

OPTIMIZATION RULES

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Abstract: *Nonlinear programming is based on a collection of definitions, theorems, and principles that must be clearly understood if the available nonlinear programming methods are to be used effectively. This article begins with the definition of the gradient vector, the Hessian matrix, and the various types of extrema (maxima and minima).*

Key words: transport, optimizations, mechanics

1.Gradient Information

The conditions that must hold at the solution point are then discussed and techniques for the characterization of the extrema are described. Subsequently, the classes of convex and concave functions are introduced. These provide a natural formulation for the theory of global convergence.

Throughout the article , we focus our attention on the nonlinear optimization problem

minimize $f = f(x)$

subject to: $x \in R$

where $f(x)$ is a real-valued function and $R \subset E^n$ is the feasible region.

In many optimization methods, gradient information pertaining to the objective function is required. This information consists of the first and second derivatives of $f(x)$ with respect to the n variables. If $f(x) \in C^1$, that is, if $f(x)$ has continuous first-order partial derivatives, the gradient of $f(x)$ is defined as

$$\begin{aligned} \mathbf{g}(\mathbf{x}) &= \left[\frac{\partial f}{\partial x_1} \quad \frac{\partial f}{\partial x_2} \quad \cdots \quad \frac{\partial f}{\partial x_n} \right]^T \\ &= \nabla f(\mathbf{x}) \end{aligned} \tag{1.1}$$

Where

$$\nabla = \left[\frac{\partial}{\partial x_1} \quad \frac{\partial}{\partial x_2} \quad \cdots \quad \frac{\partial}{\partial x_n} \right]^T \tag{1.2}$$

If $f(x) \in C^2$, that is, if $f(x)$ has continuous second-order partial derivatives, the Hessian of $f(x)$ is defined as

$$H(x) = \nabla g^T = \nabla \{ \nabla^T f(x) \} \quad (1.3)$$

Hence Eqs. (1.1) – (1.3) give

$$H(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

For a function $f(x) \in C^2$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$$

since differentiation is a linear operation and hence $H(x)$ is an $n \times n$ square symmetric matrix.

The gradient and Hessian at a point $x = x_k$ are represented by $g(x_k)$ and $H(x_k)$ or by the simplified notation g_k and H_k , respectively. Sometimes, when confusion is not likely to arise, $g(x)$ and $H(x)$ are simplified to g and H . The gradient and Hessian tend to simplify the optimization process considerably. Nevertheless, in certain applications it may be uneconomic, time-consuming, or impossible to deduce and compute the partial derivatives of $f(x)$. For these applications, methods are preferred that do not require gradient information.

Gradient methods, namely, methods based on gradient information may use only $g(x)$ or both $g(x)$ and $H(x)$. In the latter case, the inversion of matrix $H(x)$ may be required which tends to introduce numerical inaccuracies and is time-consuming. Such methods are often avoided.

2. The Taylor Series

Some of the nonlinear programming procedures and methods utilize linear or quadratic approximations for the objective function and the equality and inequality constraints, namely, $f(x)$, $a_i(x)$, and $c_j(x)$ in Eq. (1.4). Such approximations can be obtained by

using the Taylor series. If $f(x)$ is a function of two variables x_1 and x_2 such that $f(x) \in C^p$ where $P \rightarrow \infty$, that is, $f(x)$ has continuous partial derivatives of all orders, then the value of function $f(x)$ at point

$[x_1 + \delta_1, x_2 + \delta_2]$ is given by the Taylor series as

$$\begin{aligned}
 f(x_1 + \delta_1, x_2 + \delta_2) &= f(x_1, x_2) + \frac{\partial f}{\partial x_1} \delta_1 + \frac{\partial f}{\partial x_2} \delta_2 \\
 &+ \frac{1}{2} \left(\frac{\partial^2 f}{\partial x_1^2} \delta_1^2 + \frac{2\partial^2 f}{\partial x_1 \partial x_2} \delta_1 \delta_2 + \frac{\partial^2 f}{\partial x_2^2} \delta_2^2 \right) \\
 &+ O(\|\delta\|^3)
 \end{aligned}
 \tag{1,4 a}$$

where

$\delta = [\delta_1 \ \delta_2]^T$, $O(\|\delta\|^3)$ is the remainder, and $\|\delta\|$ is the Euclidean norm of δ given by

$$\|\delta\| = \sqrt{\delta^T \delta}$$

The notation $\phi(x) = O(x)$ denotes that $\phi(x)$ approaches zero at least as fast as x as x approaches zero, that is, there exists a constant $K \geq 0$ such that

$$\left| \frac{\phi(x)}{x} \right| \leq K$$

as

$$x \rightarrow 0$$

If $f(x)$ is a function of n variables, then the Taylor series of $f(x)$ at point $[x_1 + \delta_1, x_2 + \delta_2, \dots]$ is given by

$$\begin{aligned}
 f(x_1 + \delta_1, x_2 + \delta_2, \dots) &= f(x_1, x_2, \dots) + \sum_{i=1}^n \frac{\partial f}{\partial x_i} \delta_i \\
 &+ \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \delta_i \frac{\partial^2 f}{\partial x_i \partial x_j} \delta_j \\
 &+ o(\|\delta\|^2)
 \end{aligned}$$

(1.4b)

Alternatively, on using matrix notation

$$f(\mathbf{x} + \delta) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \delta + \frac{1}{2} \delta^T \mathbf{H}(\mathbf{x}) \delta + o(\delta) \quad (1.4c)$$

where $\mathbf{g}(\mathbf{x})$ is the gradient, and $\mathbf{H}(\mathbf{x})$ is the Hessian at point \mathbf{x} .

As $\delta \rightarrow 0$, second- and higher-order terms can be neglected and a linear approximation can be obtained for $f(\mathbf{x} + \delta)$ as

$$f(\mathbf{x} + \delta) \approx f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \delta \quad (1.4d)$$

Similarly, a quadratic approximation for $f(\mathbf{x} + \delta)$ can be obtained as

$$f(\mathbf{x} + \delta) \approx f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \delta + \frac{1}{2} \delta^T \mathbf{H}(\mathbf{x}) \delta \quad (1.4e)$$

Another form of the Taylor series, which includes an expression for the remainder term, is

$$\begin{aligned}
f(\mathbf{x} + \delta) = & f(\mathbf{x}) \\
& + \sum_{1 \leq k_1 + k_2 + \dots + k_n \leq P} \frac{\partial^{k_1 + k_2 + \dots + k_n} f(\mathbf{x})}{\partial x_1^{k_1} \partial x_2^{k_2} \dots \partial x_n^{k_n}} \prod_{i=1}^n \frac{\delta_i^{k_i}}{k_i!} \\
& + \sum_{k_1 + k_2 + \dots + k_n = P+1} \frac{\partial^{P+1} f(\mathbf{x} + \alpha \delta)}{\partial x_1^{k_1} \partial x_2^{k_2} \dots \partial x_n^{k_n}} \prod_{i=1}^n \frac{\delta_i^{k_i}}{k_i!}
\end{aligned} \quad (1.4f)$$

where $0 \leq \alpha \leq 1$ and

$$\sum_{1 \leq k_1 + k_2 + \dots + k_n \leq P} \frac{\partial^{k_1 + k_2 + \dots + k_n} f(\mathbf{x})}{\partial x_1^{k_1} \partial x_2^{k_2} \dots \partial x_n^{k_n}} \prod_{i=1}^n \frac{\delta_i^{k_i}}{k_i!}$$

is the sum of terms taken over all possible combinations of k_1, k_2, \dots, k_n that add up to a number in the range 1 to P .

for proof.) This representation of the Taylor series is completely general and, therefore, it can be used to obtain cubic and higher-order approximations for $f(\mathbf{x} + \delta)$. Furthermore, it can be used to obtain linear, quadratic, cubic, and higher-order exact closed-form expressions for $f(\mathbf{x} + \delta)$. If $f(\mathbf{x}) \in C^1$ and $P = 0$, Eq. (1.4f) gives

$$f(\mathbf{x} + \delta) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x} + \alpha \delta)^T \delta \quad (1.4g)$$

and if $f(\mathbf{x}) \in C^2$ and $P = 1$, then

$$f(\mathbf{x} + \boldsymbol{\delta}) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \boldsymbol{\delta} + \frac{1}{2} \boldsymbol{\delta}^T \mathbf{H}(\mathbf{x} + \alpha \boldsymbol{\delta}) \boldsymbol{\delta} \quad (1.4h)$$

where $0 \leq \alpha \leq 1$. Eq. (1.4g) is usually referred to as the mean-value theorem for differentiation.

Yet another form of the Taylor series can be obtained by regrouping the terms in Eq. (1.4f) as

$$f(\mathbf{x} + \boldsymbol{\delta}) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \boldsymbol{\delta} + \frac{1}{2} \boldsymbol{\delta}^T \mathbf{H}(\mathbf{x}) \boldsymbol{\delta} + \frac{1}{3!} D^3 f(\mathbf{x}) \boldsymbol{\delta} \boldsymbol{\delta} \boldsymbol{\delta} + \dots + \frac{1}{(r-1)!} D^{r-1} f(\mathbf{x}) \boldsymbol{\delta} \boldsymbol{\delta} \dots \boldsymbol{\delta} + \dots$$

where

$$D^r f(\mathbf{x}) = \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_r=1}^n \left\{ \delta_{i_1} \delta_{i_2} \dots \delta_{i_r} \frac{\partial^r f(\mathbf{x})}{\partial x_{i_1} \partial x_{i_2} \dots \partial x_{i_r}} \right\}$$

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