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A REVIEW OF CONCEPTS IN LINEAR, NONLINEAR AND DISCRETE OPTIMIZATION

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Abstract

A brief review of mathematical concepts in linear, nonlinear and discrete optimization is made. Following statements and classifications of problems in optimization, convexity and partial derivative concepts are discussed. An abstract approach to evaluation of first-order sensitivities is presented, indicating its relationship with the adjoint network method. Branch and bound concepts for discrete optimization are sketched out. Linear inequalities, along with descent, optimality conditions and feasible direction approaches are noted. Definitions are given of the Lagrangian function, primal and dual problems. A discussion of quadratic models, scaling and transformations leads the reader to Newton, modified Newton and quasi-Newton algorithms. Consideration of linearly constrained problems is followed by linear programming.

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Introduction

A brief review of mathematical concepts in linear, nonlinear and discrete optimization is made. Following statements and classifications of problems in optimization, convexity and partial derivative concepts are discussed. An abstract approach to evaluation of first-order sensitivities is presented, indicating its relationship with the adjoint network method. Branch and bound concepts for discrete optimization are sketched out. Linear inequalities, along with descent, optimality conditions and feasible direction approaches are noted. Definitions are given of the Lagrangian function, primal and dual problems. A discussion of quadratic models, scaling and transformations leads the reader to Newton, modified Newton and quasi-Newton algorithms. Consideration of linearly constrained problems is followed by linear programming.

The Optimization Problem

The optimization problem is to minimize with respect to parameter vector $\boldsymbol{\phi}$ restricted to the domain Φ^k the scalar objective function $U(\boldsymbol{\phi})$ subject to inequality constraints $\mathbf{c}(\boldsymbol{\phi}) \geq \mathbf{0}$[†] and equality constraints $\mathbf{h}(\boldsymbol{\phi}) = \mathbf{0}$, where

$$\boldsymbol{\phi} \triangleq \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_k \end{bmatrix}, \qquad \mathbf{c} \triangleq \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}, \qquad \mathbf{h} \triangleq \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_s \end{bmatrix} . \tag{1}$$

$\triangleq$ means "equal to by definition". Thus, $\boldsymbol{\phi}$ defines a k-dimensional parameter space. The vectors $\mathbf{c}$ and $\mathbf{h}$ contain constraint functions, which may be linear or nonlinear in $\boldsymbol{\phi}$. The symbol Φ^k is used to denote any extraneous restrictions on the k-vector $\boldsymbol{\phi}$ not covered by $\mathbf{c} \geq \mathbf{0}$ and $\mathbf{h} = \mathbf{0}$.

We may classify some optimization problems as follows:

linear programming: U, $\mathbf{c}$, $\mathbf{h}$ linear in $\boldsymbol{\phi}$

quadratic programming: U quadratic, $\mathbf{c}$, $\mathbf{h}$ linear

nonlinear programming: U, $\mathbf{c}$, $\mathbf{h}$, nonlinear in $\boldsymbol{\phi}$

integer programming: Φ^k = {integer k-vectors}

discrete programming: Φ^k = {specified[††] k-vectors}

mixed integer programming: Φ^k = {k-vectors with some components integer}

Terms such as unconstrained optimization, discrete nonlinear programming, and so on, follow in an obvious manner.

A constraint region R_c may be given by

$$R_c \triangleq \{\boldsymbol{\phi} \mid \mathbf{c}(\boldsymbol{\phi}) \geq \mathbf{0}, \mathbf{h}(\boldsymbol{\phi}) = \mathbf{0}\} . \tag{2}$$

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† The notation $\mathbf{a} \geq \mathbf{0}$ means all elements of $\mathbf{a}$ must be nonnegative.

†† A finite number of possible solutions is specified.

Convexity and Convex Programming

We present a number of important related ideas on convex functions and regions.

A function of $f(\underset{\sim}{x})$ is said to be convex if a linear interpolation between every two points $\underset{\sim}{x}^a$ and $\underset{\sim}{x}^b$ on its surface never underestimates the function, i.e.,

$$f(\underset{\sim}{x}^a + \lambda(\underset{\sim}{x}^b - \underset{\sim}{x}^a)) \leq f(\underset{\sim}{x}^a) + \lambda(f(\underset{\sim}{x}^b) - f(\underset{\sim}{x}^a)) \text{ for all } 0 \leq \lambda \leq 1 \ . \quad (6)$$

Strictly convex functions are similarly defined but must have strict inequalities in (6) for $\underset{\sim}{x}^a \neq \underset{\sim}{x}^b$. A function $f(\underset{\sim}{x})$ is concave (strictly concave) if $-f(\underset{\sim}{x})$ is convex (strictly convex).

A region (set of points or domain) is convex if for every $\underset{\sim}{x}^a$ and $\underset{\sim}{x}^b$ in the region

$$\underset{\sim}{x} = \underset{\sim}{x}^a + \lambda(\underset{\sim}{x}^b - \underset{\sim}{x}^a) \ , \text{ for all } 0 \leq \lambda \leq 1 \quad (7)$$

lies in the region. Thus, R is convex if

$$\underset{\sim}{\phi}^a, \ \underset{\sim}{\phi}^b, \ \underset{\sim}{\phi}^a + \lambda(\underset{\sim}{\phi}^b - \underset{\sim}{\phi}^a) \in R \text{ for all } 0 \leq \lambda \leq 1 \ . \quad (8)$$

Given a distinct number of points $\underset{\sim}{x}^i$, i = 1, 2, ..., n a convex combination $\underset{\sim}{x}$ of the points is described by

$$\underset{\sim}{x} = \sum_{i=1}^{n} \lambda_i \underset{\sim}{x}^i, \ \sum_{i=1}^{n} \lambda_i = 1, \ \lambda_i \geq 0, \ i = 1, 2, \ldots, n \ . \quad (9)$$

A region is convex if every possible convex combination of all sets of distinct points is in the region.

$$\underset{\sim}{G} = \nabla_{\underset{\sim}{x}} \nabla^T_{\underset{\sim}{x}} f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \tag{14}$$

and is symmetrical for twice differentiable functions. If we identify $\underset{\sim}{y}$ as $\nabla_{\underset{\sim}{x}} f$ then $\partial \underset{\sim}{y}^T / \partial \underset{\sim}{x} = \nabla_{\underset{\sim}{x}} \nabla^T_{\underset{\sim}{x}} f$, where m = n.

Consider the function, for $m \geq n$,

$$f' = \frac{1}{2} \underset{\sim}{y}^T \underset{\sim}{y} \quad . \tag{15}$$

Then

$$\nabla_{\underset{\sim}{x}} f' = \frac{\partial \underset{\sim}{y}^T}{\partial \underset{\sim}{x}} \underset{\sim}{y} = \underset{\sim}{J}^T \underset{\sim}{y} \tag{16}$$

and, neglecting second derivatives of $\underset{\sim}{y}$ w.r.t. $\underset{\sim}{x}$, it is readily shown that

$$\underset{\sim}{G}' = \nabla_{\underset{\sim}{x}} \nabla^T_{\underset{\sim}{x}} f' \simeq \underset{\sim}{J}^T \underset{\sim}{J} \quad . \tag{17}$$

The minimization of f' of (15) is called <u>least squares approximation</u>. The n x n Hessian $\underset{\sim}{G}'$ of (17) is exact if $\underset{\sim}{y}$ is assumed linear in $\underset{\sim}{x}$.

If $\underset{\sim}{x}^0$ is some reference point and $\underset{\sim}{x}$ arbitrary then Taylor's theorem gives

$$\begin{aligned} f(\underset{\sim}{x}) &= f(\underset{\sim}{x}^0) + \Delta\underset{\sim}{x}^T \nabla_{\underset{\sim}{x}} f(\underset{\sim}{x}^0 + \lambda_1 \Delta\underset{\sim}{x}) \\ &= f(\underset{\sim}{x}^0) + \Delta\underset{\sim}{x}^T \nabla_{\underset{\sim}{x}} f(\underset{\sim}{x}^0) + \frac{1}{2} \Delta\underset{\sim}{x}^T \underset{\sim}{G}(\underset{\sim}{x}^0 + \lambda_2 \Delta\underset{\sim}{x}) \Delta\underset{\sim}{x} \\ &= f(\underset{\sim}{x}^0) + \Delta\underset{\sim}{x}^T \nabla_{\underset{\sim}{x}} f(\underset{\sim}{x}^0) + \frac{1}{2} \Delta\underset{\sim}{x}^T \underset{\sim}{G}(\underset{\sim}{x}^0) \Delta\underset{\sim}{x} + \ldots \end{aligned} \tag{18}$$

for some $0 \leq \lambda_1, \lambda_2 \leq 1$, where

$$\Delta\underset{\sim}{x} \triangleq \underset{\sim}{x} - \underset{\sim}{x}^0 \quad . \tag{19}$$

Furthermore, we denote first-order changes by δ so that

$$\delta f \triangleq \Delta\underset{\sim}{x}^T \nabla_{\underset{\sim}{x}} f(\underset{\sim}{x}^0) \quad . \tag{20}$$

Sensitivity Evaluation

An abstract approach to the evaluation of first-order sensitivities will be presented. It is desired to evaluate $\nabla_{\tilde{x}} f$ where f is calculated through a set of intermediate variables $\tilde{y}$ obtained from a solution of the system

$$\tilde{A}(\tilde{x})\, \tilde{y} = \tilde{b} \tag{26}$$

which is linear in $\tilde{y}$. We assume that

$$\tilde{y} = \tilde{A}^{-1}(\tilde{x})\, \tilde{b} \implies f(\tilde{x}, \tilde{y}(\tilde{x})) \quad . \tag{27}$$

Then

$$\nabla_{\tilde{x}} f = \frac{\partial f}{\partial \tilde{x}} + \frac{\partial \tilde{y}^T}{\partial \tilde{x}} \frac{\partial f}{\partial \tilde{y}} \quad . \tag{28}$$

Differentiating (26) w.r.t. x_i we have

$$\frac{\partial \tilde{A}}{\partial x_i}(\tilde{x})\, \tilde{y} + \tilde{A}(\tilde{x}) \frac{\partial \tilde{y}}{\partial x_i} = \tilde{0} \quad . \tag{29}$$

Given $\tilde{y}$ from a solution of (26) and assuming that the calculation of $\partial \tilde{A}/\partial x_i$ presents no difficulty the calculation of $\partial \tilde{y}/\partial x_i$ is obtained from the solution of the linear system

$$\tilde{A}(\tilde{x}) \frac{\partial \tilde{y}}{\partial x_i} = - \frac{\partial \tilde{A}(\tilde{x})}{\partial x_i} \tilde{y} \quad . \tag{30}$$

Clearly, n such analyses yield the matrix $\partial \tilde{y}^T/\partial \tilde{x}$, if it is desired.

Suppose, for example, that

$$\tilde{y} = \tilde{A}^{-1}(\tilde{x})\, \tilde{b} \implies f(y_i(\tilde{x})) \text{ for some } i \, . \tag{31}$$

Then $\partial f/\partial \tilde{y}$ is zero except possibly for the ith component. Let $\tilde{u}_i$ be the ith unit vector. Then

$$\nabla_{\tilde{x}} f = \frac{\partial \tilde{y}^T}{\partial \tilde{x}} \tilde{u}_i \frac{\partial f}{\partial y_i} \tag{32}$$

follows from (28). Thus, only the ith column of $\partial \tilde{y}^T/\partial \tilde{x}$, namely $\partial y_i/\partial \tilde{x}$,

Branch and Bound

We consider the general optimization problem

$$\underset{\underset{\sim}{\phi}}{\text{minimize}}\ U(\underset{\sim}{\phi}) \quad \text{s.t. } \underset{\sim}{\phi} \in R \quad , \tag{37}$$

where R was defined by (4). The branch and bound method employs a tree enumeration approach and upper and lower bounds on the objective function to accelerate the process of finding optimal discrete solutions.

Consider a tree structure of nodes and branches. Associated with each node is a bounding procedure and a strategy for choosing the next node, or branching. The nodes are numbered in the order in which they are considered, node 0 representing the original problem. Each node has a unique predecessor tracing one's way back along the path to node 0. Constraints effective at node j are those associated with the path back to 0 as well as those defining R and result in a region R^j. Note that $R = R^0$. As constraints are added to a problem one expects the minimum objective function value to increase or stay the same.

A lower bound at node j is found as follows. Let

$$\check{U}^j = \begin{cases} \min\limits_{\underset{\sim}{\phi} \in R^j} U(\underset{\sim}{\phi}) & \text{if } \check{\underset{\sim}{\phi}}^j \text{ exists} \\ \infty & \text{if } R^j = \emptyset \\ -\infty & \text{otherwise} \end{cases} \tag{38}$$

Relax the constraints suitably to give $\underline{R}^j$ to find a lower bound $\underline{U}^j \leq \check{U}^j$. Thus $R^j \subseteq \underline{R}^j$ and let

$$\underline{U}^j = \begin{cases} \check{\underline{U}}^j = \min\limits_{\underset{\sim}{\phi} \in \underline{R}^j} U(\underset{\sim}{\phi}) & \text{if } \check{\underline{\underset{\sim}{\phi}}}^j \text{ exists} \\ \infty & \text{if } \underline{R}^j = \emptyset \\ -\infty & \text{otherwise} \end{cases} \tag{39}$$

Farkas Lemma

A statement of central importance to optimization is Farkas Lemma. Given the vectors $\{\underset{\sim}{p}_0, \underset{\sim}{p}_1, \ldots, \underset{\sim}{p}_n\}$ one can write

$$\underset{\sim}{p}_0 = \sum_{i=1}^{n} \alpha_i \underset{\sim}{p}_i, \quad \alpha_i \geq 0 \tag{40}$$

if and only if

$$\underset{\sim}{p}_0^T \underset{\sim}{q} \geq 0 \tag{41}$$

for all $\underset{\sim}{q}$ satisfying

$$\underset{\sim}{p}_i^T \underset{\sim}{q} \geq 0, \; i = 1, 2, \ldots, n \tag{42}$$

i.e., there is no $\underset{\sim}{q}$ which simultaneously satisfies $\underset{\sim}{p}_0^T \underset{\sim}{q} < 0$ and (42) if and only if $\underset{\sim}{p}_0$ is in the convex cone spanned by the $\underset{\sim}{p}_i$.

Let

$$J(\underset{\sim}{\phi}) \triangleq \{i \mid M(\underset{\sim}{\phi}) = f_i(\underset{\sim}{\phi})\} \tag{50}$$

denote the set of active functions at any point $\underset{\sim}{\phi}$. Let

$$\underset{\sim}{g}_i \triangleq \underset{\sim}{\nabla}_\phi f_i(\underset{\sim}{\phi}) \tag{51}$$

Then, for differentiable functions

$$\underset{\sim}{g}_i^{j^T} \underset{\sim}{s}^j < 0 \quad \text{for all } i \in J \tag{52}$$

implies that $\delta f_i^j < 0$ for all $i \in J$ and, corresponding to (44),

$$M(\underset{\sim}{\phi}^j + \alpha \underset{\sim}{s}^j) < M(\underset{\sim}{\phi}^j) \tag{53}$$

for sufficiently small $\alpha > 0$ and where we assume that $J(\underset{\sim}{\phi}^j + \alpha \underset{\sim}{s}^j) \subseteq J(\underset{\sim}{\phi}^j)$. $\underset{\sim}{s}^j$ can be described as a descent direction for $M(\underset{\sim}{\phi})$ at $\underset{\sim}{\phi}^j$. The condition

$$\underset{\sim}{g}_i^T \underset{\sim}{s}^j \geq 0, \; i \in J(\underset{\sim}{\phi}) \tag{54}$$

is a necessary condition for a minimum of $M(\underset{\sim}{\phi})$ w.r.t. α along $\underset{\sim}{s}^j$.

A necessary condition for a minimum $\underset{\sim}{\check{\phi}}$ assuming differentiability is the existence of u_i, $i = 1, 2, \ldots, n$ such that

$$\sum_{i=1}^{n} u_i \underset{\sim}{g}_i(\underset{\sim}{\check{\phi}}) = \underset{\sim}{0} \tag{55}$$

$$\sum_{i=1}^{n} u_i = 1 \tag{56}$$

$$u_i \geq 0, \; i = 1, 2, \ldots, n \tag{57}$$

$$u_i = 0, \; i \notin J(\underset{\sim}{\check{\phi}}) \quad , \tag{58}$$

i.e., the origin must be a convex combination of the gradient vectors of the active functions at $\underset{\sim}{\check{\phi}}$.

Consider the problem

$$\text{minimize } U(\underset{\sim}{\phi}) \text{ s.t. } \underset{\sim}{h}(\underset{\sim}{\phi}) = \underset{\sim}{0} \quad . \tag{59}$$

The Lagrangian function is given by

Since, for any $\underset{\sim}{\lambda}^0$ and $\underset{\sim}{\phi}^0$,

$$\min_{\underset{\sim}{\phi}} L(\underset{\sim}{\phi},\underset{\sim}{\lambda}^0) \le \max_{\underset{\sim}{\lambda} \ge \underset{\sim}{0}} L(\underset{\sim}{\phi}^0, \underset{\sim}{\lambda}) \tag{68}$$

the dual problem yields a lower bound for the primal problem and the solutions, if they exist, give the same L.

If $U(\underset{\sim}{\phi})$ is convex and $\underset{\sim}{c}(\underset{\sim}{\phi})$ concave and the functions are differentiable then

$$\nabla_{\underset{\sim}{\phi}} L = \underset{\sim}{g} - \sum_{i=1}^{m} \lambda_i \, \underset{\sim}{a}_i = \underset{\sim}{0}, \; \underset{\sim}{\lambda} \ge \underset{\sim}{0} \tag{69}$$

imply that the dual requirements are satisfied. Hence, maximizing L w.r.t. $\underset{\sim}{\phi}$ and $\underset{\sim}{\lambda}$ subject to the constraints (69) is an equivalent problem to the dual problem.

Assume that a minimum exists at $\underset{\sim}{\check{\phi}}$, that the functions concerned are differentiable and that <u>constraint qualifications</u> are satisfied. Then there exists an m-dimensional vector $\underset{\sim}{u}$ such that

$$\underset{\sim}{g}(\underset{\sim}{\check{\phi}}) - \sum_{i=1}^{m} u_i \, \underset{\sim}{a}_i(\underset{\sim}{\check{\phi}}) = \underset{\sim}{0} \tag{70}$$

$$u_i \ge 0, \; i = 1, 2, \ldots, m \tag{71}$$

$$u_i = 0, \; i \notin J(\underset{\sim}{\check{\phi}}) \tag{72}$$

where

$$\underset{\sim}{a}_i \triangleq \nabla_{\underset{\sim}{\phi}} c_i \tag{73}$$

The conditions (70) to (72) are usually called the <u>Kuhn-Tucker conditions</u> and the $\underset{\sim}{u}$ contains the <u>Kuhn-Tucker multipliers</u>. The multipliers are non-negative since they correspond to $c_i \ge 0$. If $c_i \le 0$ the corresponding multiplier would be nonpositive. If $c_i = 0$, then the multiplier is unrestricted.

The conditions may be interpreted as: the gradient vector of the

The feasible direction strategies outlined above are quadratic programs. A linear programming approach can be suggested with the same constraints but where we minimize $\underset{\sim}{g}^T \underset{\sim}{s}$ subject to the additional constraints $\underset{\sim}{a}_i^T \underset{\sim}{s} \geq 0$ in the general case and minimize s_{k+1} subject to the additional constraints $s_{k+1} \geq \underset{\sim}{g}_i^T \underset{\sim}{s}$ for the minimax problem.

Scaling and Transformations

Consider a nonsingular linear transformation of $\underset{\sim}{\phi}$ into $\underset{\sim}{\phi}'$, forming the image space. Thus,

$$\underset{\sim}{\phi}' = \underset{\sim}{T}^T \underset{\sim}{\phi} \quad , \tag{79}$$

where, obviously,

$$\underset{\sim}{T} = \frac{\partial \underset{\sim}{\phi}'^T}{\partial \underset{\sim}{\phi}} \quad . \tag{80}$$

Incremental changes or directions are then related by

$$\underset{\sim}{s}' = \underset{\sim}{T}^T \underset{\sim}{s} \tag{81}$$

and gradients by

$$\underset{\sim}{g} = \underset{\sim}{T}\, \underset{\sim}{g}' \quad . \tag{82}$$

Consider

$$\underset{\sim}{s} = \alpha\, \underset{\sim}{g} \quad . \tag{83}$$

Then

$$\underset{\sim}{s}' = \alpha \underset{\sim}{T}^T \underset{\sim}{T}\, \underset{\sim}{g}' \quad , \tag{84}$$

hence the conventional directions of steepest ascent, namely $\underset{\sim}{g}$ and $\underset{\sim}{g}'$, correspond if $\underset{\sim}{T}^T \underset{\sim}{T}$ is a multiple of an orthogonal matrix. Equal changes of scale and simple rotations of coordinates are permitted. Other transformations or unequal changes of scale may cause a well-conditioned problem in one set of variables to be badly conditioned in another, and vice versa. In any case we note that gradient directions are scale dependent.

The quadratic function $Q(\underset{\sim}{s})$ under the linear transformation becomes

$$Q'(\underset{\sim}{s}') = \frac{1}{2} \underset{\sim}{s}'^T \underset{\sim}{Q}' \underset{\sim}{s}' + \underset{\sim}{g}'^T \underset{\sim}{s}' + c \quad , \tag{85}$$

where

$$\underset{\sim}{Q}' = \underset{\sim}{T}^{-1} \underset{\sim}{Q}\, \underset{\sim}{T}^{T^{-1}} . \tag{86}$$

Newton and Modified Newton Methods

Following our discussion on partial derivatives we observe that the basic Newton-type iteration involves solving for $\mathbf{s}^j$ the system

$$\mathbf{G}^j \mathbf{s}^j = -\mathbf{g}^j \quad , \tag{92}$$

where $\mathbf{G}^j$ and $\mathbf{g}^j$ are calculated at $\boldsymbol{\phi}^j$. If $\mathbf{G}^j$ is positive definite we obtain a $\mathbf{s}^j$ which is downhill since $\mathbf{s}^{j^T} \mathbf{G}^j \mathbf{s}^j > 0$ for nonzero $\mathbf{s}^j$ implying that $-\mathbf{s}^{j^T} \mathbf{g}^j > 0$. To make sure of a descent direction when $\mathbf{G}^j$ is not sufficiently positive definite we may consider the solution of

$$\mathbf{G}_m^j \mathbf{s}^j = -\mathbf{g}^j \quad , \tag{93}$$

where $\mathbf{G}_m^j$ is a suitable modified matrix.

Two important possible modifications will be singled out. The first may be described as the Levenberg-Marquardt approach. In general, we let

$$\mathbf{G}_m^j = \mathbf{G}^j + \lambda^j \mathbf{1} \tag{94}$$

choosing $\lambda^j \geq 0$ to make $\mathbf{G}_m^j$ positive definite. In essence, we have added a term $\lambda(\mathbf{s}^T \mathbf{s} - h^2)$ to the objective function, λ being interpreted as a Lagrange multiplier and h as a step size. New parameters have thus been introduced which must be determined at each iteration. For $\lambda = 0$ we regain the undamped Newton step, whereas with large positive λ the steepest descent direction is obtained. Methods based on this approach would attempt to ensure a sufficient decrease in the objective function at each iteration by appropriately selecting a value of λ.

A second method is due to Gill and Murray. Here, we let

$$\mathbf{G}_m^j = \mathbf{G}^j + \mathbf{E}^j \quad , \tag{95}$$

where $\mathbf{E}^j$ is a diagonal matrix, and where $\mathbf{G}^j$ is factored as

$$\mathbf{G}^j = \mathbf{L}^j \mathbf{D}^j \mathbf{L}^{j^T} \quad , \tag{96}$$

where $\mathbf{L}^j$ is a lower triangular matrix and $\mathbf{D}^j$ is a diagonal matrix whose elements are sufficiently large to ensure stable factorization. $\mathbf{E}^j$ can be set to zero if $\mathbf{G}^j$ is sufficiently positive definite.

In general, if $\underset{\sim}{H}^0$ is a positive definite symmetric matrix then $\underset{\sim}{H}^j$ is also a positive definite symmetric matrix so that $\underset{\sim}{s}^j$ always points downhill. A consequence of Dixon's work is that for the same $\underset{\sim}{\phi}^0$ and $\underset{\sim}{H}^0$ these and other special cases of Huang's family generate the same sequence $\underset{\sim}{\phi}^1$, $\underset{\sim}{\phi}^2$, ...

Under the conditions of full linear search $\underset{\sim}{s}^{j^T} \underset{\sim}{g}^{j+1} = 0$, thus post-multiplying both sides of (98) and (99) by $\underset{\sim}{\gamma}^j$ we find that

$$\underset{\sim}{H}^{j+1} \underset{\sim}{\gamma}^j = \alpha^j \underset{\sim}{s}^j \quad . \tag{103}$$

This is a condition analogous to one which is fulfilled by positive definite quadratic functions, which the updating formulas are attempting to force.

$$\underset{\sim}{\lambda} = (\underset{\sim}{A}^T \underset{\sim}{G}^{-1} \underset{\sim}{A})^{-1} \underset{\sim}{A}^T \underset{\sim}{G}^{-1} \underset{\sim}{g} \quad , \tag{110}$$

$$\underset{\sim}{s} = -(\underset{\sim}{1} - \underset{\sim}{G}^{-1} \underset{\sim}{A} (\underset{\sim}{A}^T \underset{\sim}{G}^{-1} \underset{\sim}{A})^{-1} \underset{\sim}{A}^T) \underset{\sim}{G}^{-1} \underset{\sim}{g} \quad . \tag{111}$$

$\underset{\sim}{\lambda}$ is in effect a second-order estimate of the Lagrange multipliers at the solution, i.e., an attempt is made to satisfy the optimality conditions for the main problem with selected active constraints and a quadratic model for the objective function. $\underset{\sim}{s}$ is a projection of $-\underset{\sim}{g}$ onto the constrained space.

Suppose $\underset{\sim}{Q} = \underset{\sim}{1}$. Following through the derivations we obtain the special case

$$\underset{\sim}{\lambda} = \underset{\sim}{A}^+ \underset{\sim}{g} \quad , \tag{112}$$

$$\underset{\sim}{s} = -(\underset{\sim}{1} - \underset{\sim}{A} \underset{\sim}{A}^+) \underset{\sim}{g} \quad . \tag{113}$$

yielding a first-order estimate of the Lagrange multipliers at the solution and the constrained steepest descent direction. Letting $\underset{\sim}{P} \triangleq \underset{\sim}{A} \underset{\sim}{A}^+$ we recognize the more familar projection onto the subspace spanned by the active $\underset{\sim}{a}_i$, and $\underset{\sim}{1} - \underset{\sim}{P}$ as the orthogonal projection onto the constrained space.

Negative multipliers indicate constraints which may be dropped from the set of constraints currently held active. During minimization new constraints can be added to the active set when necessary.

Quasi-Newton methods for unconstrained minimization can be extended to the linearly constrained case.

So-called <u>reduced-gradient</u> methods use linear equality constraints to eliminate variables from the optimization problem.

where, for convenience, we have taken the first n variables are the basic variables corresponding to an admissible basis $\underset{\sim}{B}$ containing n linearly independent columns. We have set $\phi_i = 0$, $i = n+1, n+2, \ldots, k$.

By analogy with the foregoing discussion

$$\underset{\sim}{A}^T = \begin{bmatrix} \underset{\sim}{B} & \underset{\sim}{C} \\ \underset{\sim}{0} & \underset{\sim}{1} \end{bmatrix} \quad . \tag{118}$$

Equation (114) is now interpreted as

$$\begin{bmatrix} \underset{\sim}{B}^T & \underset{\sim}{0} \\ \underset{\sim}{C}^T & \underset{\sim}{1} \end{bmatrix} \begin{bmatrix} \underset{\sim}{\lambda}_b \\ \underset{\sim}{\lambda}_c \end{bmatrix} = \begin{bmatrix} \underset{\sim}{c}_b \\ \underset{\sim}{c}_c \end{bmatrix} \quad , \tag{119}$$

where $\underset{\sim}{\lambda}$ and $\underset{\sim}{c}$ have been appropriately partitioned. The solution of

$$\underset{\sim}{B}^T \underset{\sim}{\lambda}_b = \underset{\sim}{c}_b \tag{120}$$

provides the simplex multipliers for investigating

$$\underset{\sim}{\lambda}_c = \underset{\sim}{c}_c - \underset{\sim}{C}^T \underset{\sim}{\lambda}_b \quad , \tag{121}$$

namely, the Lagrange multipliers for the inequality constraints $\underset{\sim}{\phi} \geq \underset{\sim}{0}$ which are active.

Now since $\underset{\sim}{B}$ provides a basis we can expand any column $\underset{\sim}{a}_i'$ of $\underset{\sim}{A}'$ as $\underset{\sim}{B}\,\underset{\sim}{x}_i = \underset{\sim}{a}_i'$. Note that $\underset{\sim}{x}_i = \underset{\sim}{u}_i$, $i = 1, 2, \ldots, n$. Consider

$$\underset{\sim}{B}(\underset{\sim}{\phi}_b - \theta \underset{\sim}{x}_i) + \theta \underset{\sim}{a}_i' = \underset{\sim}{b} \tag{122}$$

and

$$\underset{\sim}{c}_b^T (\underset{\sim}{\phi}_b - \theta \underset{\sim}{x}_i) + \theta c_i \tag{123}$$

and suppose that $\lambda_r < 0$ for some $n+1 \leq r \leq k$ and therefore we want to move away from $\phi_r = 0$. Let the nearest constraint be $\phi_s = 0$. Choose $\theta = \theta_s$ such that $\underset{\sim}{\phi}_b - \theta \underset{\sim}{x}_r$ has a zero in the sth row, i.e.,

$$\theta_s = \frac{\phi_s}{x_{sr}} = \min_{x_{ir}>0} \frac{\phi_i}{x_{ir}} \quad . \tag{124}$$

Reference Material

Principal texts consulted in writing this review are ones by Garfinkel and Nemhauser[1], Gill and Murray[2] and Lasdon[3]. Integer and discrete problems are further discussed in considerable detail by Garfinkel and Nemhauser. Chapters by Gill and Murray, Powell and Sargent in the excellently edited book by Gill and Murray provided a wealth of illuminating material on descent, optimality, linear inequalities and constraints, projection methods, and linear programming as well as on quadratic forms and Newton based algorithms. Lasdon also provides a detailed discussion of linear programming. The review paper by Charalambous[4] was consulted, and the section on sensitivity evaluation was inspired by a paper due to Branin[5].

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1 R.S. Garfinkel and G.L. Nemhauser, Integer Programming. New York: Wiley, 1972.

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Note that R_c as given by (2) admits all its boundary points and hence this region is said to be closed. An open region does not contain any of its boundary points. The notation $\phi \in R_c$ signifies that ϕ is in the constraint region.

$U(\phi)$ generates a response hypersurface. The goal of optimization is to locate a $\check{\phi}$ in R such that

$$U(\check{\phi}) \leq U(\phi), \text{ for all } \phi \in R \quad , \tag{3}$$

where

$$R \triangleq R_c \cap \Phi^k \quad . \tag{4}$$

This gives a global minimum. A somewhat more difficult concept to define is a local minimum. A local minimum of $U(\phi)$ occurs at $\check{\phi}$ in R with respect to a suitably defined neighborhood $N(\phi)$ if

$$U(\check{\phi}) \leq U(\phi), \text{ for all } \phi \in R \cap N(\check{\phi}) \quad . \tag{5}$$

In continuous optimization the neighborhood is taken as an open hypersphere containing $\check{\phi}$.

Depending upon the nature of the problem and the algorithm employed we may find the global minimum, a local minimum, several local minima, or no minimum. The processes of determining the existence of an optimal solution, characterizing it and searching for it fall into the domain of mathematical programming.

Partial Derivatives

We consider now some important classical concepts applicable to continuous functions with continuous first and second partial derivatives, as appropriate.

Consider the differentiable functions $f(\underset{\sim}{x})$ and $\underset{\sim}{y}(\underset{\sim}{x})$, where

$$\underset{\sim}{x} \triangleq \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \qquad \underset{\sim}{y} \triangleq \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}. \tag{10}$$

Let the n-dimensional partial derivative operator w.r.t. $\underset{\sim}{x}$ be

$$\underset{\sim}{\nabla}_x \triangleq \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{bmatrix}. \tag{11}$$

Then $\underset{\sim}{\nabla}_x f$ is the gradient vector of f w.r.t. $\underset{\sim}{x}$ and $\underset{\sim}{J}$ given by

$$\underset{\sim}{J}^T = \frac{\partial \underset{\sim}{y}^T}{\partial \underset{\sim}{x}} \triangleq \left[\underset{\sim}{\nabla}_x y_1 \ \underset{\sim}{\nabla}_x y_2 \ \cdots \ \underset{\sim}{\nabla}_x y_m\right] \tag{12}$$

is termed the Jacobian matrix of $\underset{\sim}{y}$ w.r.t. $\underset{\sim}{x}$. Observe that $\underset{\sim}{\nabla}_x = \frac{\partial}{\partial \underset{\sim}{x}}$ and

$$\frac{\partial \underset{\sim}{x}^T}{\partial \underset{\sim}{x}} = \underset{\sim}{1} \triangleq \begin{bmatrix} 1 & 0 \dots 0 \\ 0 & 1 \dots 0 \\ \vdots & \vdots \quad \vdots \\ 0 & 0 \dots 1 \end{bmatrix}. \tag{13}$$

The Hessian matrix $\underset{\sim}{G}$ of $\underset{\sim}{f}$ w.r.t. $\underset{\sim}{x}$ is given by

It is a simple exercise to prove that, with respect to the Euclidean measure of distance, $\nabla_{x} f$ provides the steepest ascent direction and $-\nabla_{x} f$ the steepest descent direction. In other words, δf is maximized (minimized) for the norm $|| \Delta x || = (\Delta x^T \Delta x)^{1/2} = 1$ if Δx is aligned with the steepest ascent (descent) directions at x^0.

Now,

$$y(x) = y(x^0) + J(x^0)\ \Delta x + \ldots \tag{21}$$

The solution x^1 to $y(x) = 0$ obtained from a linear approximation at x^0 is interpreted from (21) as

$$x^1 = x^0 - J^{-1}(x^0)\ y(x^0) \tag{22}$$

Taking $y \equiv \nabla_x f$ we have, correspondingly,

$$x^1 = x^0 - G^{-1}(x^0)\ \nabla_x f(x^0) \tag{23}$$

and, for $f' = \frac{1}{2} y^T y$, we have following (15) to (17)

$$x^1 \simeq x^0 - (J^T J)^{-1} J^T y(x^0) \quad , \tag{24}$$

i.e., we have the basis for the well-known Newton methods of solving non-linear equations, function minimization and least squares approximation, respectively, x^0 being the current estimate and x^1 the next (hopefully better) estimate of the solution.

If $G(x)$ is positive semidefinite (negative semidefinite) for all x then, from Taylor's theorem (18),

$$f(x) \geq (\leq)\ f(x^0) + \delta f \tag{25}$$

from which it can be shown that $f(x)$ is convex (concave). $f(x^0) + (x - x^0)^T \nabla_x f(x^0)$ defines a tangent hyperplane at x^0.

If $G(x^0)$ is positive definite the Newton step $-G^{-1}(x^0)\ \nabla_x f(x^0)$ can be thought of as providing the steepest descent direction for the norm $|| \Delta x || = (\Delta x^T G(x^0)\ \Delta x)^{1/2} = 1$, δf being accordingly minimized.

is required. Now

$$\frac{\partial y_i}{\partial x_j} = \underset{\sim}{u}_i^T \frac{\partial \underset{\sim}{y}}{\partial x_j} = -\underset{\sim}{u}_i^T \underset{\sim}{A}^{-1}(\underset{\sim}{x}) \frac{\partial \underset{\sim}{A}(\underset{\sim}{x})}{\partial x_j} \underset{\sim}{y} \quad . \tag{33}$$

Let $\hat{\underset{\sim}{y}}_i$ be the solution to

$$\underset{\sim}{A}^T(\underset{\sim}{x}) \hat{\underset{\sim}{y}}_i = \underset{\sim}{u}_i \quad . \tag{34}$$

Then

$$\frac{\partial y_i}{\partial x_j} = -\hat{\underset{\sim}{y}}_i^T \frac{\partial \underset{\sim}{A}(\underset{\sim}{x})}{\partial x_j} \underset{\sim}{y} \quad . \tag{35}$$

Thus,

$$\frac{\partial y_i}{\partial \underset{\sim}{x}} = \left[-\hat{\underset{\sim}{y}}_i^T \frac{\partial \underset{\sim}{A}(\underset{\sim}{x})}{\partial x_1} \underset{\sim}{y} \quad -\hat{\underset{\sim}{y}}_i^T \frac{\partial \underset{\sim}{A}(\underset{\sim}{x})}{\partial x_2} \underset{\sim}{y} \quad \cdots \quad -\hat{\underset{\sim}{y}}_i^T \frac{\partial \underset{\sim}{A}(\underset{\sim}{x})}{\partial x_n} \underset{\sim}{y} \right]^T \tag{36}$$

and is obtained numerically through the solutions $\underset{\sim}{y}$ and $\hat{\underset{\sim}{y}}_i$ and matrix multiplications. Observe that if $\underset{\sim}{A}$ is factored into upper and lower triangular forms in the solution of (26) then the solution to (34) is obtained following one forward and one backward substitution. Using sparsity and system structure appropriately the sensitivity expressions (35) may reduce to simple formulas.

The relationship of the foregoing presentation to the adjoint network method should be clear. See Branin (1973).

The choice of $\underline{R}^j$ must be such as to result in a convenient problem to be solved and to yield a useful (not too low) lower bound. This lower bound is also valid for successor nodes. An example of an $\underline{R}^j$ would be one leading to a continuous optimization problem.

An upper bound $\overline{U}^j \geq \check{U}^j$ can, for example, be found by calculating U at any convenient point in R^j. We note that this bound is valid for predecessor nodes.

A node j is fathomed if $\underline{U}^j = \overline{U}^j$ (for obvious reasons) or if $\underline{U}^j \geq \overline{U}^0$, since $\overline{U}^0$ represents the best discrete solution available and a successor to node j can not improve the situation. No further branching takes place from fathomed nodes.

Descent and Optimality

During minimization of $U(\tilde{\phi})$ a sequence of points $\{\tilde{\phi}^0, \tilde{\phi}^1, \ldots\}$ is generated. If

$$U(\tilde{\phi}^{j+1}) < U(\tilde{\phi}^j) \tag{43}$$

then the step from $\tilde{\phi}^j$ to $\tilde{\phi}^{j+1}$ is a descent step.

The vector $\tilde{s}^j$ is said to be a downhill direction at $\tilde{\phi}^j$ if

$$U(\tilde{\phi}^j + \alpha\, \tilde{s}^j) < U(\tilde{\phi}^j) \tag{44}$$

for sufficiently small $\alpha > 0$. It is also a feasible direction if the constraints are satisfied.

Descent algorithms usually attempt to obtain a suitable value α^j such that

$$\tilde{\phi}^{j+1} = \tilde{\phi}^j + \alpha^j\, \tilde{s}^j \quad , \tag{45}$$

where $\tilde{s}^j$ is a downhill search direction at $\tilde{\phi}^j$ and (43) is satisfied.

Differentiating $U(\tilde{\phi}^j + \alpha\, \tilde{s}^j)$ w.r.t. α at $\tilde{\phi} = \tilde{\phi}^j + \alpha\, \tilde{s}^j$ we have

$$\frac{\partial U}{\partial \alpha} = \tilde{g}^T\, \tilde{s}^j \quad , \tag{46}$$

where

$$\tilde{g} \triangleq \nabla_{\tilde{\phi}}\, U \tag{47}$$

so that, for a differentiable function U,

$$\tilde{g}^{j^T}\, \tilde{s}^j < 0$$

implies that $\delta U^j < 0$, (44) is satisfied and $\tilde{s}^j$ is downhill. The condition

$$\tilde{g}^T\, \tilde{s}^j = 0 \tag{48}$$

is a necessary condition for a minimum of a differentiable function $U(\tilde{\phi})$ w.r.t. α along $\tilde{s}^j$. An exact linear search for a minimum gives $\tilde{g}^{j+1^T}\, \tilde{s}^j = 0$.

Consider minimax optimization for which

$$M(\tilde{\phi}) \triangleq \max_{1 \leq i \leq n} f_i(\tilde{\phi}) \quad . \tag{49}$$

$$L(\underset{\sim}{\phi}, \underset{\sim}{\lambda}) = U(\underset{\sim}{\phi}) - \underset{\sim}{\lambda}^T \underset{\sim}{h}(\underset{\sim}{\phi}) \quad , \tag{60}$$

where $\underset{\sim}{\lambda}$ is an s-vector of Lagrange multipliers. A stationary point $\underset{\sim}{\phi}^0$, $\underset{\sim}{\lambda}^0$ is found from the solution of

$$\underset{\sim}{\nabla}_\phi L = \underset{\sim}{g} - \sum_{i=1}^{s} \lambda_i \underset{\sim}{\nabla}_\phi h_i = \underset{\sim}{0} \tag{61}$$

$$\underset{\sim}{\nabla}_\lambda L = \underset{\sim}{h} = \underset{\sim}{0} \quad , \tag{62}$$

where the multipliers are unrestricted in sign.

Now consider the problem

$$\underset{\underset{\sim}{\phi}}{\text{minimize}}\ U(\underset{\sim}{\phi}) \text{ s.t. } \underset{\sim}{c}(\underset{\sim}{\phi}) \geq \underset{\sim}{0} \quad . \tag{63}$$

Let

$$J(\underset{\sim}{\phi}) \triangleq \{i \mid c_i(\underset{\sim}{\phi}) = 0\} \tag{64}$$

denote the set of active functions at any feasible point $\underset{\sim}{\phi}$, where $c_i(\underset{\sim}{\phi}) > 0$ for all $i \notin J$. We can write down the Lagrangian

$$L(\underset{\sim}{\phi}, \underset{\sim}{\lambda}) = U(\underset{\sim}{\phi}) - \underset{\sim}{\lambda}^T \underset{\sim}{c}(\underset{\sim}{\phi}) \tag{65}$$

where $\underset{\sim}{\lambda}$ is an m-vector.

Observe that $\max\limits_{\underset{\sim}{\lambda} \geq \underset{\sim}{0}} L(\underset{\sim}{\phi}, \underset{\sim}{\lambda})$ is simply $U(\underset{\sim}{\phi})$ where $\underset{\sim}{c} \geq \underset{\sim}{0}$ and $+\infty$ where $\underset{\sim}{c} \not\geq \underset{\sim}{0}$. This is called the primal function. The problem

$$\underset{\underset{\sim}{\phi}}{\text{minimize}}\ \max_{\underset{\sim}{\lambda} \geq \underset{\sim}{0}} L(\underset{\sim}{\phi}, \underset{\sim}{\lambda}) \tag{66}$$

is referred to as the primal problem which is essentially the original nonlinear programming problem.

The problem

$$\underset{\underset{\sim}{\lambda} \geq \underset{\sim}{0}}{\text{maximize}}\ \min_{\underset{\sim}{\phi}} L(\underset{\sim}{\phi}, \underset{\sim}{\lambda}) \tag{67}$$

is referred to as the dual problem. The function $\min\limits_{\underset{\sim}{\phi}} L(\underset{\sim}{\phi}, \underset{\sim}{\lambda})$ is called the dual function.

objective function is in the cone spanned by the gradient vectors of the active constraints at $\check{\underset{\sim}{\phi}}$.

If we identify a new independent variable ϕ_{k+1} and reinterpret the Kuhn-Tucker conditions for the special problem, for m = n,

$$U = \phi_{k+1} \tag{74}$$

$$c_i = \phi_{k+1} - f_i(\underset{\sim}{\phi}) \tag{75}$$

we have $\underset{\sim}{g} = \underset{\sim}{0}$, $\partial U/\partial\phi_{k+1} = 1$, $\underset{\sim}{a}_i = -\underset{\sim}{g}_i$, $\partial c_i/\partial\phi_{k+1} = 1$ and, given $\underset{\sim}{\phi}$, $c_i = 0$ corresponds to $\phi_{k+1} = M(\underset{\sim}{\phi})$ so that the conditions (55) to (58) and (70) to (72) correspond. In fact, this special nonlinear (linear) program is often set up to solve nonlinear (linear) minimax approximation problems.

If at some point $\underset{\sim}{\phi}$ the vector $\underset{\sim}{g}$ is not in the convex cone spanned by the active gradient vectors we would normally expect a feasible descent direction. Thus, if there exists an $\underset{\sim}{s}$ such that $\underset{\sim}{a}_i^T \underset{\sim}{s} \geq 0$ for all $i \in J$ and $\underset{\sim}{g}^T \underset{\sim}{s} < 0$ then $\underset{\sim}{g}$ is not in the cone. It can be proved that the smallest $\underset{\sim}{s}$ in the Euclidean sense w.r.t. α_i subject to

$$\underset{\sim}{s} = -\underset{\sim}{g} + \sum_{i \in J} \alpha_i \underset{\sim}{a}_i, \; \alpha_i \geq 0 \tag{76}$$

provides the steepest feasible descent direction also in the Euclidean sense. This is the principle of the <u>method of feasible directions</u>. Indeed, if the minimal $\underset{\sim}{s} = \underset{\sim}{0}$ the necessary conditions for optimality are satisfied.

Similarly, the smallest $\underset{\sim}{s}$ w.r.t. α_i subject to

$$\underset{\sim}{s} = -\sum_{i \in J} \alpha_i \underset{\sim}{g}_i, \quad \sum_{i \in J} \alpha_i = 1, \; \alpha_i \geq 0 \tag{77}$$

provides the steepest downhill direction in the Euclidean sense for the minimax problem, with appropriate optimality conditions satisfied.

Quadratic Models

The most common model with respect to which, for example, unconstrained minimization methods are derived is the positive definite quadratic model. By analogy with (18) we consider

$$Q(\underset{\sim}{s}) = \frac{1}{2} \underset{\sim}{s}^T \underset{\sim}{Q} \underset{\sim}{s} + \underset{\sim}{g}^T \underset{\sim}{s} + c \quad , \tag{78}$$

where $\underset{\sim}{Q}$ is a k x k constant symmetric matrix, $\underset{\sim}{g}$ is a k-vector of constants and c is a constant. The gradient vector is $\underset{\sim}{Q}\,\underset{\sim}{s} + \underset{\sim}{g}$ and the Hessian matrix is $\underset{\sim}{Q}$. The solution of $\underset{\sim}{Q}\,\underset{\sim}{s} + \underset{\sim}{g} = \underset{\sim}{0}$, if $\underset{\sim}{Q}$ is positive definite, yields a unique minimum of Q and can be found in a finite number of steps. If $\underset{\sim}{Q}$ is the Hessian matrix of the nonlinear objective function under consideration and $\underset{\sim}{g}$ is the gradient vector then Q is a <u>quadratic approximation</u> to the objective function. If $\underset{\sim}{Q} = \underset{\sim}{1}$ then the step to the minimum $\underset{\sim}{s} = -\underset{\sim}{g}$. This indicates that the minimum lies in the direction of the negative gradient when the contours of the function are spherical, which brings us to the important subject of scaling.

We are at liberty to set $\underset{\sim}{Q}' = \underset{\sim}{1}$ which can be effected if

$$\underset{\sim}{T} = \underset{\sim}{X}\, \underset{\sim}{\Lambda}^{1/2} \quad , \tag{87}$$

where $\underset{\sim}{X}$ contains the unit eigenvectors of $\underset{\sim}{Q}$ and $\underset{\sim}{\Lambda}$ is a diagonal matrix with corresponding distinct eigenvalues. The transformation $\underset{\sim}{X}^{-1}\, \underset{\sim}{Q}\, \underset{\sim}{X} = \underset{\sim}{\Lambda}$ is called the diagonalization of $\underset{\sim}{Q}$.

Steepest descent algorithms might benefit from such an analysis, however, it is not convenient to implement, in general, minimization algorithms less sensitive to scaling being more desirable.

A nonlinear transformation is given, for example, by

$$\underset{\sim}{\phi}' = \underset{\sim}{f}(\underset{\sim}{\phi}) \quad . \tag{88}$$

A matrix $\underset{\sim}{T}$ can be defined as in (80) leading to

$$\delta\underset{\sim}{\phi}' = \underset{\sim}{T}^{T}\, \Delta\, \underset{\sim}{\phi} \quad , \tag{89}$$

$$\underset{\sim}{g}' = \underset{\sim}{T}^{-1}\, \underset{\sim}{g} \quad , \tag{90}$$

which should be compared with (81) and (82), respectively.

Suppose

$$\underset{\sim}{\phi}' = \log_e \underset{\sim}{\phi} \quad , \tag{91}$$

hence $\underset{\sim}{T}$ is a diagonal matrix with ith element $1/\phi_i$. We have $\delta\phi_i' = \Delta\phi_i/\phi_i$ and $g_i' = \phi_i\, g_i$, hence first-order changes and gradients in the $\underset{\sim}{\phi}'$ space are scale independent.

Quasi-Newton Methods

Instead of using local second partial derivative information at the jth iteration, quasi-Newton methods, using only first derivatives, can be thought of as building up information from previous iterations to ensure good downhill directions of search. The information results in a matrix $\underset{\sim}{H}^j$ which may tend under certain conditions to approximate the inverse of the Hessian.

The direction $\underset{\sim}{s}^j$ is obtained from

$$\underset{\sim}{s}^j = -\underset{\sim}{H}^j \underset{\sim}{g}^j \quad . \tag{97}$$

Two important and effective updating formulas for $\underset{\sim}{H}^j$ can be stated. The first is the Davidon-Fletcher-Powell (DFP) formula

$$\underset{\sim}{H}^{j+1} = \underset{\sim}{H}^j + \frac{\alpha^j \underset{\sim}{s}^j \underset{\sim}{s}^{j^T}}{\underset{\sim}{s}^{j^T} \underset{\sim}{\gamma}^j} - \frac{\underset{\sim}{H}^j \underset{\sim}{\gamma}^j \underset{\sim}{\gamma}^{j^T} \underset{\sim}{H}^j}{\underset{\sim}{\gamma}^{j^T} \underset{\sim}{H}^j \underset{\sim}{\gamma}^j} \tag{98}$$

and the complementary DFP formula

$$\underset{\sim}{H}^{j+1} = \underset{\sim}{H}^j - \frac{\underset{\sim}{s}^j \underset{\sim}{\gamma}^{j^T} \underset{\sim}{H}^j}{\underset{\sim}{s}^{j^T} \underset{\sim}{\gamma}^j} - \frac{\underset{\sim}{H}^j \underset{\sim}{\gamma}^j \underset{\sim}{s}^{j^T}}{\underset{\sim}{s}^{j^T} \underset{\sim}{\gamma}^j} + \left(\alpha^j + \frac{\underset{\sim}{\gamma}^{j^T} \underset{\sim}{H}^j \underset{\sim}{\gamma}^j}{\underset{\sim}{s}^{j^T} \underset{\sim}{\gamma}^j} \right) \frac{\underset{\sim}{s}^j \underset{\sim}{s}^{j^T}}{\underset{\sim}{s}^{j^T} \underset{\sim}{\gamma}^j} \quad , \tag{99}$$

where

$$\underset{\sim}{\gamma}^j \triangleq \underset{\sim}{g}^{j+1} - \underset{\sim}{g}^j \quad , \tag{100}$$

which was discovered by Fletcher, Broyden and Goldfarb.

The formulas are special cases of a general family derived by Huang. On a positive definite quadratic function the minimum is attained in at most k iterations if a full linear search for a minimum is made along each of the k conjugate directions which are generated and $\underset{\sim}{H}^k$ is the inverse Hessian. Thus,

$$\underset{\sim}{g}^k = \underset{\sim}{0} \quad , \tag{101}$$

$$\underset{\sim}{H}^k = \underset{\sim}{A}^{-1} \quad . \tag{102}$$

<u>Linearly Constrained Problems</u>

An important class of problems features constraints of the form

$$\tilde{a}_i^T \tilde{\phi} \geq b_i \quad , \quad i = 1, 2, \ldots, m \quad . \tag{104}$$

Consider a point $\tilde{\phi}$ at which one or more of these constraints are satisfied as equalities. In particular, let

$$\tilde{A}^T \tilde{\phi} = \tilde{b} \tag{105}$$

represent the active set, when $\tilde{A}$ is a rectangular matrix assumed of full rank, necessarily less than k, the number of variables, and $\tilde{b}$ is a vector of corresponding dimension.

Let $Q(\tilde{s})$ be a suitable quadratic model to the objective function at $\tilde{\phi}$. Then a steepest descent direction $\tilde{s}$ may be found by solving the quadratic program

$$\underset{\tilde{s}}{\text{minimize}}\ Q(\tilde{s}) \ , \ \text{s.t.}\ \tilde{A}^T \tilde{s} = \tilde{0} \quad . \tag{106}$$

The directions $\tilde{s}$ are thus forced to be orthogonal to the gradient vectors $\tilde{a}_i$ of the active constraints, i.e., they are to be kept active.

The Lagrange multiplier solution to this problem provides the basis for minimization algorithms subject to linear constraints. We have, taking $\tilde{Q} \equiv \tilde{G}$,

$$\tilde{G}\, \tilde{s} + \tilde{g} = \tilde{A}\, \tilde{\lambda} \quad . \tag{107}$$

Observing that the form is the same as that of a least squares problem linear in $\tilde{\lambda}$ we can write down the solution as

$$\tilde{\lambda} = \tilde{A}^+ (\tilde{G}\, \tilde{s} + \tilde{g}) \quad . \tag{108}$$

If we premultiply both sides of (107) by $\tilde{A}^T \tilde{G}^{-1}$, however, we obtain using the fact that $\tilde{A}^T \tilde{s} = \tilde{0}$

$$\tilde{A}^T \tilde{G}^{-1} \tilde{g} = \tilde{A}^T \tilde{G}^{-1} \tilde{A}\, \tilde{\lambda} \tag{109}$$

from which

Linear Programming

In linear programming we have the linear objective function $\underset{\sim}{c}^T \underset{\sim}{\phi}$ where $\underset{\sim}{c}$ is constant k-vector. The gradient vector $\underset{\sim}{g} \equiv \underset{\sim}{c}$. In linear programming m > k and the solution will lie at a vertex of the feasible region. Suppose we consider k active constraints at a time. The Lagrange multipliers are found from the k equations in k unknowns

$$\underset{\sim}{A}\, \underset{\sim}{\lambda} = \underset{\sim}{c} \quad . \tag{114}$$

If any of the multipliers is negative, $\underset{\sim}{c}^T \underset{\sim}{\phi}$ can be reduced by dropping the corresponding constraint and moving in a direction parallel to the remaining k-1 constraints. This is effected by solving

$$\underset{\sim}{A}^T \underset{\sim}{s} = \underset{\sim}{u}_i \tag{115}$$

for $\underset{\sim}{s}$. Observe that $\underset{\sim}{A}^T \underset{\sim}{s} = \underset{\sim}{0}$ has been relaxed and that $\underset{\sim}{a}_i$ and $\underset{\sim}{s}$ are no longer orthogonal. The procedure is repeated when a new constraint is encountered resulting in a new $\underset{\sim}{A}$ matrix.

The <u>standard form</u> has the constraints

$$\underset{\sim}{A}' \underset{\sim}{\phi} = \underset{\sim}{b} \,, \underset{\sim}{\phi} \geq \underset{\sim}{0} \quad . \tag{116}$$

Assume $\underset{\sim}{A}'$ is of full rank n < k. A <u>basic solution</u> is obtained by letting k - n variables be zero and solving the remaining n equations in n unknowns. A <u>basic feasible solution</u> is a basic solution satisfying $\underset{\sim}{\phi} \geq \underset{\sim}{0}$. Note that $\underset{\sim}{A}' \underset{\sim}{\phi} = \underset{\sim}{b}$ is always active. A <u>nondegenerate basic feasible solution</u> occurs when the n variables corresponding to the n linearly independent columns of $\underset{\sim}{A}'$ are all positive.

The Simplex Method

Partition $\underset{\sim}{A}'$ as

$$\underset{\sim}{A}' = [\underset{\sim}{B} \;\; \underset{\sim}{C}] \quad , \tag{117}$$

Thus, $\underset{\sim}{a}_s'$ has been removed from the basis and replaced by $\underset{\sim}{a}_r'$. Clearly, the new parameter values are

$$\phi_i \leftarrow \begin{cases} \phi_i - \theta_s x_{ir} & i \neq s,\ 1 \leq i \leq n \\ \theta_s & i = r \\ 0 & \text{otherwise} \end{cases} \tag{125}$$

and the value of the objective function has decreased by $\theta_s(\underset{\sim}{c}_b^T \underset{\sim}{x}_r - c_r)$. In fact, from (119)

$$\underset{\sim}{c}_b^T \underset{\sim}{x}_r - c_r = \underset{\sim}{\lambda}_b^T \underset{\sim}{B}\, \underset{\sim}{x}_r - c_r = \underset{\sim}{\lambda}_b^T \underset{\sim}{a}_r' - c_r = -\lambda_r \quad . \tag{126}$$

Duality in Linear Programming

Consider

$$\underset{\underset{\sim}{\phi}}{\text{minimize}}\ \underset{\sim}{c}^T \underset{\sim}{\phi} \text{ s.t. } \underset{\sim}{\bar{A}}^T \underset{\sim}{\phi} \geq \underset{\sim}{b}, \underset{\sim}{\phi} \geq \underset{\sim}{0} \quad . \tag{127}$$

The Lagrangian is

$$\underset{\sim}{c}^T \underset{\sim}{\phi} - \underset{\sim}{\pi}_1^T (\underset{\sim}{\bar{A}}^T \underset{\sim}{\phi} - \underset{\sim}{b}) - \underset{\sim}{\pi}_2^T \underset{\sim}{\phi} \ , \tag{128}$$

where $\underset{\sim}{\pi}_1$ and $\underset{\sim}{\pi}_2$ are vectors of dual variables. The function can be rewritten as

$$\underset{\sim}{\pi}_1^T \underset{\sim}{b} - \underset{\sim}{\phi}^T (\underset{\sim}{\bar{A}}\ \underset{\sim}{\pi}_1 + \underset{\sim}{\pi}_2 - \underset{\sim}{c}) \tag{129}$$

where $\underset{\sim}{\bar{A}}\ \underset{\sim}{\pi}_1 + \underset{\sim}{\pi}_2 - \underset{\sim}{c} = \underset{\sim}{0}$ leads to a dual function $\underset{\sim}{\pi}_1^T \underset{\sim}{b}$. $\underset{\sim}{\pi}_2 \geq \underset{\sim}{0}$ is handled by $\underset{\sim}{\bar{A}}\ \underset{\sim}{\pi}_1 - \underset{\sim}{c} \leq \underset{\sim}{0}$ so that the dual problem is succinctly stated as

$$\underset{\underset{\sim}{\lambda}}{\text{maximize}}\ \underset{\sim}{b}^T \underset{\sim}{\lambda} \text{ s.t. } \underset{\sim}{\bar{A}}\ \underset{\sim}{\lambda} \leq \underset{\sim}{c},\ \underset{\sim}{\lambda} \geq \underset{\sim}{0} \quad . \tag{130}$$

The pair of problems we have considered are called the symmetric primal-dual problems. An important consequence of this analysis is that we are at liberty to choose either the primal or the dual problem to solve. Generally, if the primal has many inequalities and relatively few variables, the dual problem will have few inequalities and many variables and may be easier to solve.