Second Order Conditions of Optimality for Constrained Optimization Problems in Finite Dimensional Spaces

by

E. Polak and E. J. Messerli

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ABSTRACT

First-order necessary conditions of optimality for many problems in optimal control, nonlinear programming, and the calculus of variations can be obtained by transcribing these problems into a simple canonical form. In finite dimensional space this form reads:

(1) Basic Problem: Let $f : E^n \to E^1$, $r : E^n \to E^m$ be continuously differentiable functions and Ω a given subset of E^n. Find $\hat{x} \in \Omega$ such that $r(\hat{x}) = 0$, and, for all $x \in \Omega$ satisfying $r(x) = 0$, $f(\hat{x}) \le f(x)$.

Roughly, the most general necessary condition for the Basic Problem (1) is of the form:

(2) If $\hat{x}$ is an optimal solution to the Basic Problem (1), then there is a nonzero vector $\psi \in E^{m+1}$ with $\psi^o \le 0$ such that

$$\langle \psi^o \nabla f(\hat{x}) + \sum_{i=1}^{m} \psi^i \nabla r^i(\hat{x}), \delta x \rangle \le 0$$ for all δx in a convex cone which "approximates" the set Ω at the optimal solution $\hat{x}$.

This general necessary condition can be satisfied trivially in some cases, such as when the gradients $\nabla f(\hat{x}), \nabla r^1(\hat{x}), \ldots, \nabla r^m(\hat{x})$ are linearly dependent, leading to a need for auxiliary necessary conditions for these cases.

In this paper the special case of linear dependence caused by the gradient $\nabla f(\hat{x})$ being zero is investigated. A new condition, involving second order partial derivatives of the equality constraint function $r(\cdot)$, and first order partial derivatives of the equality constraint function $r(\cdot)$, is obtained. This new condition holds for all perturbation vectors in the convex cone associated with the general (first order) necessary condition (2) - a set which is larger than the one usually considered in obtaining second order conditions.

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SUMMARY

Introduction: In the last few years it has been shown [1, 2] that problems of the calculus of variations, nonlinear programming and optimal control can be treated in a unified manner as far as necessary conditions of optimality are concerned. This was done by establishing that all these problems can be transcribed into a simple canonical form, for which necessary conditions were developed. Specialized necessary conditions of optimality for any particular problem then followed from the structure of the problem.

For finite dimensional problems the canonical form mentioned above reads as follows:

1. Basic Problem: Let $f : E^n \to E^1$, $r : E^n \to E^m$ be continuously differentiable functions, and let Ω be a subset of E^n. Find a vector $\hat{x} \in \Omega$ such that: (i) $r(\hat{x}) = 0$ and (ii) for every x in Ω with $r(x) = 0$, $f(x) \geq f(\hat{x})$.

Thus, for example, the usual Nonlinear Programming Problem, $\min\{f(x) \mid r(x) = 0,\ q(x) \leq 0\}$, where $f: E^n \to E^1$, $r: E^n \to E^m$ and $q: E^n \to E^k$ are continuously differentiable, is recognized to be the Basic Problem (1) with $\Omega = \{x \mid q(x) \leq 0\}$. Examples of the transcription of discrete optimal control problems to Basic Problem form may be found in [1].

Before giving the necessary condition for the Basic Problem (1) we require an "approximation" of the set Ω at a given point.

2. Definition: A convex cone $C(\hat{x}, \Omega)$ will be called a conical approximation of the constraint set Ω at $\hat{x}$ if for any collection $\{\delta x_1, \dots, \delta x_k\}$ of linearly independent vectors in $C(\hat{x}, \Omega)$ there exists an $\varepsilon > 0$ (possibly depending on $\hat{x}$, $\delta x_1, \dots, \delta x_k$), and a continuous map $\zeta(\cdot)$ from the convex hull (co) of $\{0, \delta x_1, \dots, \delta x_k\}$ into $\Omega - \hat{x}$ such that $\zeta(\delta x) = \varepsilon\,\delta x + 0(\varepsilon\,\delta x)$ where $\|0(\varepsilon\,\delta x)\| / \|\varepsilon\,\delta x\| \to 0$ as $\varepsilon \to 0$, uniformly for $\delta x \in \text{co}\{0, \delta x_1, \dots, \delta x_k\}$.

The most general necessary condition for the Basic Problem (1) is the following one.

3. Fundamental Theorem: If $\hat{x}$ is a solution to the Basic Problem (1), and $C(\hat{x}, \Omega)$ is a conical approximation of Ω at $\hat{x}$, then there exists a nonzero vector $\psi = (\psi^0, \dots, \psi^m)$ in E^{m+1} with $\psi^0 \leq 0$ such that for every δx in the closure, $\overline{C(\hat{x}, \Omega)}$, of $C(\hat{x}, \Omega)$:

4. $$\langle \psi^0 \nabla f(\hat{x}) + \sum_{i=1}^{m} \lambda^i \nabla r^i(\hat{x}),\ \delta x \rangle \leq 0$$

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Note that the Fundamental Theorem (3) may become degenerate in two ways. The first occurs when ψ^o must be chosen to be zero, and hence no information about the cost function $f(\cdot)$ enters into the necessary condition (4). This most often occurs when there is only one $x \in \Omega$ satisfying $r(x) = 0$, and may be avoided by introducing a regularity condition, such as the Kuhn-Tucker constraint qualification, on $r(\cdot)$ and Ω. The Fundamental Theorem also becomes degenerate when the vectors $\nabla f(\hat{x})$, $\nabla r^1(\hat{x}), \ldots, \nabla r^m(\hat{x})$ are linearly dependent since then one can always choose a $\psi \neq 0$ which satisfies $\psi^o \nabla f(\hat{x}) + \sum_{i=1}^{m} \psi^i \nabla r^i(\hat{x}) = 0$, and hence (4), without reference to the optimality of $\hat{x}$.

When a degeneracy in the first-order condition occurs, it is obviously desirable to have a second-order necessary condition. However, there are other cases when a second-order condition is also meaningful. Thus, suppose that in $C(\hat{x}, \Omega)$ there are "critical" vectors y which satisfy $\langle \nabla f(\hat{x}), y \rangle = 0$ and $\langle \nabla r^i(\hat{x}), y \rangle = 0 \quad i = 1, \ldots, m$. Then, under suitable assumptions, one obtains for these vectors relations of the form:

5. $$y^T \frac{\partial^2 f}{\partial x^2} (\hat{x})\, y \geq 0$$

or

6. $$y^T \left(\frac{\partial^2 f}{\partial x^2} (\hat{x}) - \sum_{i=1}^{m} \lambda^i \frac{\partial^2 r^i}{\partial x^2} (\hat{x}) - \sum_{i=1}^{k} u^i \frac{\partial^2 q^i}{\partial x^2} (\hat{x}) \right) y \geq 0$$

(see, for example [3], [4]).

In this paper we consider a special case of degeneracy in the first-order condition (4), namely the case when $\nabla f(\hat{x}) = 0$, which causes the vectors $\nabla f(\hat{x})$, $\nabla r^1(\hat{x}), \nabla r^2(\hat{x}), \ldots, \nabla r^m(\hat{x})$ to be linearly dependent. However, we shall not restrict ourselves to critical directions only as in [3], [4], and, instead, we shall obtain a condition similar to (4), but with $\delta x^T \frac{\partial^2 f}{\partial x^2} (\hat{x})\, \delta x$ playing the role of $\langle \nabla f(\hat{x}), \delta x \rangle$.

II. <u>A Second-Order Condition</u>: Let us assume that $\hat{x}$ is a solution to the Basic Problem (1) such that $\nabla f(\hat{x}) = 0$, and suppose that $f(\cdot)$ is twice continuously differentiable. Then to the Fundamental Theorem (3) we can add the following new second-order condition:

7. <u>Theorem</u>: If $\hat{x}$ is a solution to the Basic Problem (1) such that $\nabla f(\hat{x}) = 0$, and $C(\hat{x}, \Omega)$ is a conical approximation of Ω at the point $\hat{x}$, then the ray R,

8. $$R \triangleq \{ y \in E^{m+1} \mid y = \beta(-1, 0, 0, 0 \ldots, 0) \quad \beta \geq 0 \}$$

has no points in the interior of the set L defined by:

9. $$L \triangleq \{ (y^o, y) \mid y^o = \delta x^T \frac{\partial^2 f}{\partial x^2} (\hat{x})\, \delta x, \; y = \frac{\partial r}{\partial x} (\hat{x})\, \delta x; \; \delta x \in C(\hat{x}, \Omega) \}$$

An equivalent statement of the Fundamental Theorem (3) is that the ray R given by (8) has no points in the interior of the set L^o defined by:

10. $$L_o \triangleq \{ (y^o, y) \mid y^o = \langle \nabla f(\hat{x}), \delta x \rangle, \; y = \frac{\partial r}{\partial x} (\hat{x})\, \delta x, \; \delta x \in C(\hat{x}, \Omega) \}.$$

Since L_o is also a convex cone, L_o and R must be separated, which is the essence of the statement of Theorem (3) in the original form given.

Since L defined in (9) is not in general convex it is natural to inquire if there is a curved surface which separates R and L - rather than a plane. In fact a parboloid of the form:

11. $$\tilde{g}_\lambda(y) = \lambda^o y^o + \sum_{i=1}^{m} \lambda^i (y^i)^2 \qquad \text{with} \qquad \lambda^o \leq 0$$

is the logical candidate, which, on substituting $y \epsilon L$ gives the following quadratic in δx,

12. $$g_\lambda(\delta x) = \lambda^o \delta x^T \frac{\partial^2 f}{\partial x^2} \delta x + \sum_{i=1}^{m} \lambda^i \delta x^T (\nabla r^i(\hat{x})) \langle \nabla r^i(\hat{x})) \delta x .$$

We are thus led to the following consequence of Theorem (7).

13. Theorem: If $\hat{x}$ is a solution to the Basic Problem (1) such that $\nabla f(\hat{x}) = 0$, and $C(\hat{x}, \Omega)$ is a conical approximation of Ω at $\hat{x}$, then there is a nonzero vector $\lambda \epsilon E^{m+1}$ with $\lambda^o \leq 0$ such that for every δx in $C(\hat{x}, \Omega)$,

14. $$\lambda^o \delta x^T \frac{\partial^2 f}{\partial x^2}(\hat{x}) \delta x + \sum_{i=1}^{m} \lambda^i \langle r^i(\hat{x}), \delta x \rangle^2 \leq 0$$

15. Moreover, if the ray R (8) is not a boundary ray of the set L (9), λ^o may be taken as -1.

16. Remark: The relation (14) can always be satisfied trivially if we allow $\lambda^o = 0$. While there are cases in which λ^o must be chosen to be zero, the qualification (15) allows a nontrivial statement for many problems.

Thus, let us again consider the Nonlinear Programming Problem,

17. $$\min \{f(x) \mid r(x) = 0, \ q(x) \leq 0\}$$

where $f: E^n \rightarrow E'$ is assumed twice continuously differentiable, and $r: E^n \rightarrow E^m$, $q: E^n \rightarrow E^k$ are continuously differentiable.

Define $I(x) = \{i \epsilon \{1, \ldots, k\} \mid q^i(x) = 0\}$ and $I\,C(x) = \{y \mid \langle \nabla q^i(x), y \rangle < 0 \ i \epsilon I(x)\}$.

We now obtain the following condition from Theorem (14).

18. Theorem: If $\hat{x}$ is a solution to the Nonlinear Programming Problem (17) such that $\nabla f(\hat{x}) = 0$, $I\,C(\hat{x})$ is not empty, and the Kuhn-Tucker Constraint Qualification [5] is satisfied, then there is a vector λ in E^m such that

19. $$-y^T \frac{\partial^2 f}{\partial x^2}(\hat{x}) y + \sum_{i=1}^{m} \lambda^i \langle \nabla r^i(\hat{x}), y \rangle^2 \leq 0 \qquad \forall y \epsilon \overline{IC(\hat{x})}$$

III. Conclusions: We have shown in this paper that, when first-order necessary conditions of optimality fail because the gradient of the cost function at the optimal point is zero, it is possible to replace these first-order conditions with a new condition. This new condition, involving second-order partial derivatives of the cost function and first-order partial derivatives of the equality constraint function, holds for all perturbation vectors in a set which is larger than the one usually considered in obtaining second-order conditions.

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