$$

for arbitrary $0 < \epsilon < 1$).

By definition, the LQP is singular if $R(t) = 0$, $t \in [t_0,t_f]$; for nonsingular minimization problems, $R(t) > 0$, $t \in [t_0,t_f]$. From Eq. (6), note that the A-operator has a component $T^* PT$ for both types of problems, and thus properties of the $T^* PT$ operator are of interest.

Definition 2: A set S of elements is *bounded* if there exists a constant c such that for all $u \in S$, $\|u\| \leq c$. A set S is *compact* if each sequence $\{u_n\}$ of elements in S contains a convergence subsequence. A linear operator is *completely continuous* if it transforms bounded sets into compact sets.

Theorem 3: The linear operator $T^* PT$ defined in Eq. (6) is a completely continuous operator. For the proof, see Ref. 14, pp. 91-92.

Theorem 4: Suppose $Z: L_2[t_0,t_f] \to L_2[t_0,t_f]$ is a completely continuous operator. If $\{u_k\}$ is a weakly convergent sequence (i.e., $\lim_{k \to \infty} \langle u_k,f \rangle = \langle \tilde{u},f \rangle$ for each $f \in L_2[t_0,t_f]$), then $\{Zu_k\}$ converges uniformly (i.e., $\lim_{k \to \infty} \| Zu_k - Z\tilde{u} \| = 0$). For the proof, see Ref. 13, Sec. 85.

Theorems 3 and 4 are very important in the development of rate of convergence results for nonsingular optimal control problems which are presented in the next section.

III. Nonsingular Case

In this section properties of the nonsingular LQP (i.e., $R(t) > 0$, $t \in [t_0,t_f]$, in Eqs. (1) and (6)) will be summarized for comparison with corresponding properties of the singular problem in the next section, and to show the effectiveness of the function-space DFP method on nonsingular problems. It is well known that if $P(t)$ is positive semi-definite for $t \in [t_0,t_f]$, then the LQP possesses a unique solution. The only way that a solution cannot exist is if $P(t)$ is not positive semidefinite and a conjugate point exists on the interval $[t_0,t_f)$. The conjugate point test is actually a positivity test for the second-variation operator A.

Theorem 5: The operator A of Eq. (5) is bounded and strongly positive if $R(t) > 0$, $t \in [t_0,t_f]$, and the matrix $K(t)$ is finite for each $t \in [t_0,t_f]$, where

$$\dot{K} = -KF - F^T K - P + KGR^{-1} G^T K, \; K(t_f) = 0 \tag{23}$$

Furthermore, if A is strongly positive there exists a unique optimal control for the LQP. For the proof, see Ref. 15, pp. 35-38.

The last part of Theorem 5 is an existence theorem for the nonsingular case of Eq. (5), and it is of interest to compare it with the general existence theorem, Theorem 2. Condition (1) is satisfied since A strongly positive implies $A \geq 0$. Condition (2) follows from the fact that $w \in R(A)$ is always satisfied for a strongly positive operator (i.e., $\tilde{u} = A^{-1} w$ is an element such that $A\tilde{u} = w$, where A^{-1} exists and is bounded by Theorem 1). This implies that if A is strongly positive, then the existence of an optimal solution is not a function of w in Eq. (5), and thus, is not a function of the initial condition x_0 (since A is independent of x_0 and w is strongly dependent upon x_0). This is the fundamental reason why the nonsingular problem is less dependent upon the particular initial condition, whereas the singular problem is not.

As noted in the previous section the analysis of sufficient conditions for optimal control and convergence of algorithms is basically a study of positivity properties of operators. Thus, the hypotheses for the two areas should be the same. Indeed this is the case, as shown in the following theorem.

Theorem 6: Consider the application of the function-space gradient, conjugate gradient, and DFP methods to the problem defined by Eqs. (1) and (2). All of the algorithms converge uniformly (i.e., $\lim_{k \to \infty} \| u_k - \tilde{u} \| = 0$) if A is strongly positive (which is guaranteed if $R(t) > 0$ and the Riccati Equation, Eq. (23), is finite on $[t_0,t_f)$; the sufficient conditions for an optimal control). For the proof, see Ref. 15, pp. 55-58.

From a practical point of view, the rate of convergence is the main factor in the choice of an algorithm. Numerous simulations[6-8] have shown that function space conjugate gradient and DFP methods converge more rapidly than the gradient method on optimal control problems, especially singular problems. Thus, one is led to a theoretical study of the rates of convergence for these algorithms. It is well known that the gradient method has a linear convergence rate for nonsingular problems,[16] i.e.,

$$\lim_{k \to \infty} \frac{\| u_{k+1} - \tilde{u} \|}{\| u_k - \tilde{u} \|} = c \qquad (0 < c < 1) \tag{24}$$

It can also be shown, using arguments similar to those for the development of Eq. (24), that the conjugate gradient and DFP methods converge linearly. However, simulation results indicate a more rapid convergence rate. By noting that the operator A is a sum of a nonsingular component and a completely continuous operator (i.e., Eq. (6) and Theorem 3), a better rate of convergence can be developed.

Theorem 7: Suppose A of Eq. (6) is strongly positive. Then, both the conjugate gradient and the DFP methods converge superlinearly, i.e.,

$$\lim_{k \to \infty} \frac{\| u_{k+1} - \tilde{u} \|}{\| u_k - \tilde{u} \|} = 0 \tag{25}$$

For the proof, see Ref. 16.

To summarize this section, it has been noted that if the nonsingular sufficient conditions are satisfied, then the second variation operator is strongly positive. This allows one to show then that: 1) the existence of nonsingular arcs is not a function of the initial state, 2) all of the gradient-type algorithms mentioned converge uniformly without any further assumptions, and 3) the superlinear rate of convergence of the conjugate gradient and DFP algorithms can be proved without any further assumptions (after noting that the T^*PT-component of the A-operator is completely continuous). As will be shown in the next section, none of these properties hold for the singular case.

IV. Singular Case

In this section, the singular case, i.e., $R(t) \equiv 0$ in Eqs. (1) and (6), will be considered. The format will be to determine results that correspond to Theorems 5-7 of the nonsingular problem. Since $A = T^*PT$ for the singular case, the A-operator is at least a completely continuous operator. With respect to positivity properties, we have the following.

Theorem 8: The operator A of Eq. (5) is bounded and positive (but not strongly positive) for the $R(t) \equiv 0$ case if the following conditions hold:

1) $G^TPG>0$ for each $t \in [t_0,t_f]$ (generalized Legendre-Clebsch condition); (26)

2) $K(t)$ is finite for $t \in [t_0,t_f)$, where

$$\dot{K} = -KF - F^TK - P + [K(FG-\dot{G}) + PG][G^TPG]^{-1} \times [K(FG-\dot{G}) + PG]^T$$

$$K(t_f) = 0 \text{ (generalized Jacobi test)} \tag{27}$$

The complete proof is quite lengthy (see Ref. 15, pp. 39-48), so only the major ideas of the proof will be presented. The Goh transformation

$$v(t) = \int_{t_0}^{t} u(\tau)\mathrm{d}\tau \equiv Wu \tag{28}$$

was employed in Ref. 2 to develop a sufficient condition for singular control, and the same idea is applied here. Note that the Goh transformation is simply an integral operator or smoothing process. It is noted in Ref. 14, pp. 84-89, that in problems with nonclosed range for the operator (which is the case for the singular control problem), a standard technique in functional analysis is to define a new inner product in the range space of A such that A becomes a strongly positive operator (which implies closed range) in this new setting. It is then shown in Ref. 14 that Goh's transformation is equivalent to a change of space from $L_2[t_0,t_f]$ to $V \equiv \{$absolutely continuous functions with derivative in $L_2[t_0,t_f]\}$ with inner product

$$[v_1,v_2] \equiv v_1(t_0)^Tv_2(t_0) + \langle v_1,v_2\rangle \tag{29}$$

which is itself a Hilbert space (Ref. 17, p. 231). This gives some indication why the Goh transformation is useful in singular optimal control problems.

Upon substitution of Eq. (28) into Eq. (5) (with $R \equiv 0$), an unconstrained functional in v is formed:

$$J = \tfrac{1}{2}\langle v,\hat{A}v\rangle + \langle v,\hat{w}\rangle + \hat{J}_0 \tag{30}$$

where

$$A = W^*\hat{A}W \tag{31}$$

$$\hat{A}v = \int_t^{t_f}\int_{t_0}^{s} [F(t)G(t) - \dot{G}(t)]^T\phi^T(s,t)P(s)\phi(s,\tau) \times [F(\tau)G(\tau) - \dot{G}(\tau)]v(\tau)\mathrm{d}\tau\mathrm{d}s + \int_{t_0}^{t_f} G^T(t)P(t)\phi(t,\tau) \times [F(\tau)G(\tau) - \dot{G}(\tau)]v(\tau)\mathrm{d}\tau + G(t)^TP(t)G(t)v(t) \tag{32}$$

If $G^TPG>0$, $t \in [t_0,t_f]$, and $K(t)$ is finite on $[t_0,t_f)$, then $\hat{A}$ can be shown to be strongly positive (since Eq. (30) is then of the same form as the problem for Theorem 5). Thus, there exist constants $0<\hat{m} \le \hat{M}$ such that

$$\hat{m}\|v\|^2 \le \langle v,\hat{A}v\rangle \le \hat{M}\|v\|^2 \tag{33}$$

But,

$$\langle v,\hat{A}v\rangle = \langle Wu,\hat{A}Wu\rangle = \langle u,W^*\hat{A}Wu\rangle = \langle u,Au\rangle \tag{34}$$

which implies

$$\hat{m}\|Wu\|^2 \le \langle u,Au\rangle \le \hat{M}\|Wu\|^2 \tag{35}$$

The integral operator W is bounded and its null space consists of the zero element only, i.e.,

$$\|Wu\| \le B\|u\| \ (0<B<\infty), \ 0<\|Wu\| \ (u \ne 0) \tag{36}$$

Thus, upon substitution into Eq. (35),

$$\langle u,Au\rangle \le \hat{M}B^2\|u\|^2 \equiv M\|u\|^2 \tag{37}$$

$$\langle u,Au\rangle \ge \hat{m}\|Wu\| > 0 \text{ for } u \ne 0 \tag{38}$$

which implies A is a bounded and positive operator.

Note that Theorem 8 does not require the Jacobson necessary condition[5]; this is because there are no terms outside the integral and no xu-type terms under the integral in Eq. (1), which implies the Jacobson condition is satisfied trivially. Also, note that Theorem 8 is a sufficient condition for positivity of the A-operator. If the singular problem is of an order greater than one, then $G^TPG=0$ and further Goh transformations are required (i.e., higher order smoothing).

Since A is, at most, a positive operator in a singular problem, w of Eq. (5) is not necessarily in $R(A)$ (which implies existence is not guaranteed, by Theorem 5). In terms of problem variables [i.e., Eqs. (1) and (2)], a sufficient condition for the existence and uniqueness of a singular arc is as follows.

Theorem 9: There exists a unique singular control for the problem defined by Eqs. (1) and (2), with $R(t) \equiv 0$, if Eqs. (26) and (27) are satisfied, $v(t)$ is differentiable, and $v(t_0) = 0$, where

$$v(t) = -(G^TPG)^{-1}[G^TP + (FG-\dot{G})^TS]y \tag{39}$$

$$\dot{y} = Fy + (FG-\dot{G})v, y(t_0) = x_0 \tag{40}$$

The optimal control is

$$\bar{u}(t) = \frac{\mathrm{d}v(t)}{\mathrm{d}t} \tag{41}$$

This type of existence condition was first proved in Ref. 18 (pp. 282-287) and generalized in Ref. 15 (pp. 49-51) and Ref. 14 (pp. 78-83). Note that Eq. (39) evaluated at t_0 must be zero, and this corresponds to the $w \in R(A)$ requirement, which as previously noted is strongly dependent upon the initial condition. In Example 1, $v(t_0)=0$ only if $x_0=0$. As with Theorem 8, this theorem is a sufficient condition for the first-order singular problem. (Theorem 5, of course, is applicable to all singular problems, but it is not expressed as a convenient test.)

Assuming that an optimal control exists, the next problem is to develop conditions for the convergence of algorithms in the computation of singular controls. In the previous section it was shown that for the nonsingular problem all of the gradient-type methods mentioned converge if the sufficient condition for an optimal control is satisfied (i.e., Theorem 6). The singular case is not as straightforward, and two results are developed: 1) convergence characteristics when the existence condition of Theorem 9 is assumed, and 2) development of a uniform convergence result by employing an operator theory approach.

Theorem 10: Consider the application of the function-space gradient, conjugate gradient, and DFP methods to the problem defined by Eqs. (1) and (2) with $R(t)\equiv 0$. The sequences $\{v_i(t)\equiv Wu_i\}$ and $\{J(u_i)\}$ converge uniformly (i.e., $\lim_{i\to\infty}\|Wu_i-W\bar{u}\|=0$ and $\lim_{i\to\infty}|J(u_i)-\bar{J}|=0$) for all of the algorithms if $\hat{A}$ (defined in Eq. (30)) is strongly positive (which is guaranteed if Eqs. (26) and (27) are satisfied; the sufficient condition for a singular optimal control) and $v(t_0)=0$ and $v(t)$ differentiable.

Proof: As with Theorem 8, since the A operator is only positive, the Goh transformation is introduced and the operator $\hat{A}$ is formed. By Theorem 8, $\hat{A}$ is strongly positive and Theorem 6 can be applied to the sequence $\{v_i\}\equiv\{Wu_i\}$, i.e., $\lim_{i\to\infty}\|Wu_i-W\bar{u}\|=0$, where the uniqueness and existence of $\bar{u}$ are guaranteed since all of the hypotheses of Theorem 9 are satisfied. The fact that $\{J(u_i)\}$ converges is shown by observing that

$$\begin{aligned}|J(u_i)-J(\bar{u})| &= |J(v_i)-J(\bar{v})| = |\tfrac{1}{2}\langle v_i,\hat{A}v_i\rangle+\langle v_i,\hat{w}\rangle \\ &+J_0-\tfrac{1}{2}\langle\bar{v},\hat{A}\bar{v}\rangle-\langle\bar{v},\hat{w}\rangle-J_0| = |\langle v_i,\hat{A}\bar{v}\rangle \\ &-\tfrac{1}{2}\langle\bar{v},\hat{A}\bar{v}\rangle+\tfrac{1}{2}\langle v_i-\bar{v},\hat{A}(v_i-\bar{v})\rangle+\langle v_i-\bar{v},\hat{w}\rangle \\ &-\tfrac{1}{2}\langle\bar{v},\hat{A}\bar{v}\rangle| = |\langle v_i-\bar{v},\hat{A}\bar{v}+\hat{w}\rangle+\tfrac{1}{2}\langle v_i-\bar{v},\hat{A}(v_i-\bar{v})\rangle|\to 0\end{aligned} \tag{42}$$

since $\lim_{i\to\infty}v_i=\bar{v}$.

To develop a convergence result for the sequence $\{u_i\}$, it is convenient to introduce the function space generalization of the pseudo-inverse (PI) operator. (This is motivated by convergence results for the finite-dimensional singular case developed in Ref. 19 which involves the finite-dimensional PI.) The following definitions and properties are adapted from Ref. 20.

Definition 3: Consider the linear operator equation

$$-w=Au \tag{43}$$

where the notation is motivated by the gradient equation for Eq. (5). The element $\tilde{u}\in L_2[t_0,t_f]$ is a *best approximate solution (BAS)* of Eq. (43) if

$$\|-w-A\tilde{u}\|=\delta_w \tag{44}$$

and

$$\|\tilde{u}\|<\|u\| \tag{45}$$

for any other u which attains the infinum Eq. (44), where

$$\delta_w\equiv\inf_{u\in L_2[t_0,t_f]}\|-w-Au\|, w\in R(A) \tag{46}$$

Property 1: A BAS exists if and only if $w\in F_A$, where

$$F_A\equiv\{w\,|\,P_Rw\in R(A)\} \tag{47}$$

where $P_R\equiv$ orthogonal projection on $\overline{R(A)}$ (i.e., the closure of the range of A).

Definition 4: An operator A^+ is called a *pseudo-inverse (PI)* if $D(A^+)=F_A$, and if for each $w\in F_A$,

$$\tilde{u}=-A^+w \tag{48}$$

is the BAS, where $D(A^+)\equiv$ the domain of the A^+ operator.

Property 2: The PI exists as the uniquely defined linear closed densely defined operator

$$A^+=A_r^{-1}P_R \tag{49}$$

where A denotes the restriction of A to the subspace $N(A)^\perp\equiv$ the orthogonal complement of the null space of A.

With this characterization of the function-space PI, the following theorem can be proved.

Theorem 11: Let $\{u_i\}$ be a sequence of elements generated by the DFP method applied to Eqs. (1) and (2) with $R(t)\equiv 0$, $H_0=I$, and $u_0\in\overline{R(A)}$. Suppose A is positive (which implies $\overline{R(A)}=L_2[t_0,t_f]$) and $w\in R(A)$. Then, the sequence $\{u_i\}$ converges to the unique solution $\bar{u}=-A^+w$. The proof is long and involves mainly operator theory arguments, so it will not be presented here. See Ref. 15, pp. 63-71.

An important aspect of Theorem 11, in addition to showing the uniform convergence of the sequence $\{u_i\}$, is that the solution to the totally singular optimal control problem is naturally expressed in terms of the function-space PI operator. The full ramifications of this have not been analyzed, but it appears that this is a natural way to study theoretical properties of singular arcs (just as the finite-dimensional PI is the natural way to study finite-dimensional singular problems). Also, note that Theorem 11 only assumes general existence conditions [i.e., $A>0$ and $w\in R(A)$], whereas Theorem 10 (as it stands) is restricted to first-order singular problems.

The major remaining area of concern is the development of a rate of convergence for the DFP method. For the LQP (singular or nonsingular), the conjugate gradient and DFP methods produce identical search directions if $H_0=I$. The only published rate of convergence for positive (but not strongly positive) quadratic functionals with the conjugate gradient (or equivalently, the DFP) method is a linear convergence result in Ref. 21. Such a convergence rate appears to be too conservative compared to numerous simulation results.

Numerous theoretical approaches have been attempted to develop a superlinear convergence rate for at least the sequence of cost functionals $\{J(u_i)\}$ (see Ref. 15, pp. 72-76). To date these attempts have been unsuccessful, so a number of careful simulations have been constructed to develop insight into determining factors which strongly affect the rate of convergence.

Example 2: Consider the numerical solution of Example 1 [i.e., Eqs. (15) and (16)] with $x_0=0$. The rate of convergence result in Ref. 21 requires that $u_0\in R(A)$ [as opposed to $\overline{R(A)}$] if A is a positive operator, whereas the convergence result of Theorem 11 requires only $u_0\in\overline{R(A)}=L_2[t_0,t_f]$. Thus, it is of interest to compare the rates of simulations with $u_0\in R(A)$ and $u_0\notin R(A)$ (but, of course, $u_0\in\overline{R(A)}$). Consider the following cases:

Case 1:

$$u_0(t)\equiv 1-t^2\in R(A) \tag{50}$$

Case 2:

$$u_0(t)\equiv 1\notin R(A) \tag{51}$$

where an element $u_0\in R(A)$ if there exists $z(t)\in L_2[t_0,t_f]$ such that (see Eq. (17))

$$u_0=Az=T^*Tz=\int_t^1\left[\int_0^\tau z(s)\,\mathrm{d}s\right]\mathrm{d}\tau \tag{52}$$

Case 1 is in $R(A)$ because $z(t)\equiv 2\in L_2[t_0,t_f]$ causes $u_0=1-t^2$, while Case 2 is not in $R(A)$ because any $u_0(1)\neq 0$ cannot satisfy Eq. (52). The numerical results are presented in Fig. 1, and the rate of convergence of Case 1 is clearly superior to Case 2. The control for Case 2 is shown in Fig. 2.

Since $u_0\notin R(A)$ can cause a poor convergence rate for gradient-type algorithms in their standard form either the algorithm should be modified or $u_0\in R(A)$ should be guaranteed. The latter suggestion is not possible in general problems, so modifications of the algorithms are required if $u_0\notin R(A)$ appears to be a possibility. This will be the case in singular problems which require the gradient to be zero at t_f as a necessary condition. This is a common occurrence in applications (see Ref. 10), e.g., if the original control variable u in a singular problem is required to be continuous and

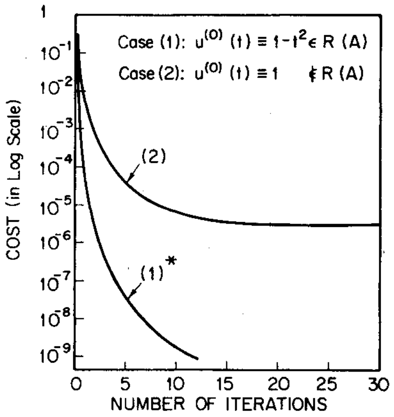

Fig. 1 Cost functional vs number of iterates for Example 2.

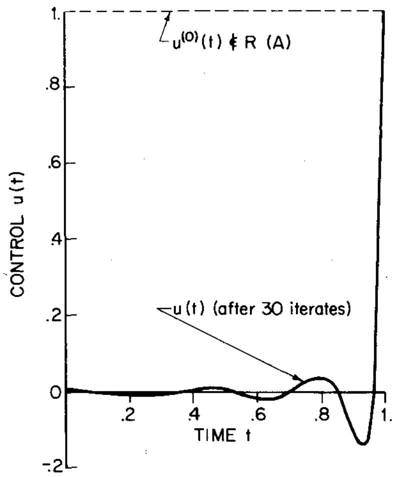

Fig. 2 Control profiles for Example 2, Case 2.

$|\dot{u}| \leq K$, then a new state variable, x_{n+1}, is usually introduced with $x_{n+1} \equiv u$, $\dot{x}_{n+1} = \dot{u} \equiv \tilde{u}$, with $|\tilde{u}| \leq K$; since $x_{n+1}(t_f)$ is not specified, $\lambda_{n+1}(t_f) = H_{\tilde{u}}(t_f) = 0$ is a necessary condition of optimality, where $H_{\tilde{u}}$ is the function-space gradient for the new problem. Procedures for modifying gradient-type algorithms to cause the terminal value of u to converge to $\bar{u}(t_f)$ (i.e., the optimal value) are presented in Refs. 14 (pp. 98-108) and 15 (pp. 88-91).

Example 3: In Ref. 19 it is shown that the rate of convergence for the DFP method applied to the finite-dimensional singular problem is better than or equal to the rate for a well-defined set of associated nonsingular problems, while the gradient method has exactly the opposite behavior. In Theorem 7 it was shown that the function-space DFP method converges superlinearly for the nonsingular problem. Thus, even though a useful rate of convergence result cannot be developed for the singular problem, it is of interest to compare the behavior of the gradient and DFP methods as a problem tends to singularity. Consider the problem:

Minimize:

$$J = \tfrac{1}{2}\left[x_1\left(\frac{\pi}{4}\right)\right]^2 + \tfrac{1}{2}\left[x_2\left(\frac{\pi}{4}\right) + 2^{-\frac{1}{2}}\right]^2 + \tfrac{1}{2}\int_0^{\pi/4} [x_2^2 - x_1^2 + \epsilon u^2]\,\mathrm{d}t \tag{53}$$

subject to:

$$\dot{x}_1 = x_2, \quad x_1(0) = 1$$
$$\dot{x}_2 = u, \quad x_2(0) = 0 \tag{54}$$

When $\epsilon > 0$, the problem is nonsingular, and when $\epsilon = 0$, the problem is singular with optimal control $\bar{u}(t) = -\cos t$. To study the behavior as the problem tends to singularity, the gradient and DFP methods were applied for values of $\epsilon = 1.0$, 0.1, 0.001, and 0 (the singular case). The computations were performed in double precision on an Amdahl 470 computer with the stopping criterion $|J(u_i)| < 3 \times 10^{-7}$.

From Table 1, the number of iterates remains nearly constant for the DFP method as $\epsilon \to 0$ (recall that superlinear convergence is guaranteed for $\epsilon > 0$ by Theorem 7), while the gradient method deteriorates rapidly as $\epsilon \to 0$. Thus, for this example, the singular aspect of the problem does not adversely affect the DFP method, whereas the gradient method is affected strongly.

The properties and examples presented above emphasize certain infinite-dimensional aspects of singular and nonsingular problems. However, the numerical solution on a digital computer requires a finite-dimensional representation of the problem, and there exist numerous realistic ways to discretize the problem. Furthermore, the solution will be different for the case where the control is first discretized and then the finite-dimensional DFP method is applied than for the case where the function-space DFP method is applied with the numerical integrator and the finite-dimensional projection of the control causing the discrete representation. For the problem of Examples 1 and 2, an interesting difference between the given singular problem and associated nonsingular problems results if the former method of discretization is employed.

Example 4: Consider the problem defined by Eqs. (15) and (16) with $x_0 = 0$. Suppose the control is approximated by a sequence of N piecewise constant functions on [0,1], say $\{a_1, \ldots, a_N\}$. Then,

$$x(t) \equiv \begin{cases} a_1 t & t_0 \equiv 0 \leq t \leq t_1 \\ a_2(t-t_1) + a_1 \Delta t & t_1 \leq t \leq t_2 \\ a_N(t-t_{N-1}) + (a_1 + \ldots + a_{N-1})\Delta t & t_{N-1} \leq t \leq 1 \equiv t_N \end{cases} \tag{55}$$

where $\Delta t \equiv t_{i+1} - t_i \; (i = 0, \ldots, N-1)$. Upon substitution into the performance index and integration, the following unconstrained, finite-dimensional, quadratic parameter optimization problem is formed:

$$J(a) = \tfrac{1}{2}[(a_1^2/3)(\Delta t)^3 + (a_2^2/3)(\Delta t)^3 + a_2 a_1 (\Delta t)^2 + a_1^2(\Delta t)^3 + \ldots + (a_N^2/3)(\Delta t)^3 + a_N(a_1 + \ldots + a_{N-1})(\Delta t)^3 + (a_1 + \ldots + a_{N-1})^2(\Delta t)^3] \tag{56}$$

or

$$J(a) \equiv \tfrac{1}{2} a^T Q a \tag{57}$$

where

$$Q \equiv (\Delta t)^3 \begin{bmatrix} q_{11} & & \\ \cdot & q_{22} & 0 \\ \cdot & \cdot & \\ \cdot & & \cdot \\ q_{N1} & \cdots & q_{NN} \end{bmatrix} \tag{58}$$

$$\begin{aligned} q_{ij} &\equiv \tfrac{1}{3} + N - i && (i=j) \\ q_{ij} &\equiv 2(N-i) + 1 && (j<i) \\ q_{ij} &\equiv 0 && (j>i) \end{aligned} \tag{59}$$

Table 1 Computational results for example 3

	Number of iterations[a]			
	$\epsilon=1$	$\epsilon=0.1$	$\epsilon=0.001$	$\epsilon=0$
Gradient	4	16	49	45
DFP	3	4	4	4

[a] In all cases, an exact one-dimensional search is employed to determine the parameter α_i in each iteration; $u^{(0)}(t)\equiv 1$.

Note that the resultant parameter optimization problem is nonsingular since the eigenvalues of Q are its diagonal elements (which are all positive). Furthermore, the conditioning of Q is determined by the ratio of the largest to smallest eigenvalue, which is

$$\text{Ratio}\,|_{\text{Singular}} = [\,1/3 + (N-1)\,]\,/\,1/3 = 3N-2 \qquad (60)$$

Note that as N increases (i.e., a finer discretization), the spread of the eigenvalues increases with a corresponding negative impact on convergence rate, especially for the gradient method.

Now consider the set of associated nonsingular problems $\{J_\epsilon\}$, where

$$J_\epsilon = 1/2\int_0^1 (x^2+\epsilon u^2)\,dt \qquad (\epsilon>0) \qquad (61)$$

With $x(t)$ defined by Eq. (55), the performance index can be written as

$$J_\epsilon = 1/2\, a^T Q_N a \qquad (62)$$

with Q_N of the same form as Eq. (58) with

$$\begin{aligned} q_{N_{ii}} &\equiv 1/3 + N - i + \epsilon/(\Delta t)^2 \qquad & i=j \\ q_{N_{ij}} &\equiv 2(N-i)+1 & j<i \\ q_{N_{ij}} &\equiv 0 & j>i \end{aligned} \qquad (63)$$

Again the matrix is nonsingular, but the spread of the eigenvalues is

$$\text{Ratio}\,|_{\text{Nonsingular}} = [\,1/3 + N - 1 + N^2\epsilon\,]\,/\,[\,1/3 + N^2\epsilon\,] \qquad (64)$$

Thus,

$$\lim_{N\to\infty} \text{Ratio}\,|_{\text{Nonsingular}} = 1 \quad (\epsilon>0)$$

which implies that the finer the discretization, the better the conditioning (which is exactly the opposite of the $\epsilon=0$ or singular case).

V. Concluding Remarks

The existence theorem for the minimization of a quadratic functional has been employed to develop insight into the inherent differences between singular and nonsingular control problems. Concrete realizations of the main existence theorem result in sufficient, existence, and uniqueness conditions for optimal controls as well as convergence conditions for gradient-type algorithms.

In Section IV a number of examples were presented to determine guidelines for the computation of optimal singular controls:

1) The gradient method is ill-suited for singular problems, whereas the conjugate gradient and DFP methods are not.

2) If the necessary conditions for a singular problem require a zero gradient at t_f, then the rate of convergence for the standard application of gradient-type methods is adversely affected.

Although these guidelines were developed for the totally singular problem, they apply as well to problems with both singular and nonsingular subarcs since the existence of singular subarcs in such problems is strongly dependent upon initial conditions and/or the attainment of intermediate state vector values from which singular subarcs are possible.

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