11. GRADIENT-BASED NONLINEAR OPTIMIZATION METHODS

While linear programming and its various related methods provide powerful tools for use in water resources systems analysis, there are many water-related problems that cannot be adequately represented only in terms of a linear objective function and linear constraints. When the objective function and/or some or all of the constraints of a problem are nonlinear, other problem solution methods must be used. A class of such solution techniques used information about the problem geometry obtained from the gradient of the objective function. These solution methods are collectively categorized here as "gradient-based" methods.

The purpose of this section is to provide a simple introduction to gradient solution methods. Those interested in greater detail regarding the many gradient-based methods and the mathematical theory upon which they are based should refer to Wagner (1975), MacMillan (1975), among many others.

11.1 INTRODUCTION TO NONLINEAR PROBLEMS

11.1.1 Convex and Concave Functions

The geometry of nonlinear problems places certain requirements on the topology of the objective function and constraint set before the solution found by certain gradient methods can be guaranteed to be an optimum solution. In Section 3 of these notes, the concepts of convex and concave sets were introduced. The notions of convex and concave functions were illustrated in Section 8, but now we offer more formal definitions.

A function is convex if it satisfies the following inequality:

$$
f(\mathbf{x}) \le \theta f(\mathbf{x}_1) + (1 - \theta) f(\mathbf{x}_2) \tag{11.1}
$$

where the point:

$$
\mathbf{x} = \mathbf{x}(\theta) = \theta \mathbf{x}_1 + (1 - \theta) \mathbf{x}_2 \tag{11.2}
$$

lies on a line segment that connects the points \mathbf{x}_1 and \mathbf{x}_2 ($0 \le \theta \le 1$). This notion is illustrated in Figure 11.1 for a nonlinear function of two variables.

A function, f(**x**), is said to be concave if:

$$
f(\mathbf{x}) = f(\theta \mathbf{x}_1 + (1 - \theta) \mathbf{x}_2) \ge \theta \ f(\mathbf{x}_1) + (1 - \theta) \ f(\mathbf{x}_2)
$$
...(11.3)

where θ and the n-tuple **x** are as defined above.

Figure 11.1: A Convex Function of Two Variables

11.1.2 Kuhn-Tucker Conditions

The Kuhn-Tucker conditions extend the concept of Lagrange multipliers to mathematical models with active and inactive inequality constraints. They supply a set of necessary and sufficient conditions to determine if a solution to a nonlinear optimization problem is a global optimum.

Consider a problem where the objective function and constraints might be nonlinear:

$$
g_k(\mathbf{x}) \ge b_k
$$
 ...[11.6]

$$
g_m(\mathbf{x}) = b_m \tag{11.7}
$$

$$
\mathbf{x} \ge 0 \tag{11.8}
$$

where
$$
\mathbf{x} = \begin{cases} x_1 \\ x_2 \\ \dots \\ x_n \end{cases}
$$
.

The approach in using the Kuhn-Tucker conditions to obtain a solution to a nonlinear optimization problem is to introduce Lagrange multipliers to transform the problem into a single objective function with no constraints. Applying this to Expressions [11.4] through [11.7] gives:

$$
L(\mathbf{x}, \lambda, \mu, \mathbf{v}) = f(\mathbf{x}) + \sum_{i} \lambda_{i} (b_{i} - g_{i}(\mathbf{x})) + \sum_{k} \mu_{k} (b_{k} - g_{k}(\mathbf{x})) + \sum_{m} v_{m} (b_{m} - g_{m}(\mathbf{x})) \qquad \qquad \dots [11.9]
$$

where λ , μ , and ν are vectors of control variables/Lagrange multipliers associated with the "lessthan", "greater-than", and "equal-to" constraints, respectively.

Necessary Conditions. The necessary conditions for a solution to [11.4] through [11.7] to be a critical or stationary point are:

$$
\nabla_{\mathbf{x}} \mathbf{L} = 0 \tag{11.10}
$$

$$
\nabla_{\lambda} L = 0 \tag{11.11}
$$

$$
\nabla_{\mu} L = 0 \tag{11.12}
$$

$$
\nabla_{\mathbf{v}} \mathbf{L} = \mathbf{0} \tag{11.13}
$$

Sufficient Conditions: These conditions (i.e., Equations $[11.10]$ through $[11.13]$) are identical to the requirements of Lagrange multipliers for equality constraints. The Kuhn-Tucker conditions, however, specify additional requirements for a stationary point to be a global optimum. Further, the specifications differ, depending upon whether is a global minimum or a global maximum that is sought for the objective function.

For a minimization problem, such as:

$$
\text{Min } Z = f(\mathbf{x}) \tag{11.14}
$$

 $g_k(\mathbf{x}) \geq b_k$ $(k = 1, 2, ...)$ \ldots [11.16]

 $g_m(\mathbf{x}) = b_m$ $(m = 1, 2, ...)$ \ldots [11.17] the Kuhn-Tucker approach becomes:

Min L(
$$
\mathbf{x}, \lambda, \mu, \mathbf{v}
$$
) = f(\mathbf{x}) + \sum_{i} λ_i (b_i - g_i(\mathbf{x})) + \sum_{k} μ_k (b_k - g_k(\mathbf{x}))
+ \sum_{m} ν_m (b_m - g_m(\mathbf{x})) ...[11.18]

s.t.:

necessary conditions:

(1) xj ≥ 0 and ∂^L ∂xj ≥ 0 (j = 1, 2, ..., n) ...[11.19]

(2a) If
$$
\lambda_i = 0
$$
, then $b_i - g_i(\mathbf{x}) \ge 0$ (inactive constraint) ...[11.20a]

- (2b) Else if $b_i g_i(x) = 0$, then $\lambda_i \le 0$ (active constraint) ...[11.20b]
- (3a) If $\mu_k = 0$, then $b_k g_k(x) \le 0$ (inactive constraint) ...[11.21a]
- (3b) Else if $b_k g_k(x) = 0$, then $\mu_k \ge 0$ (active constraint) ...[11.21b]

(4)
$$
v_m
$$
 is unrestricted in sign and $b_m - g_m(\mathbf{x}) = 0$...(11.22)

sufficient conditions:

- (5) $f(x)$ is a convex function
- $(6a)$ (**x**) is a convex function
- (6b) $g_k(x)$ is a concave function
- (6c) $g_m(x)$ is a linear function

For a maximization problem, such as:

$$
Max Z = f(x) \t\t\t\t\t\t\t....[11.23]
$$

s.t.: $g_i(\mathbf{x}) \leq b_i$ $(i = 1, 2, ...)$...[11.24]

gk(**x**) ≥ bk (k = 1, 2, ...) ...[11.25]

$$
g_m(\mathbf{x}) = b_m \tag{11.26}
$$

the Kuhn-Tucker formulation and conditions become:

$$
\text{Max } L(\mathbf{x}, \lambda, \mu, \mathbf{v}) = f(\mathbf{x}) + \sum_{i} \lambda_{i} (b_{i} - g_{i}(\mathbf{x})) + \sum_{k} \mu_{k} (b_{k} - g_{k}(\mathbf{x})) + \sum_{m} v_{m} (b_{m} - g_{m}(\mathbf{x})) \qquad \qquad \dots [11.27]
$$

s.t.:

necessary conditions:

(1)
$$
x_j \ge 0
$$
 and $\frac{\partial L}{\partial x_j} \le 0$
 (j = 1, 2, ..., n) ...[11.28]

- (2a) If $\lambda_i = 0$, then $b_i g_i$ (**x**) ≥ 0 (inactive constraint) ...[11.29a]
- (2b) Else if $b_i g_i(x) = 0$, then $\lambda_i \ge 0$ (active constraint) ...[11.29b]
- (3a) If $\mu_k = 0$, then $b_k g_k(x) \le 0$ (inactive constraint) ...[11.30a]
- (3b) Else if $b_k g_k(x) = 0$, then $\mu_k \le 0$ (active constraint) ...[11.30b]

(4)
$$
v_m
$$
 is unrestricted in sign and $b_m - g_m(\mathbf{x}) = 0$...(11.31)

sufficient conditions:

- (5) f(**x**) is a concave function
- $(6a)$ $g_i(x)$ is a convex function
- (6b) $g_k(x)$ is a concave function
- (6c) $g_m(x)$ is a linear function

Note that neither the Kuhn-Tucker conditions nor the Lagrangian approach require $x_i \ge 0$ (as opposed to the LP simplex method).

11.1.3 Example of the Kuhn-Tucker Method

Solve the following problem by applying the Kuhn-Tucker conditions:

Min
$$
f = 2 x_1 + x_1 x_2 + 3 x_2
$$
 ...(11.32)

s.t.:
$$
x_1^2 + x_2 \ge 3
$$
 ...(11.33)

Solution: First, re-write the nonlinear constraint as:

$$
g = x_1^2 + x_2 - 3 \ge 0 \tag{11.34}
$$

and formulate the Kuhn-Tucker problem and conditions:

Min h = 2 x₁ + x₁ x₂ + 3 x₂ -
$$
\lambda
$$
 (x₁² + x₂ - 3) ...[11.35]

(1)
$$
\frac{\partial \mathbf{h}}{\partial \mathbf{x}_1} = 2 + \mathbf{x}_2 - 2 \lambda \mathbf{x}_1 = 0 \qquad \qquad \dots [11.36]
$$

(2)
$$
\frac{\partial h}{\partial x_2} = x_1 + 3 - \lambda = 0
$$
...(11.37)

(3)
$$
\frac{\partial h}{\partial \lambda} = x_1^2 + x_2 - 3 \ge 0
$$
...(11.38)

(4)
$$
\lambda (x_1^2 + x_2 - 3) = 0
$$
 ...(11.39)

$$
\lambda \ge 0 \qquad \qquad \lambda \ge 0 \qquad \qquad \ldots [11.40]
$$

The solution approach for resolving Expressions [11.36] through [11.40] is to assume the constraint is non-binding (i.e., assume $\lambda = 0$) and then obtain a solution for x_1, x_2 , and g. This solution is checked to verify that the other Kuhn-Tucker conditions are met. If so, the solution is optimal. If not, the assumption must have been incorrect, and the constraint must be binding. In this case, a different solution for x_1, x_2 , and λ can be found.

Setting $\lambda = 0$ and solving [11.36] and [11.37] yields: $x_1 = -3$, $x_2 = -2$, and $g = 4 \ge 0$.

11.1.4 Geometric Interpretation of the Kuhn-Tucker Conditions

For a maximization or minimization problem subject to a single, equality constraint, the Lagrangian solution seeks a point where the slope of the objective function, f, is equal to the slope of the constraint, g. As illustrated in Figure 11.2, this occurs at a point, A.

Figure 11.2: Lagrangian Solution to an Optimization Problem with an Equality Constraint

For a maximization or minimization problem subject to multiple equality constraints, the Lagrangian seeks a point where the gradient of the objective function, f, is within the "feasible cone" of slopes defined by the perpendiculars to the equality constraints, i.e., the g's, as shown in Figure 11.3. That is, if f has a gradient within the "cone", θ , then the Lagrangian will find point A as the optimal solution.

The same is true of the Kuhn-Tucker inequalities, but instead of a one-point solution space, there are an infinite number of possible solutions, as illustrated in Figure 11.4. However, the cone of feasible vectors has the same meaning as in the Lagrangian condition for equality constraints.

Figure 11.3: Lagrangian Solution of a Problem with Multiple Nonlinear Equality Constraints

Figure 11.4: Kuhn-Tucker Solution of a Problem with Multiple Nonlinear Inequality Constraints

11.2 GRADIENT-BASED OPTIMIZATION

11.2.1 Overview

A number of gradient-based methods are available for solving constrained and unconstrained nonlinear optimization problems. A common characteristic of all of these methods is that they employ a numerical technique to calculate a direction in n-space in which to search for a better estimate of the optimum solution to a nonlinear problem. This search direction relies on the estimation of the value of the gradient of the objective function at a given point.

Gradient-based methods are used to solve nonlinear constrained or unconstrained problems where other techniques:

are not feasible (e.g., LP)

do not yield desired information about the problem geometry (e.g., DP)

Gradient-based methods have the advantages that they are applicable to a broader class of problems than LP and they provide much more information about the problem geometry. They have the disadvantages that they are computationally complex and costly, and they are much more mathematically sophisticated and difficult than LP.

11.2.2 Common Gradient-Based Methods

The most commonly used gradient techniques are:

steepest ascent (or, for constrained problems, steepest feasible ascent)

conjugate gradient

reduced gradient

Each of these methods can be found in commercially available mathematical programming software. The method of steepest ascent is mathematically simple and easy to program, but converges to an optimal solution only slowly. On the other end of the spectrum is the reduced gradient method, which has a high rate of convergence, but is much more mathematically complex and difficult to program.

11.2.3 An Example of the Method of Steepest Ascent

Before presenting an example of the method of steepest feasible ascent, we must develop some terminology. Define the gradient of a function, f(**x**), to be the vector of first partial derivatives of the function:

$$
\nabla f = \begin{cases} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \dots \\ \frac{\partial f}{\partial x_n} \end{cases}
$$
...(11.41)

The value of ∇f at a point P_o [where P_o is an n-tuple equal to $(x_{1_0}, x_{2_0}, ..., x_{n_0})$] is a vector, V_{P_0} , with entries equal to

$$
\mathbf{V}_{P_{O}} = \nabla f \Big|_{P_{o}} = \begin{cases} \n\frac{\partial f}{\partial x_{1}} \Big|_{P_{o}} \\ \n\frac{\partial f}{\partial x_{2}} \Big|_{P_{o}} \\ \n\cdots \\ \n\frac{\partial f}{\partial x_{n}} \Big|_{P_{o}} \n\end{cases} \tag{11.42}
$$

The vector, V_{P_0} , gives the direction in n-space of the steepest ascent from the point P_0 , i.e., the direction in which the rate of increase in the objective function, f, is maximum.

Define a unit vector in the direction of V_{P_0} to be v_{P_0} , calculated as

$$
\mathbf{v}_{\mathrm{P}_o} = \frac{\mathbf{V}_{\mathrm{P}_o}}{\|\mathbf{V}_{\mathrm{P}_o}\|} \tag{11.43}
$$

where $\|\mathbf{V}_{P_{o}}\|$ is the norm of the gradient vector.

Consider the following optimization problem:

$$
\text{Max } f(x_1, x_2) = 7 x_1 + 4 x_2 + x_1 x_2 - x_1^2 - x_2^2 \tag{11.44}
$$

s.t.:
$$
\frac{2}{3}x_1 + x_2 \le 8
$$
 ...(11.45)

$$
-\frac{5}{12}x_1 + x_2 \le 2 \tag{11.46}
$$

$$
x_2 \le 4 \tag{11.47}
$$

$$
x_1, x_2 \ge 0 \tag{11.48}
$$

The constraint set for this problem is illustrated in Figure 11.5. Note that the solution to the unconstrained problem is $\mathbf{x} = (x_1, x_2) = (6, 5)$.

The method of steepest feasible ascent will be used to solve the constrained problem. This method is an iterative procedure whereby, with each iteration, information is garnered at a particular point in solution space to determine the direction and distance to go to find another point which is feasible and at which an improvement in the objective function is found. This continues until no further improvement in the objective function is possible.

To begin, evaluate an expression for the gradient:

$$
\nabla f = \begin{cases} 7 + x_2 - 2x_1 \\ 4 + x_1 - 2x_2 \end{cases}
$$
...(11.49)

Assume a starting point of $P_0 = (8,2)$ (refer to Figure 11.5), and calculate the value of the gradient at this point:

$$
\mathbf{V}_{\mathbf{P}_0} = \nabla f \big|_{\mathbf{P}_0} = \begin{Bmatrix} 7 & + & 2 & - & 2 & (8) \\ 4 & + & 8 & - & 2 & (2) \end{Bmatrix} = \begin{Bmatrix} -7 \\ 8 \end{Bmatrix} \tag{11.50}
$$

and calculate a unit vector pointing in this direction:

$$
\mathbf{v}_{P_0} = \frac{\mathbf{V}_{P_o}}{\|\mathbf{V}_{P_o}\|} = \begin{cases} -0.659\\ 0.753 \end{cases}
$$
...(11.51)

Note, as shown in Figure 11.5, moving from the point P_0 in the direction of v_{P_0} will violate a constraint before the unconstrained optimum is reached.

If we assume the constrained optimum lies at a corner point of the constraint set, all we have to do is project from P_0 along v_{P_0} to the nearest constraint. Thence we can move along that constraint to a corner point, and then to another corner, etc., until an optimum is found. If the optimum is not at a corner point, then there will be an iteration in our search when the optimum search direction (as projected along a constraint) will reverse itself. If this happens, we will know that we have overshot the optimum, and that we must search for it between the most recent two corner points we have visited.

Figure 11.5: Steepest Ascent Method Search **Figure 11.5: Steepest Ascent Method Search**

We can determine how far to move by calculating the distance from our current point to the nearest constraint in the direction of v_{P_0} . To do this, we must compute the following for each constraint:

$$
\alpha_{i} = \frac{c_{i} - \left[x_{O_{1}} \quad x_{O_{2}}\right] \begin{Bmatrix} a_{i} \\ b_{i} \end{Bmatrix}}{\left[v_{1} \quad v_{2}\right] \begin{Bmatrix} a_{i} \\ b_{i} \end{Bmatrix}} \qquad \qquad \dots [11.52]
$$

where:

 α_i is the distance from the current point, P_o, to constraint i, in the direction of \mathbf{v}_{P_0}

 $[x_{O_1}, x_{O_2}]$ are the coordinates of the current point, P_o

 $\begin{Bmatrix} a_i \\ b_i \end{Bmatrix}$ are the coefficients on x_1 and x_2 in constraint i

[v_1 , v_2] are the elements of the vector v_{P_Q}

Table 11.1 summarizes the values of α_i for the five constraints of the problem.

To determine the next point in our search, we select that distance in Table 11.1 which is smallest, but non-negative. Clearly, in the direction of, the first constraint is the closest, and to get to that constraint we must move a distance of 2.2 units. The new point, P_1 , can be found from:

$$
P_1 = P_o + \alpha_1 (v_1, v_2) = (8 + \alpha_1 (-0.659), 2 + \alpha_1 (0.753)) = (6.599, 3.601) \quad \dots [11.53]
$$

and is shown in Figure 11.5.

From P_1 , we wish to move along constraint 1 (i.e., the currently binding constraint) in the direction of a vector, G_1 , that results from the projection of the gradient (calculated at P₁) onto the constraint. The direction of the "gradient projection" is the direction of "steepest feasible ascent".

To find G_1 (projected from P₁), we must make the following calculations:

$$
K = \frac{\begin{bmatrix} r & s \end{bmatrix} \begin{Bmatrix} b_k \\ -a_k \end{Bmatrix}}{\begin{bmatrix} a_k & b_k \end{bmatrix} \begin{bmatrix} a_k \\ b_k \end{bmatrix}}
$$
...(11.54)

and

$$
\mathbf{G} = \mathbf{K} \begin{Bmatrix} \mathbf{b}_{k} \\ -\mathbf{a}_{k} \end{Bmatrix} \tag{11.55}
$$

where:

 $\overline{}$

$$
\begin{Bmatrix} r \\ s \end{Bmatrix} = \nabla f \Big|_{P_1}
$$

and a_k and b_k are coefficients on x_1 and x_2 , respectively, of the constraint along which G is to be projected.

The gradient evaluated at P_1 is:

$$
\begin{Bmatrix} \mathbf{r} \\ \mathbf{s} \end{Bmatrix} = \nabla \mathbf{f} \bigg|_{\mathbf{P}_1} = \begin{Bmatrix} -2.597 \\ 3.397 \end{Bmatrix}
$$
...(11.56)

From this, K and G_1 can be calculated as:

$$
K = \frac{\begin{bmatrix} -2.597 & 3.397 \end{bmatrix} \begin{bmatrix} 1 \\ -(\frac{2}{3}) \end{bmatrix}}{\begin{bmatrix} (2/3) & 1 \end{bmatrix} \begin{bmatrix} 1 \\ (2/3) \end{bmatrix}} = -3.366
$$
...(11.57)

$$
G_1 = -3.366 \begin{bmatrix} 1 \\ -(\frac{2}{3}) \end{bmatrix} = \begin{bmatrix} -3.366 \\ 2.244 \end{bmatrix}
$$
...(11.58)

This establishes a new search direction from point P_1 in which to travel to find a corner point with a (hopefully) better objective function value. A unit vector in this direction is:

$$
\mathbf{v}_{P_1} = \frac{\mathbf{G}_1}{|\mathbf{G}_1|} = \begin{cases} -0.832\\ 0.555 \end{cases}
$$
...(11.59)

We can now reproduce the calculations shown in Table 11.1, except that we are projecting from point P_1 along a vector specified by \mathbf{v}_{P_1} . The nearest constraint in that direction will be constraint 3, at a distance of $\alpha_3 = 0.71$. A new search point, P_2 , can now be established from:

$$
P_2 = P_1 + \alpha_3 (v_1, v_2) = (6.599 + 0.71 (-0.832), 3.601 + 0.71 (0.555))
$$

= (6.0,4.0) ...[11.60]

As shown in Figure 11.5, point P_2 is at the intersection between constraints 1 and 3.

A similar set of calculations will yield a point P_3 (at the intersection of constraints 2 and 3). However, evaluation of the gradient projection at point P_3 indicates that the optimum solution lies in a direction back toward point P_2 . This means that the optimum is not at a corner point, but somewhere between points P_2 and P_3 . We must invoke another search technique to look between these points for the solution.

Any number of search methods could be used to evaluate the interval between P_2 and P_3 to find the constrained optimum (e.g., bisection search, Golden Section search, etc.). One very efficient method for this particular problem would be to parameterize the objective function in terms of the position of a point along a line segment connecting P_2 and P_3 , and then maximize the parameterized equation. It can be done as follows:

Let: (y_1, y_2) be the coordinates of P₂, and

 (z_1, z_2) be the coordinates of P₃.

Now, define:

$$
x_1 = y_1 + t (z_1 - y_1) \tag{11.61}
$$

and

$$
x_2 = y_2 + t (z_2 - y_2) \tag{11.62}
$$

We can specify the coordinates of any arbitrary point between P_2 and P_3 simply by picking the appropriate value of t, where $0 \le t \le 1$. In particular, we can substitute Equations [11.61] and [11.62] into the objective function for x_1 and x_2 , turning the objective into a function of a single variable, t. The maximum of the objective function, f, can now be found simply by differentiating it with respect to t, setting the result equal to zero, and solving for t.

11.3 PROBLEMS

- 1. Complete the solution to the constrained nonlinear problem of Section 11.2 by:
	- a. performing the calculations to find points P_2 and P_3
	- b. solving the parameterization problem at the end of the section (i.e., finding the optimal solution which lies somewhere between P_2 and P_3)
- 2. A narrow, confined aquifer is penetrated by three wells (refer to Figure 11.6, below). Assume the aquifer is isotropic and homogeneous, that the land surface is horizontal, and that datum is at the land surface. Within the aquifer, the governing equation for porous media flow is:

$$
\frac{\partial^2 \mathbf{h}}{\partial \mathbf{x}^2} + \frac{\partial^2 \mathbf{h}}{\partial \mathbf{y}^2} = \tilde{\mathbf{Q}} \qquad \qquad \dots [11.63]
$$

where $\tilde{Q} = \frac{Q}{10,000}$, and Q is pumping rate from a well located at point (x,y). Units of \tilde{Q} are inverse length.

If the combined output of the three wells must be at least 2 gpm, determine the optimal pumping rates for each of the wells in order to minimize total cost of pumping.

Figure 11.6: A Simple Groundwater Optimization Problem