C

Parameter Optimization Methods

IN this appendix classical necessary and sufficient conditions for solution of unconstrained and equality-constrained parameter optimization problems are summarized. We also summarize two iterative techniques for unconstrained minimization, and discuss the relative merits of these approaches.

C.1 Unconstrained Extrema

Suppose we wish to determine a vector $\mathbf{x}$ that minimizes (or maximizes) the following *loss function*:

$$\vartheta \equiv \vartheta(\mathbf{x}) \tag{C.1}$$

with $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}^T$. Without loss in generality, we assume our task is to minimize eqn. (C.1). It is evident that a simple change of sign converts a maximization problem to a minimization problem. To obtain the most fundamental classical results, we restrict initial attention to ϑ and $\mathbf{x}$ of class C_2 (smooth, continuous functions having two continuous derivatives with respect to all arguments). Using the matrix calculus differentiation rules developed in §A.5, it follows that a "stationary" or "critical" point can be determined by solving the following necessary condition:

$$\nabla_{\mathbf{x}} \vartheta \equiv \frac{\partial \vartheta}{\partial \mathbf{x}} = \mathbf{0} \tag{C.2}$$

where $\nabla_{\mathbf{x}}$ is the Jacobian (see Appendix A). Unfortunately, satisfying the condition in eqn. (C.2) does not guarantee a *local minimum* in general. If $\mathbf{x}$ is scalar, then the classic test for a local minimum is to check the second derivative of ϑ, which must be positive. This concept can be expanded to a vector of unknown variables by using a matrix check.[1, 2] The sufficiency condition requires that one determine the definiteness of the matrix of partial derivatives, known as the Hessian matrix (see Appendix A). Suppose we have a stationary point, denoted by $\mathbf{x}^*$. This point is a local minimum if the following sufficient condition is satisfied:

$$\nabla_{\mathbf{x}}^2 \vartheta \equiv \left. \frac{\partial^2 \vartheta}{\partial \mathbf{x} \, \partial \mathbf{x}^T} \right|_{\mathbf{x}^*} \text{ must be positive definite} \tag{C.3}$$

where $\nabla^2_{\mathbf{x}}\vartheta$ is the Hessian (see Appendix A). If this matrix is negative definite, then the point is a maximum. If the matrix is indefinite, then a *saddle point* exists, which corresponds to a relative minimum or maximum with respect to the individual components of $\mathbf{x}^*$. A global minimum is much more difficult to establish though. Consider the minimization of the following function (known as Himmelblau's function):[3]

$$\vartheta(\mathbf{x}) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \tag{C.4}$$

A plot of the contours (lines of constant ϑ) is shown in Figure C.1. Also shown in this plot are the numerical iteration points for the method of gradients (see §C.3.2) from various starting guesses. There is a set of four stationary points which provide local minimums, each of approximately the same importance:

- $\mathbf{x}_1^* = \begin{bmatrix} 3 & 2 \end{bmatrix}^T$, with $\vartheta(\mathbf{x}_1^*) = 0$.
- $\mathbf{x}_2^* = \begin{bmatrix} -3.7792 & -3.2831 \end{bmatrix}^T$, with $\vartheta(\mathbf{x}_2^*) = 0.0054$.
- $\mathbf{x}_3^* = \begin{bmatrix} -2.8051 & 3.1313 \end{bmatrix}^T$, with $\vartheta(\mathbf{x}_3^*) = 0.0085$.
- $\mathbf{x}_4^* = \begin{bmatrix} 3.5843 & -1.8483 \end{bmatrix}^T$, with $\vartheta(\mathbf{x}_4^*) = 0.0011$.

Clearly, a numerical technique such as the method of gradients can converge to any one of these four points from various starting guesses. Fortunately a resourceful analyst can often achieve a high degree of confidence that a stationary point is a global minimum through intimate knowledge of the loss function (e.g., the Hessian matrix for a *quadratic loss function* is constant).

Example C.1: In this example we consider finding the extreme points of the following loss function:[1]

$$\vartheta(\mathbf{x}) = x_1^3 + x_2^3 + 2x_1^2 + 4x_2^2 + 6$$

The necessary conditions for x_1 and x_2, given by eqn. (C.2), are

$$\frac{\partial \vartheta}{\partial x_1} = x_1(3x_1 + 4) = 0$$
$$\frac{\partial \vartheta}{\partial x_2} = x_2(3x_2 + 8) = 0$$

These equations are satisfied at the following stationary points:

$$\mathbf{x}_1^* = \begin{bmatrix} 0 & 0 \end{bmatrix}^T, \quad \mathbf{x}_2^* = \begin{bmatrix} 0 & -\frac{8}{3} \end{bmatrix}^T$$
$$\mathbf{x}_3^* = \begin{bmatrix} -\frac{4}{3} & 0 \end{bmatrix}^T, \quad \mathbf{x}_4^* = \begin{bmatrix} -\frac{4}{3} & -\frac{8}{3} \end{bmatrix}^T$$

The Hessian matrix is given by

$$\nabla^2_{\mathbf{x}}\vartheta = \begin{bmatrix} 6x_1 + 4 & 0 \\ 0 & 6x_2 + 8 \end{bmatrix}$$

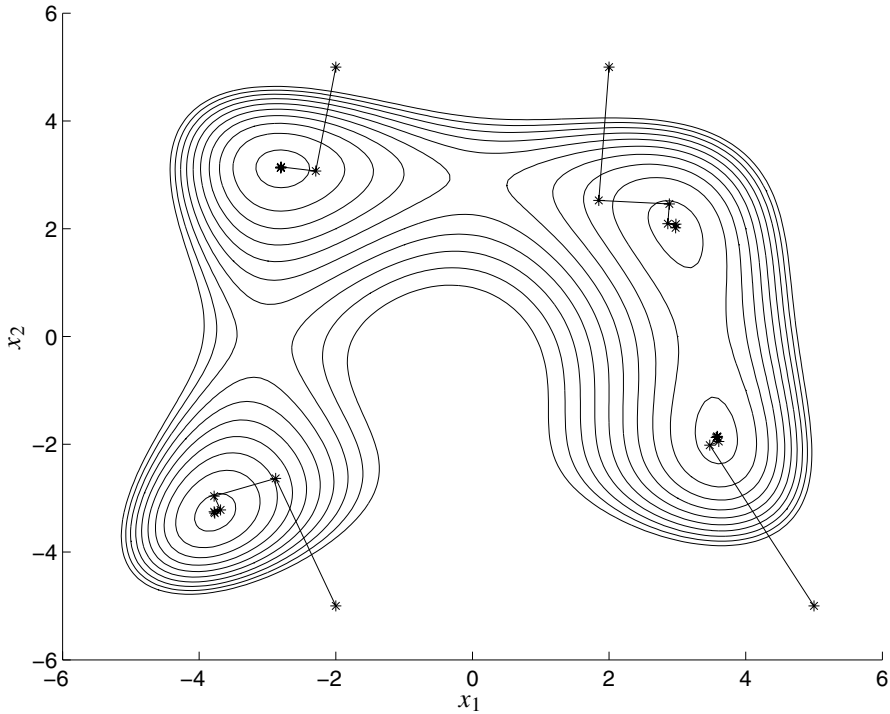

Figure C.1: Himmelblau's Function

Table C.1 gives the nature of the Hessian and the value of the loss function at the stationary points. The first point gives a local minimum, the next two points are saddle points, and the last point gives a local maximum.

C.2 Equality Constrained Extrema

One often encounters problems that must extremize

$$\vartheta \equiv \vartheta(\mathbf{x}) \tag{C.5}$$

subject to the following set of $m \times 1$ *equality constraints*:

$$\boldsymbol{\psi} \equiv \boldsymbol{\psi}(\mathbf{x}) = \mathbf{0} \tag{C.6}$$

Table C.1: Nature of the Hessian and Values for the Loss Function

Point $\mathbf{x}_i^*$	Nature of $\nabla_{\mathbf{x}}^2 \vartheta\|_{\mathbf{x}_i^*}$	Nature of $\mathbf{x}_i^*$	$\vartheta(\mathbf{x}_i^*)$
$\mathbf{x}_1^* = \begin{bmatrix} 0 & 0 \end{bmatrix}^T$	Positive Definite	Relative Minimum	6
$\mathbf{x}_2^* = \begin{bmatrix} 0 & -\frac{8}{3} \end{bmatrix}^T$	Indefinite	Saddle Point	418/27
$\mathbf{x}_3^* = \begin{bmatrix} -\frac{4}{3} & 0 \end{bmatrix}^T$	Indefinite	Saddle Point	194/27
$\mathbf{x}_4^* = \begin{bmatrix} -\frac{4}{3} & -\frac{8}{3} \end{bmatrix}^T$	Negative Definite	Relative Maximum	50/3

where $m < n$. Let us consider the case where $n = 2$ and $m = 1$. Suppose (x_1^*, x_2^*) locally minimizes eqn. (C.5) while satisfying eqn. (C.6). If this is true, then arbitrary admissible differential variations $(\delta x_1, \delta x_2)$ in the differential neighborhood of (x_1^*, x_2^*) in the sense $(x_1, x_2) = (x_1^* + \delta x_1, x_2^* + \delta x_2)$ result in a stationary value of ϑ:

$$\delta\vartheta = \frac{\partial\vartheta}{\partial x_1}\delta x_1 + \frac{\partial\vartheta}{\partial x_2}\delta x_2 = 0 \tag{C.7}$$

Since we restrict attention to neighboring points that satisfy the constraint given by eqn. (C.6), we also require the first variation of the constraint to vanish as a condition on the admissibility of $(\delta x_1, \delta x_2)$ as

$$\delta\psi = \frac{\partial\psi}{\partial x_1}\delta x_1 + \frac{\partial\psi}{\partial x_2}\delta x_2 = 0 \tag{C.8}$$

For notational convenience, we suppress the truth that all partials in eqns. (C.7) and (C.8) are evaluated at (x_1^*, x_2^*). Since eqn. (C.8) constrains the admissible variations, we can solve for either variable and eliminate the constraint equation. The two solutions of the constraint equations are obviously

$$\delta x_1 = -\left(\frac{\dfrac{\partial\psi}{\partial x_2}}{\dfrac{\partial\psi}{\partial x_1}}\right)\delta x_2 \quad \text{and} \quad \delta x_2 = -\left(\frac{\dfrac{\partial\psi}{\partial x_1}}{\dfrac{\partial\psi}{\partial x_2}}\right)\delta x_1 \tag{C.9}$$

Substitution of the "differential eliminations" into the differential of the loss function allows us to locally constrain the variations of ϑ and reduce the dimensionality either of two ways. The first way is given by using

$$\delta\vartheta = \left[\frac{\partial\vartheta}{\partial x_2} - \left(\frac{\dfrac{\partial\vartheta}{\partial x_1}}{\dfrac{\partial\psi}{\partial x_1}}\right)\frac{\partial\psi}{\partial x_2}\right]\delta x_2 = 0 \tag{C.10}$$

The second way is given by using

$$\delta\vartheta = \left[\frac{\partial\vartheta}{\partial x_1} - \left(\frac{\dfrac{\partial\vartheta}{\partial x_2}}{\dfrac{\partial\psi}{\partial x_2}} \right) \frac{\partial\psi}{\partial x_1} \right] \delta x_1 = 0 \tag{C.11}$$

It is evident that either of eqns. (C.10) or (C.11) can be used to argue that the local variations are arbitrary and the coefficient within the brackets must vanish as a necessary condition for a local minimum at (x_1^*, x_2^*). The first form of the necessary conditions is given by

$$\frac{\partial\vartheta}{\partial x_1} - \left(\frac{\dfrac{\partial\vartheta}{\partial x_2}}{\dfrac{\partial\psi}{\partial x_2}} \right) \frac{\partial\psi}{\partial x_1} = 0 \tag{C.12a}$$

$$\psi(x_1, x_2) = 0 \tag{C.12b}$$

The second form of the necessary conditions is given by

$$\frac{\partial\vartheta}{\partial x_2} - \left(\frac{\dfrac{\partial\vartheta}{\partial x_1}}{\dfrac{\partial\psi}{\partial x_1}} \right) \frac{\partial\psi}{\partial x_2} = 0 \tag{C.13a}$$

$$\psi(x_1, x_2) = 0 \tag{C.13b}$$

When this approach is carried to higher dimensions, the number of differential elimination possibilities is obviously much greater, and some of these forms of the necessary conditions may be poorly conditioned if the partial derivatives in the denominator approaches zero.

Lagrange noticed a pattern in the above and decided to "automate" all possible differential eliminations by linearly combining eqns. (C.7) and (C.8) with an unspecified scalar *Lagrange multiplier* λ as

$$\delta\vartheta + \lambda\,\delta\psi = \left[\frac{\partial\vartheta}{\partial x_1} + \lambda\frac{\partial\psi}{\partial x_1} \right] \delta x_1 + \left[\frac{\partial\vartheta}{\partial x_2} + \lambda\frac{\partial\psi}{\partial x_2} \right] \delta x_2 = 0 \tag{C.14}$$

While it "isn't legal" to set the two brackets to zero using the argument that $(\delta x_1, \delta x_2)$ are independent, we can set either one of the brackets to zero to determine λ. Notice that setting the first bracket to zero and substituting the resulting equation for $\lambda = -\left(\frac{\partial\vartheta}{\partial x_1}\right) / \left(\frac{\partial\psi}{\partial x_1}\right)$ into the second bracket renders the second bracket equal to eqn. (C.13a), whereas setting the second bracket to zero, solving for λ and substituting renders the first bracket equal to eqn. (C.12a). Thus the following necessary generalized Lagrange form of the necessary conditions captures all possible differ-

ential constraint eliminations (only two in this case):

$$\frac{\partial \vartheta}{\partial x_1} + \lambda \frac{\partial \psi}{\partial x_1} = 0 \tag{C.15a}$$

$$\frac{\partial \vartheta}{\partial x_2} + \lambda \frac{\partial \psi}{\partial x_2} = 0 \tag{C.15b}$$

$$\psi(x_1, x_2) = 0 \tag{C.15c}$$

It is apparent by inspection of eqn. (C.15) that these equations are the gradient of the augmented function $\phi \equiv \vartheta + \lambda \psi$ with respect to (x_1, x_2, λ) and thus the Lagrange multiplier rule is validated. The necessary conditions for a constrained minimum of eqn. (C.5) subject to eqn. (C.6) has the form of an unconstrained minimum of the augmented function ϕ:

$$\frac{\partial \phi}{\partial x_1} = \frac{\partial \vartheta}{\partial x_1} + \lambda \frac{\partial \psi}{\partial x_1} = 0 \tag{C.16a}$$

$$\frac{\partial \phi}{\partial x_2} = \frac{\partial \vartheta}{\partial x_2} + \lambda \frac{\partial \psi}{\partial x_2} = 0 \tag{C.16b}$$

$$\psi(x_1, x_2) = 0 \tag{C.16c}$$

Equations (C.16) provide four equations; all points (x_1^*, x_2^*, λ) satisfying these equations are *constrained stationary points*.

Expanding this concept to the general case results in the necessary conditions for a stationary point, which is applied by the unconstrained necessary condition of eqn. (C.2) to the following *augmented function*:

$$\phi \equiv \phi(\mathbf{x}, \boldsymbol{\lambda}) = \vartheta(\mathbf{x}) + \boldsymbol{\lambda}^T \boldsymbol{\psi}(\mathbf{x}) \tag{C.17}$$

The necessary conditions are now given by

$$\nabla_{\mathbf{x}} \phi \equiv \frac{\partial \phi}{\partial \mathbf{x}} = \frac{\partial \vartheta}{\partial \mathbf{x}} + \left[\frac{\partial \boldsymbol{\psi}}{\partial \mathbf{x}}\right]^T \boldsymbol{\lambda} = \mathbf{0} \tag{C.18a}$$

$$\nabla_{\boldsymbol{\lambda}} \phi \equiv \frac{\partial \phi}{\partial \boldsymbol{\lambda}} = \boldsymbol{\psi}(\mathbf{x}) = \mathbf{0} \tag{C.18b}$$

where $\boldsymbol{\lambda}$ is an $m \times 1$ vector of Lagrange multipliers. The $(n+m)$ equations shown in eqn. (C.18), which define the *Lagrange multiplier rule*, are solved for the $(n+m)$ unknowns $\mathbf{x}$ and $\boldsymbol{\lambda}$. Suppose we have a stationary point, denoted by $\mathbf{x}^*$ with a corresponding Lagrange multiplier $\boldsymbol{\lambda}^*$. The point $\mathbf{x}^*$ is a local minimum if the following sufficient condition is satisfied:

$$\nabla_{\mathbf{x}}^2 \phi \equiv \left.\frac{\partial^2 \phi}{\partial \mathbf{x} \partial \mathbf{x}^T}\right|_{(\mathbf{x}^*, \boldsymbol{\lambda}^*)} \text{ must be positive definite.} \tag{C.19}$$

The sufficient condition can be simplified by checking the positive definiteness of a matrix that is always smaller than the $n \times n$ matrix shown by eqn. (C.19). Let us rewrite the loss function in eqn. (C.5) as

$$\vartheta(x_1, \ldots, x_m, x_{m+1}, \ldots, x_n) \equiv \vartheta(\mathbf{y}, \mathbf{z}) \tag{C.20}$$

where $\mathbf{y}$ is an $m \times 1$ vector and $\mathbf{z}$ is a $p \times 1$ vector (with $p = n - m$). The necessary conditions are still given by eqn. (C.18) with $\mathbf{x} \equiv \left[\mathbf{y}^T \ \mathbf{z}^T\right]^T$. But the sufficient condition can now be determined by checking the definiteness of the following $p \times p$ matrix:[2]

$$Q \equiv \left\{ [\nabla_{\mathbf{z}}\psi]^T \left[\nabla_{\mathbf{y}}\psi\right]^{-T} \left[\nabla_{\mathbf{y}}^2\phi\right] \left[\nabla_{\mathbf{y}}\psi\right]^{-T} [\nabla_{\mathbf{z}}\psi] + \nabla_{\mathbf{z}}^2\phi \right. \\ \left. - \left[\nabla_{\mathbf{z}}\nabla_{\mathbf{y}}\phi\right] \left[\nabla_{\mathbf{y}}\psi\right]^{-1} [\nabla_{\mathbf{z}}\psi] - [\nabla_{\mathbf{z}}\psi]^T \left[\nabla_{\mathbf{y}}\psi\right]^{-T} \left[\nabla_{\mathbf{y}}\nabla_{\mathbf{z}}\phi\right] \right\} \Bigg|_{(\mathbf{y}^*, \mathbf{z}^*, \boldsymbol{\lambda}^*)} \tag{C.21}$$

where $\left[\nabla_{\mathbf{z}}\nabla_{\mathbf{y}}\phi\right]$ and $\left[\nabla_{\mathbf{y}}\nabla_{\mathbf{z}}\phi\right]$ are $p \times m$ and $m \times p$ matrices, respectively, made up of the partial derivatives with respect to $\mathbf{y}$ and $\mathbf{z}$. A stationary point is a local minimum (maximum) if Q is positive (negative) definite. Note that the inverse of an $m \times m$ matrix must be taken. Still, the matrix in eqn. (C.21) is usually simpler to check than using the $n \times n$ matrix in eqn. (C.19).

Example C.2: In this example we consider finding the extreme points of the following loss function, which represents a plane:

$$\vartheta = 6 - \frac{y}{2} - \frac{z}{3}$$

subject to a constraint represented by an elliptic cylinder:

$$\psi(\mathbf{x}) = 9(y-4)^2 + 4(z-5)^2 - 36 = 0$$

where $\mathbf{x} \equiv \left[x \ y\right]^T$. The augmented function of eqn. (C.17) for this problem is given by

$$\phi(\mathbf{x}, \lambda) = 6 - \frac{y}{2} - \frac{z}{3} - \lambda\left[9(y-4)^2 + 4(z-5)^2 - 36\right]$$

From the necessary conditions of eqn. (C.18) we have

$$\frac{\partial\phi}{\partial y} = -\frac{1}{2} + 18\lambda(y-4) = 0$$
$$\frac{\partial\phi}{\partial z} = -\frac{1}{3} + 8\lambda(y-5) = 0$$
$$\psi(\mathbf{x}) = 9(y-4)^2 + 4(z-5)^2 - 36 = 0$$

Solving these equations for λ gives $\lambda = \pm 1/(36\sqrt{2})$. Therefore, the stationary points are given by

$$y^* = 4 + \frac{1}{36\lambda} = 4 \pm \sqrt{2}$$
$$z^* = 45 + \frac{1}{24\lambda} = 5 \pm \frac{3}{2}\sqrt{2}$$
$$\lambda^* = \pm\frac{1}{36\sqrt{2}}$$

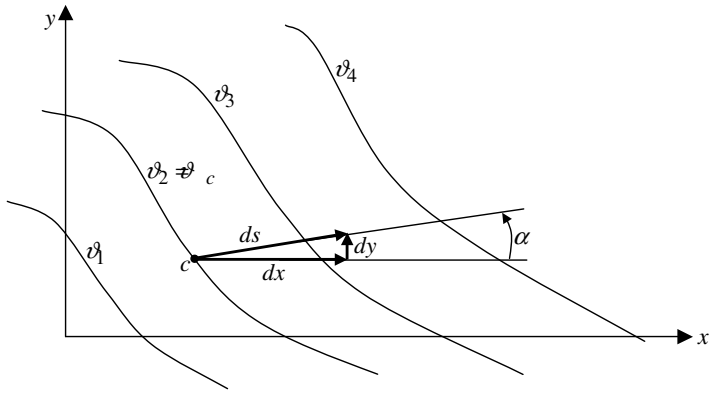

Figure C.2: The Directional Derivative Concept

The sufficient condition of eqn. (C.19) for this problem is given by

$$\nabla_{\mathbf{x}}^2 \phi = \begin{bmatrix} 18\lambda^* & 0 \\ 0 & 8\lambda^* \end{bmatrix}$$

Also, eqn. (C.21) gives

$$Q \equiv q = 8\lambda^* \left[\frac{(z^* - 5)^2}{(y^* - 4)^2} + 1 \right]$$

Clearly, if $\lambda^* = +1/(36\sqrt{2})$ then the stationary point given by $y^* = 4 + \sqrt{2}$ and $z^* = 5 + (3/2)\sqrt{2}$ is a local minimum with $\phi = (7/3) - \sqrt{2}$. Likewise, if $\lambda^* = -1/(36\sqrt{2})$ then the stationary point given by $y^* = 4 - \sqrt{2}$ and $z^* = 5 - (3/2)\sqrt{2}$ is a local maximum with $\phi = (7/3) + \sqrt{2}$.

C.3 Nonlinear Unconstrained Optimization

In this section two iterative methods are shown that can be used to solve nonlinear unconstrained optimization problems. Several approaches can be used to numerically solve these problems, but are beyond the scope of the present text. The interested reader is encouraged to pursue other approaches in the open literature (e.g., see Refs. [1] and [3]).

C.3.1 Some Geometrical Insights

Consider the function $\vartheta(x, y)$ of two variables whose contours are sketched in Figure C.2. rom the geometry of Figure C.2 it is evident that

$$\tan\alpha = \frac{dy}{dx} \tag{C.22a}$$

$$\sin\alpha = \frac{dy}{ds} \tag{C.22b}$$

$$\cos\alpha = \frac{dx}{ds} \tag{C.22c}$$

For arbitrary small displacements (dx, dy) away from the "current" point (x_c, y_c), the differential change in ϑ is given by

$$d\vartheta = \left.\frac{\partial\vartheta}{\partial x}\right|_c dx + \left.\frac{\partial\vartheta}{\partial y}\right|_c dy \tag{C.23}$$

If s is the distance measured along an arbitrary line through c, then the rate of change ("differential derivative") of ϑ in the direction of the line is

$$\left.\frac{d\vartheta}{ds}\right|_c = \left.\frac{\partial\vartheta}{\partial x}\right|_c \left.\frac{dx}{ds}\right|_c + \left.\frac{\partial\vartheta}{\partial y}\right|_c \left.\frac{dy}{ds}\right|_c \tag{C.24}$$

Making use of eqns. (C.22b) and (C.22c), we have

$$\left.\frac{d\vartheta}{ds}\right|_c = \left.\frac{\partial\vartheta}{\partial x}\right|_c \cos\alpha + \left.\frac{\partial\vartheta}{\partial y}\right|_c \sin\alpha \tag{C.25}$$

Now, let's look at a couple of particularly interesting cases. Suppose we wish to select the particular line for which $\left.\frac{d\vartheta}{ds}\right|_c = 0$. Equation (C.25) tells us that the angle $\alpha_1 = \alpha$ orienting this line is given by

$$\tan\alpha_1 = \frac{-\left.\frac{\partial\vartheta}{\partial x}\right|_c}{\left.\frac{\partial\vartheta}{\partial y}\right|_c} \tag{C.26}$$

which gives the "contour direction." Now let's also find the particular direction of which results in the minimum or maximum $\left.\frac{d\vartheta}{ds}\right|_c$. The necessary condition for the extremum of $\left.\frac{d\vartheta}{ds}\right|_c$ requires

$$\frac{d}{d\alpha}\left(\left.\frac{d\vartheta}{ds}\right|_c\right) = -\left.\frac{\partial\vartheta}{\partial x}\right|_c \sin\alpha + \left.\frac{\partial\vartheta}{\partial y}\right|_c \cos\alpha = 0 \tag{C.27}$$

From eqn. (C.27) the angle $\alpha_2 = \alpha$ which orients the direction of "steepest descent" or "steepest ascent" is given by

$$\tan\alpha_2 = \frac{\left.\frac{\partial\vartheta}{\partial y}\right|_c}{\left.\frac{\partial\vartheta}{\partial x}\right|_c} \tag{C.28}$$

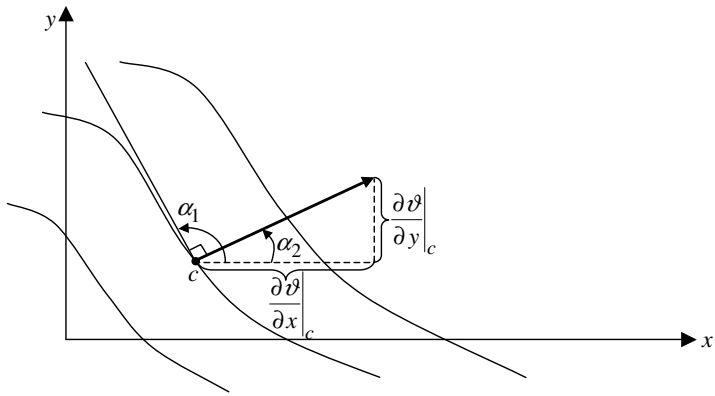

Figure C.3: Geometrical Interpretation of the Gradient Line

which gives the "gradient direction." Notice that $(\tan\alpha_1)(\tan\alpha_2) = -1$. Therefore, α_1 and α_2 orient lines that are perpendicular. So, the contour line is perpendicular to the gradient line, as shown in Figure C.3. These geometrical concepts are difficult to conceptualize rigorously in higher dimensional spaces, but fortunately, the mathematics does generalize rigorously and in a straightforward fashion.

C.3.2 Methods of Gradients

One immediate conclusion of the foregoing is that (based only upon the first derivative information), the most favorable direction to take a small step toward minimizing (or maximizing) the function ϑ is down (or up) the locally evaluated gradient of ϑ. The "method of gradients" (also known as the "method of steepest descent" for minimizing ϑ or the "method of steepest ascent" for maximizing ϑ) is a sequence of one-dimensional searches along the lines established by successively evaluated local gradients of ϑ. Consider ϑ to be a function of n variables which are the elements of $\mathbf{x}$. Let the local evaluations be denoted by superscripts. For example,

$$\vartheta^{(k)} = \vartheta\left(\mathbf{x}^{(k)}\right) \tag{C.29}$$

denotes $\vartheta(\mathbf{x})$ evaluated at the k^{th} set of $\mathbf{x}$-values. The k^{th} one-dimensional search determines a scalar $\alpha^{(k)}$ such that

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)}[\nabla_{\mathbf{x}}\vartheta]^{(k)} \tag{C.30}$$

results in

$$\vartheta^{(k+1)} = \vartheta\left(\mathbf{x}^{(k+1)}\right) \tag{C.31}$$

being a local minimum or maximum. The one-dimensional search for $\alpha^{(k)}$ can be determined analytically or numerically using various methods (see Refs. [1] and [3]).

It is important to develop a geometrical feel for the method of gradients to understand the circumstances under which it works best, to anticipate failures, and to decide upon remedial action when failure occurs. Sequences of iterations from various starting guesses for Himmelblau's function are shown in Figure C.1. Observe the orthogonality of successive gradients. The successive gradients will be exactly orthogonal only if the one-dimensional minima or maxima are perfectly located. Note, for the case of two unknowns only one gradient calculation may be necessary, since all successive gradients are either parallel or perpendicular to the first. However, this orthogonality condition is obviously insufficient to establish the gradient directions for the case of three or more unknowns (e.g., for three unknowns there exists a *plane* that is perpendicular to the gradient vector).

The convergence of the gradient method is heavily dependent upon the circularity of the contours (see Figure C.5 for a function with nonlinear trenches). As an aside, in 3-space the "contours" most desired are "spherical surfaces"; in n-space the "contours" most desired are "hyperspheres." Also, the gradient method often converges rapidly for the first few iterations (far from the solution), but is usually a very poor algorithm during the final iterations. For any function ϑ with non-spherical contours, the number of iterations to converge exactly is generally unbounded. Satisfactory convergence accuracy often requires an unacceptably large number of one-dimensional searches. This can be overcome by using the Levenberg-Marquardt algorithm shown in §1.6.3, which combines the least squares differential correction process with a gradient search.

Example C.3: In this example the method of gradients is used to determine the minimum of the following quadratic function:

$$\vartheta(\mathbf{x}) = 4x_1^2 + 3x_2^2 - 4x_1x_2 + x_1$$

The starting guess is given by $\mathbf{x}^{(0)} = \begin{bmatrix} -1 & 3 \end{bmatrix}^T$. A plot of the iterations superimposed on the contours is shown in Figure C.4. This function has low eccentricity contours with the minimum of $\mathbf{x}^* = \begin{bmatrix} -3/16 & -1/8 \end{bmatrix}^T$. The Hessian matrix is constant and symmetric for this function:

$$\nabla_{\mathbf{x}}^2 \vartheta = \begin{bmatrix} 8 & -4 \\ -4 & 6 \end{bmatrix}$$

The eigenvalues of this matrix are all positive, which states that the function is well behaved. The iterations are given by

$$\begin{aligned}
\mathbf{x}^{(1)} &= \begin{bmatrix} 0.7576 & 0.9649 \end{bmatrix}^T \\
\mathbf{x}^{(2)} &= \begin{bmatrix} -0.2456 & 0.1003 \end{bmatrix}^T \\
\mathbf{x}^{(3)} &= \begin{bmatrix} -0.1192 & -0.0462 \end{bmatrix}^T \\
\mathbf{x}^{(4)} &= \begin{bmatrix} -0.1917 & -0.1088 \end{bmatrix}^T \\
\mathbf{x}^{(5)} &= \begin{bmatrix} -0.1826 & -0.1194 \end{bmatrix}^T
\end{aligned}$$

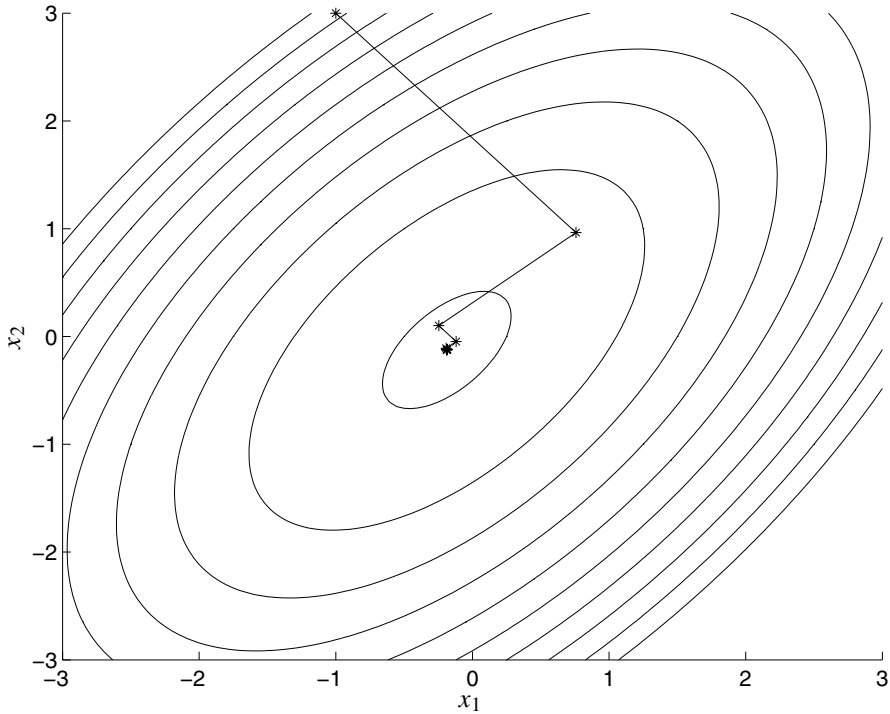

Figure C.4: Minimization of a Quadratic Loss Function

$$\mathbf{x}^{(6)} = \begin{bmatrix} -0.1878 & -0.1238 \end{bmatrix}^T$$
$$\mathbf{x}^{(7)} = \begin{bmatrix} -0.1871 & -0.1246 \end{bmatrix}^T$$
$$\mathbf{x}^{(8)} = \begin{bmatrix} -0.1875 & -0.1250 \end{bmatrix}^T$$

This clearly shows the typical performance of the gradient method, where rapid convergence is given far from the minimum, but slow progress is given near the minimum. Still, the algorithm converges to the true minimum. This behavior is also seen from various other starting guesses.

C.3.3 Second-Order (Gauss-Newton) Algorithm

The Gauss-Newton algorithm is probably the most powerful unconstrained optimization method. We will discuss a "curvature pitfall" that necessitates care in applying this algorithm, however. Say a loss function ϑ is evaluated at a local point

$\mathbf{x}^{(k)}$. It is desired to modify $\mathbf{x}^{(k)}$ by $\Delta\mathbf{x}^{(k)}$ according to

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \Delta\mathbf{x}^{(k)} \tag{C.32}$$

in such a fashion that ϑ is decreased or increased. The behavior of ϑ near $\mathbf{x}^{(k)}$ can be approximated by a second-order Taylor's series:

$$\vartheta \cong \vartheta\left(\mathbf{x}^{(k)}\right) + \Delta\mathbf{x}^T\mathbf{g}^{(k)} + \frac{1}{2}\Delta\mathbf{x}^T H^{(k)}\Delta\mathbf{x} \tag{C.33}$$

where $\mathbf{g}^{(k)} \equiv \nabla_{\mathbf{x}}\vartheta^{(k)}$ (the gradient of ϑ) and $H^{(k)} \equiv \nabla^2_{\mathbf{x}}\vartheta^{(k)}$ (the Hessian of ϑ). The local strategy is to determine the particular correction vector $\Delta\mathbf{x}^{(k)}$ which minimizes (maximizes) the second-order prediction of ϑ. Investigating eqn. (C.33) for an extreme leads to the following:

necessary condition

$$\nabla_{\Delta\mathbf{x}}\vartheta = \mathbf{g}^{(k)} + H^{(k)}\Delta\mathbf{x} = \mathbf{0} \tag{C.34}$$

sufficient condition

$$\nabla^2_{\Delta\mathbf{x}}\vartheta = H^{(k)} \begin{cases} \text{must be positive definite for minimum.} \\ \text{must be negative definite for maximum.} \\ \text{must be indefinite for saddle.} \end{cases} \tag{C.35}$$

From the necessary condition of eqn. (C.34), the local corrections are then given by

$$\Delta\mathbf{x}^{(k)} = -\left[H^{(k)}\right]^{-1}\mathbf{g}^{(k)} \tag{C.36}$$

Substituting eqn. (C.36) into eqn. (C.32) gives the Gauss-Newton second-order optimization algorithm:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \left[H^{(k)}\right]^{-1}\mathbf{g}^{(k)} \tag{C.37}$$

It is important to note that this algorithm converges in exactly one iteration for a quadratic loss function, regardless of the starting guesses used. For example, the second-order correction for the loss function shown in example C.3 is given by

$$\mathbf{x}^{(1)} = \begin{bmatrix} x_1^{(0)} \\ x_2^{(0)} \end{bmatrix} - \begin{bmatrix} \frac{3}{16} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} 8x_1^{(0)} - 4x_2^{(0)} + 1 \\ 6x_2^{(0)} - 4x_1^{(0)} \end{bmatrix} = -\begin{bmatrix} \frac{3}{16} \\ \frac{1}{8} \end{bmatrix} \tag{C.38}$$

which gives the optimal solution in one iteration! In many (probably most) solvable unconstrained optimization problems, the second-order approximation underlying eqn. (C.37) becomes valid during the final iterations; the terminal convergence of eqn. (C.37) is usually exceptionally rapid.

There is a pitfall though! If the sufficient condition of eqn. (C.35) is not satisfied, then the correction will be in the wrong direction. It is difficult to attempt minimizing

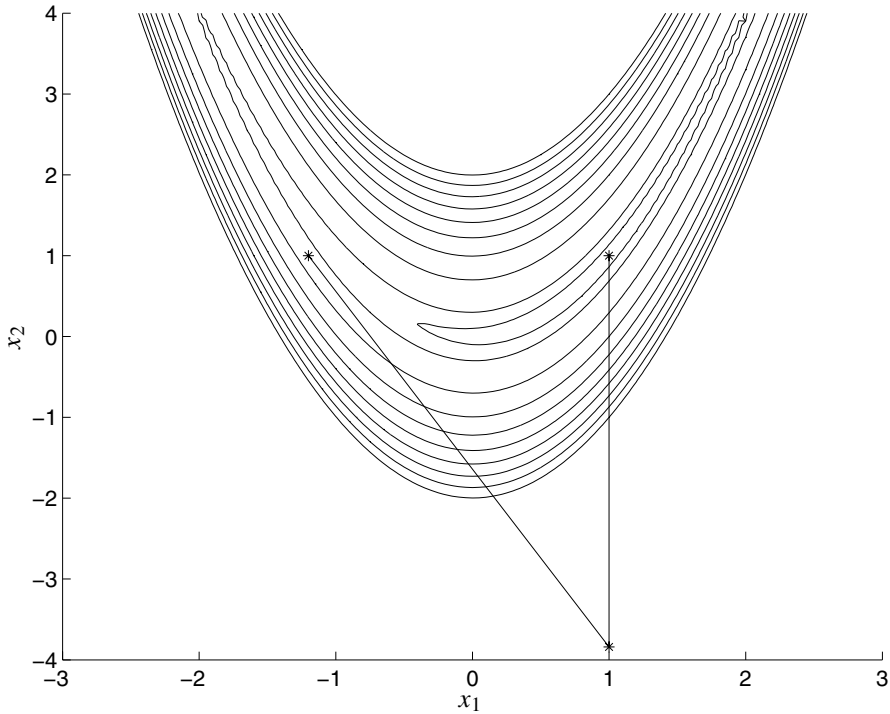

Figure C.5: Minimization of Rosenbrock's Loss Function

a function by solving for local maxima. This pitfall can be circumvented by using a gradient algorithm until the neighborhood of the solution is reached, then testing the sufficient condition of eqn. (C.35) and employing the second-order algorithm if it is satisfied.

Example C.4: In this example the Gauss-Newton algorithm is used to determine the minimum of Rosenbrock's loss function, which has been devised to be a specific challenge to gradient-based approaches:

$$\vartheta(\mathbf{x}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

A plot of the contours for this function is shown in Figure C.5. Note the highly nonlinear trenches for this function. The starting guess is given by $\mathbf{x}^{(0)} = \begin{bmatrix} -1.2 & 1 \end{bmatrix}^T$. For this particular problem, the gradient method of §C.3.2 does not converge to the true minimum of $\mathbf{x}^* = \begin{bmatrix} 1 & 1 \end{bmatrix}^T$ even after 1,000 iterations. However, the second-order algorithm converges in just two iterations, shown in Figure C.5. The iterations are given by

$$\mathbf{x}^{(1)} = \begin{bmatrix} 1.0000 & -3.8400 \end{bmatrix}^T$$

$$\mathbf{x}^{(2)} = \begin{bmatrix} 1.0000 & 1.0000 \end{bmatrix}^T$$

The Hessian matrix evaluated for this function is given

$$\nabla^2_{\mathbf{x}} \vartheta = \begin{bmatrix} -400(x_2 - x_1^2) + 800x_1^2 + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix}$$

which is always positive definite at all the iterations. This example clearly shows the advantages of using a second-order correction in the optimization process.

The overwhelmingly most significant drawback of the second-order correction is the necessity of calculating the matrix of second derivatives. For complicated loss function models, it is usually an expensive consideration to simply determine the n elements of the gradient vector. One is thus motivated to ask the question: "Is it possible to approximate quadratic convergence without the expense of calculating second partial derivatives?" The answer turns out to be yes! Observe that some "second-order information" is contained in the sequence of local function and gradient calculations. Two such techniques have been developed that are in common use today (the Fletcher-Powell[4] and Fletcher-Reeves[5] algorithms). These algorithms are not developed here due to space limitations; the interested reader should see Refs. [1] and [3] for theoretical development and numerical examples of these important algorithms.

It is also significant to note that when the loss function is the sum of squares of a set of functions whose first derivatives are available, that second-order convergence can be approximated by linearizing the functions *before squaring*. The result is a local quadratic approximation of ϑ; this local approximation can be minimized rigorously. The classical example use of this approach is the *Gaussian least squares differential correction*, which is also known as *nonlinear least squares*. This algorithm is developed in §1.4 and is applied to numerous examples in this text.

References

[1] Rao, S.S., *Engineering Optimization: Theory and Practice*, John Wiley & Sons, New York, NY, 3rd ed., 1996.

[2] Bryson, A.E. and Ho, Y.C., *Applied Optimal Control*, Taylor & Francis, London, England, 1975.

[3] Reklaitis, G.V., Ravindran, A., and Ragsdell, K.M., *Engineering Optimization: Methods and Applications*, John Wiley & Sons, New York, NY, 1983.

[4] Fletcher, R. and Powell, M., "A Rapidly Convergent Descent Method for Minimization," *Computer Journal*, Vol. 6, No. 2, July 1963, pp. 163–168.

[5] Fletcher, R. and Reeves, C.M., "Function Minimization by Conjugate Gradients," *Computer Journal*, Vol. 7, No. 2, July 1964, pp. 149–154.