The secant method was able to find the more accurate answer $p_5 = 0.4501836$.

Although the golden search is slower in this example, it has the desirable feature that it can be applied in cases where $f(x)$ is not differentiable. ■

Finding Extreme Values of $f(x, y)$

Definition 8.1 is easily extended to functions of several variables. Suppose that $f(x, y)$ is defined in the region

$$R = \{(x, y) : (x - p)^2 + (y - q)^2 < r^2\}. \tag{3}$$

The function $f(x, y)$ has a local minimum at (p, q) provided that

$$f(p, q) \le f(x, y) \quad \text{for each point } (x, y) \in R. \tag{4}$$

The function $f(x, y)$ has a local maximum at (p, q) provided that

$$f(x, y) \le f(p, q) \quad \text{for each point } (x, y) \in R. \tag{5}$$

The second derivative test for an extreme value is an extension of Theorem 8.4.

Theorem 8.5 (Second Derivative Test). Assume that $f(x, y)$ and its first- and second-order partial derivatives are continuous on a region R. Suppose that $(p, q) \in R$ is a critical point where both $f_x(p, q) = 0$ and $f_y(p, q) = 0$. The higher-order partial derivatives are used to determine the nature of the critical point.

(i) If $f_{xx}(p, q)f_{yy}(p, q) - f_{xy}^2(p, q) > 0$ and $f_{xx}(p, q) > 0$, then $f(p, q)$ is a local minimum of f.

(ii) If $f_{xx}(p, q)f_{yy}(p, q) - f_{xy}^2(p, q) > 0$ and $f_{xx}(p, q) < 0$, then $f(p, q)$ is a local maximum of f.

(iii) If $f_{xx}(p, q)f_{yy}(p, q) - f_{xy}^2(p, q) < 0$, then $f(x, y)$ does not not have a local extremum at (p, q).

(iv) If $f_{xx}(p, q)f_{yy}(p, q) - f_{xy}^2(p, q) = 0$, this test is inconclusive.

Example 8.3. Find the minimum of $f(x, y) = x^2 - 4x + y^2 - y - xy$.

The first-order partial derivatives are

$$f_x(x, y) = 2x - 4 - y \quad \text{and} \quad f_y(x, y) = 2y - 1 - x. \tag{6}$$

Setting these partial derivatives equal to zero yields the linear system

$$\begin{aligned} 2x - y &= 4 \\ -x + 2y &= 1. \end{aligned} \tag{7}$$

The solution to (7) is $(x, y) = (3, 2)$. The second-order partial derivatives of $f(x, y)$ are

$$f_{xx}(x, y) = 2, \quad f_{yy}(x, y) = 2, \quad \text{and} \quad f_{xy}(x, y) = -1.$$

It is easy to see that we have case (i) of Theorem 8.5, that is

$$f_{xx}(3, 2)f_{yy}(3, 2) - f_{xy}^2(3, 2) = 3 > 0 \quad \text{and} \quad f_{xx}(3, 2) = 2 > 0.$$

Hence $f(x, y)$ has a local minimum $f(3, 2) = -7$ at the point $(3, 2)$. ■

The Nelder-Mead Method

A simplex method for finding a local minimum of a function of several variables has been devised by Nelder and Mead. For two variables, a simplex is a triangle, and the method is a pattern search that compares function values at the three vertices of a triangle. The worst vertex, where $f(x, y)$ is largest, is rejected and replaced with a new vertex. A new triangle is formed and the search is continued. The process generates a sequence of triangles (which might have different shapes), for which the function values at the vertices get smaller and smaller. The size of the triangles is reduced and the coordinates of the minimum point are found.

The algorithm is stated using the term simplex (a generalized triangle in N dimensions) and will find the minimum of a function of N variables. It is effective and computationally compact.

The Initial Triangle BGW

Let $f(x, y)$ be the function that is to be minimized. To start, we are given three vertices of a triangle: $\mathbf{V}_k = (x_k, y_k)$, $k = 1, 2, 3$. The function $f(x, y)$ is then evaluated at each of the three points $z_k = f(x_k, y_k)$ for $k = 1, 2, 3$. The subscripts are then reordered so that $z_1 \le z_2 \le z_3$. We use the notation

$$\mathbf{B} = (x_1, y_1), \quad \mathbf{G} = (x_2, y_2), \quad \text{and} \quad \mathbf{W} = (x_3, y_3) \tag{8}$$

to help remember that $\mathbf{B}$ is the best vertex, $\mathbf{G}$ is good (next to best), and $\mathbf{W}$ is the worst vertex.

Midpoint of the Good Side

The construction process uses the midpoint of the line segment joining $\mathbf{B}$ and $\mathbf{G}$. It is found by averaging the coordinates:

$$\mathbf{M} = \frac{\mathbf{B} + \mathbf{G}}{2} = \left(\frac{x_1 + x_2}{2}, \frac{y_1 + y_2}{2}\right). \tag{9}$$

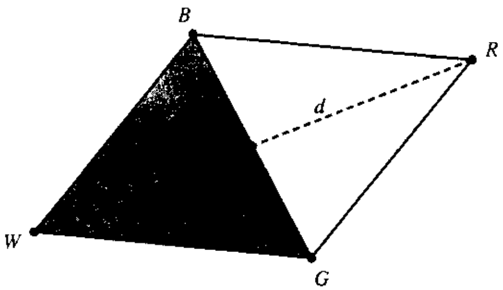


Figure 8.4 The triangle $\triangle BGW$ and midpoint $\boldsymbol{M}$ and reflected point $\boldsymbol{R}$ for the Nelder-Mead method.

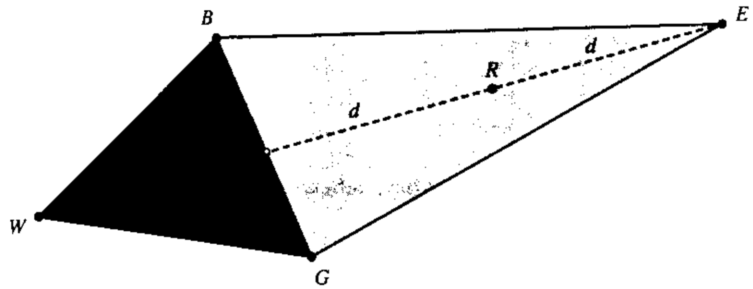


Figure 8.5 The triangle $\triangle BGW$ and point $\boldsymbol{R}$ and extended point $\boldsymbol{E}$.

Reflection Using the Point R

The function decreases as we move along the side of the triangle from $\boldsymbol{W}$ to $\boldsymbol{B}$, and it decreases as we move along the side from $\boldsymbol{W}$ to $\boldsymbol{G}$. Hence it is feasible that $f(x, y)$ takes on smaller values at points that lie away from $\boldsymbol{W}$ on the opposite side of the line between $\boldsymbol{B}$ and $\boldsymbol{G}$. We choose a test point $\boldsymbol{R}$ that is obtained by "reflecting" the triangle through the side $\overline{BG}$. To determine $\boldsymbol{R}$, we first find the midpoint $\boldsymbol{M}$ of the side $\overline{BG}$. Then draw the line segment from $\boldsymbol{W}$ to $\boldsymbol{M}$ and call its length d. This last segment is extended a distance d through $\boldsymbol{M}$ to locate the point $\boldsymbol{R}$ (see Figure 8.4). The vector formula for $\boldsymbol{R}$ is

(10) $$\boldsymbol{R} = \boldsymbol{M} + (\boldsymbol{M} - \boldsymbol{W}) = 2\boldsymbol{M} - \boldsymbol{W}.$$

Expansion Using the Point E

If the function value at $\boldsymbol{R}$ is smaller than the function value at $\boldsymbol{W}$, then we have moved in the correct direction toward the minimum. Perhaps the minimum is just a bit farther than the point $\boldsymbol{R}$. So we extend the line segment through $\boldsymbol{M}$ and $\boldsymbol{R}$ to the point $\boldsymbol{E}$. This forms an expanded triangle BGE. The point $\boldsymbol{E}$ is found by moving an additional distance d along the line joining $\boldsymbol{M}$ and $\boldsymbol{R}$ (see Figure 8.5). If the function value at $\boldsymbol{E}$ is less than the function value at $\boldsymbol{R}$, then we have found a better vertex than $\boldsymbol{R}$. The vector formula for $\boldsymbol{E}$ is

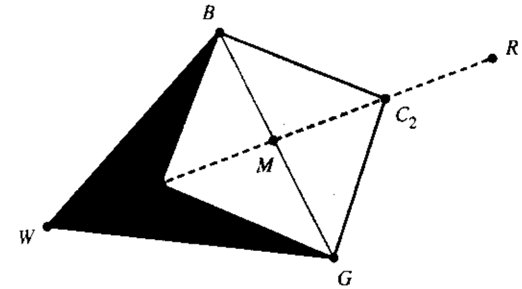


Figure 8.6 The contraction point C_1 or C_2 for Nelder-Mead method.

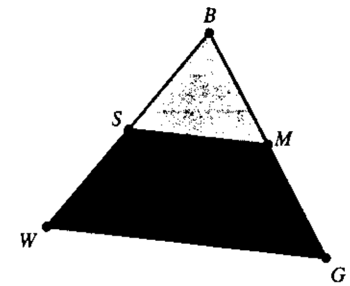


Figure 8.7 Shrinking the triangle toward $\boldsymbol{B}$.

(11) $$\boldsymbol{E} = \boldsymbol{R} + (\boldsymbol{R} - \boldsymbol{M}) = 2\boldsymbol{R} - \boldsymbol{M}.$$

Contraction Using the Point C

If the function values at $\boldsymbol{R}$ and $\boldsymbol{W}$ are the same, another point must be tested. Perhaps the function is smaller at $\boldsymbol{M}$, but we cannot replace $\boldsymbol{W}$ with $\boldsymbol{M}$ because we must have a triangle. Consider the two midpoints $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$ of the line segments $\overline{WM}$ and $\overline{MR}$, respectively (see Figure 8.6). The point with the smaller function value is called $\boldsymbol{C}$, and the new triangle is BGC. *Note:* the choice between $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$ might seem inappropriate for the two-dimensional case, but it is important in higher dimensions.

Shrink toward B

If the function value at $\boldsymbol{C}$ is not less than the value at $\boldsymbol{W}$, the points $\boldsymbol{G}$ and $\boldsymbol{W}$ must be shrunk toward $\boldsymbol{B}$ (see Figure 8.7). The point $\boldsymbol{G}$ is replaced with $\boldsymbol{M}$, and $\boldsymbol{W}$ is replaced with $\boldsymbol{S}$, which is the midpoint of the line segment joining $\boldsymbol{B}$ with $\boldsymbol{W}$.

Table 8.3 Logical Decisions for the Nelder-Mead Algorithm

IF $f(R) < f(G)$, THEN Perform Case (i) {either reflect or extend} ELSE Perform Case (ii) {either contract or shrink}	
BEGIN {Case (i).}	BEGIN {Case (ii).}
IF $f(B) < f(R)$ THEN	IF $f(R) < f(W)$ THEN
replace W with R	replace W with R
ELSE	Compute $C = (W + M)/2$
	or $C = (M + R)/2$ and $f(C)$
Compute E and $f(E)$	IF $f(C) < f(W)$ THEN
IF $f(E) < f(B)$ THEN	replace W with C
replace W with E	ELSE
ELSE	Compute S and $f(S)$
replace W with R	replace W with S
ENDIF	replace G with M
ENDIF	ENDIF
END {Case (i).}	END {Case (ii).}

Logical Decisions for Each Step

A computationally efficient algorithm should perform function evaluations only if needed. In each step, a new vertex is found, which replaces $\boldsymbol{W}$. As soon as it is found, further investigation is not needed, and the iteration step is completed. The logical details for two-dimensional cases are explained in Table 8.3.

Example 8.4. Use the Nelder-Mead algorithm to find the minimum of $f(x, y) = x^2 - 4x + y^2 - y - xy$. Start with the three vertices

$$\boldsymbol{V}_1 = (0, 0), \quad \boldsymbol{V}_2 = (1.2, 0.0), \quad \boldsymbol{V}_3 = (0.0, 0.8).$$

The function $f(x, y)$ takes on the values

$$f(0, 0) = 0.0, \quad f(1.2, 0.0) = -3.36, \quad f(0.0, 0.8) = -0.16.$$

The function values must be compared to determine $\boldsymbol{B}$, $\boldsymbol{G}$, and $\boldsymbol{W}$;

$$\boldsymbol{B} = (1.2, 0.0), \quad \boldsymbol{G} = (0.0, 0.8), \quad \boldsymbol{W} = (0, 0).$$

The vertex $\boldsymbol{W} = (0, 0)$ will be replaced. The points $\boldsymbol{M}$ and $\boldsymbol{R}$ are

$$\boldsymbol{M} = \frac{\boldsymbol{B} + \boldsymbol{G}}{2} = (0.6, 0.4) \quad \text{and} \quad \boldsymbol{R} = 2\boldsymbol{M} - \boldsymbol{W} = (1.2, 0.8).$$

The function value $f(\boldsymbol{R}) = f(1.2, 0.8) = -4.48$ is less than $f(\boldsymbol{G})$, so the situation is case (i). Since $f(\boldsymbol{R}) \le f(\boldsymbol{B})$, we have moved in the right direction, and the vertex $\boldsymbol{E}$ must be constructed:

$$\boldsymbol{E} = 2\boldsymbol{R} - \boldsymbol{M} = 2(1.2, 0.8) - (0.6, 0.4) = (1.8, 1.2).$$

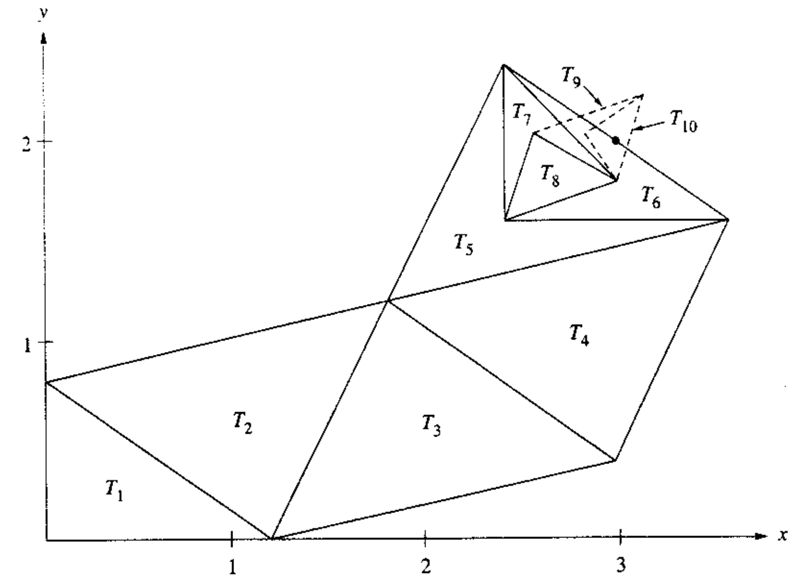


Figure 8.8 The sequence of triangles $\{T_k\}$ converging to the point $(3, 2)$ for the Nelder-Mead method.

The function value $f(\boldsymbol{E}) = f(1.8, 1.2) = -5.88$ is less than $f(\boldsymbol{B})$, and the new triangle has vertices

$$\boldsymbol{V}_1 = (1.8, 1.2), \quad \boldsymbol{V}_2 = (1.2, 0.0), \quad \boldsymbol{V}_3 = (0.0, 0.8).$$

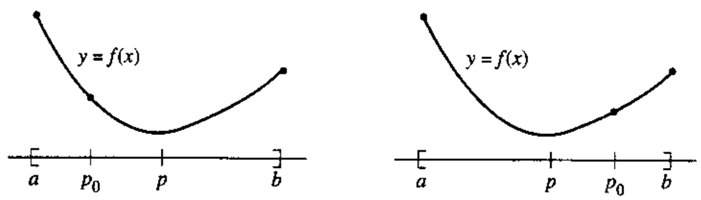
The process continues and generates a sequence of triangles that converges down on the solution point $(3, 2)$ (see Figure 8.8). Table 8.4 gives the function values at vertices of the triangle for several steps in the iteration. A computer implementation of the algorithm continued until the thirty-third step, where the best vertex was $\boldsymbol{B} = (2.99996456, 1.99983839)$ and $f(\boldsymbol{B}) = -6.99999998$. These values are approximations to $f(3, 2) = -7$ found in Example 8.3. The reason that the iteration quit before $(3, 2)$ was obtained is that the function is flat near the minimum. The function values $f(\boldsymbol{B})$, $f(\boldsymbol{G})$, and $f(\boldsymbol{W})$ were checked and found to be the same (this is an example of round-off error), and the algorithm was terminated. ∎

Minimization Using Derivatives

Suppose that $f(x)$ is unimodal over $[a, b]$ and has a unique minimum at $x = p$. Also, assume that $f'(x)$ is defined at all points in (a, b). Let the starting value p_0 lie in (a, b). If $f'(p_0) < 0$, the minimum point p lies to the right of p_0. If $f'(p_0) > 0$, p lies to the left of p_0 (see Figure 8.9).

Table 8.4 Function Values at Various Triangles for Example 8.4

k	Best point	Good point	Worst point
1	$f(1.2, 0.0) = -3.36$	$f(0.0, 0.8) = -0.16$	$f(0.0, 0.0) = 0.00$
2	$f(1.8, 1.2) = -5.88$	$f(1.2, 0.0) = -3.36$	$f(0.0, 0.8) = -0.16$
3	$f(1.8, 1.2) = -5.88$	$f(3.0, 0.4) = -4.44$	$f(1.2, 0.0) = -3.36$
4	$f(3.6, 1.6) = -6.24$	$f(1.8, 1.2) = -5.88$	$f(3.0, 0.4) = -4.44$
5	$f(3.6, 1.6) = -6.24$	$f(2.4, 2.4) = -6.24$	$f(1.8, 1.2) = -5.88$
6	$f(2.4, 1.6) = -6.72$	$f(3.6, 1.6) = -6.24$	$f(2.4, 2.4) = -6.24$
7	$f(3.0, 1.8) = -6.96$	$f(2.4, 1.6) = -6.72$	$f(2.4, 2.4) = -6.24$
8	$f(3.0, 1.8) = -6.96$	$f(2.55, 2.05) = -6.7725$	$f(2.4, 1.6) = -6.72$
9	$f(3.0, 1.8) = -6.96$	$f(3.15, 2.25) = -6.9525$	$f(2.55, 2.05) = -6.7725$
10	$f(3.0, 1.8) = -6.96$	$f(2.8125, 2.0375) = -6.95640625$	$f(3.15, 2.25) = -6.9525$



If $f'(p_0) < 0$ then p lies in $[p_0, b]$.

If $f'(p_0) > 0$ then p lies in $[a, p_0]$.

Figure 8.9 Using $f'(x)$ to find the minimum value of the unimodal function $f(x)$ on the interval $[a, b]$.

Bracketing the Minimum

Our first task is to obtain three test values,

$$(12) \qquad p_0, \quad p_1 = p_0 + h, \quad \text{and} \quad p_2 = p_0 + 2h,$$

so that

$$(13) \qquad f(p_0) > f(p_1) \quad \text{and} \quad f(p_1) < f(p_2).$$

Suppose that $f'(p_0) < 0$; then $p_0 < p$ and the step size h should be chosen positive. It is an easy task to find a value for h so that the three points in (12) satisfy (13). Start with $h = 1$ in formula (12) (provided that $a + 1 < b$).

Case (i): If (13) is satisfied, we are done.

Case (ii): If $f(p_0) > f(p_1)$ and $f(p_1) > f(p_2)$, then $p_2 < p$. We need to check points that lie farther to the right. Double the step size and repeat the process.

Case (iii): If $f(p_0) \le f(p_1)$, we have jumped over p and h is too large. We need to check values closer to p_0. Reduce the step size by a factor of $\frac{1}{2}$ and repeat the process.

When $f'(p_0) > 0$, the step size h should be chosen negative and then cases similar to (i) to (iii) can be used.

Quadratic Approximation to Find p

Finally, we have three points (12) that satisfy (13). We will use quadratic interpolation to find $p_{\min}$, which is an approximation to p. The Lagrange polynomial based on the nodes in (12) is

$$(14) \qquad Q(x) = \frac{y_0(x - p_1)(x - p_2)}{2h^2} - \frac{y_1(x - p_0)(x - p_2)}{h^2} + \frac{y_2(x - p_0)(x - p_1)}{2h^2}.$$

The derivative of $Q(x)$ is

$$(15) \qquad Q'(x) = \frac{y_0(2x - p_1 - p_2)}{2h^2} - \frac{y_1(2x - p_0 - p_2)}{h^2} + \frac{y_2(2x - p_0 - p_1)}{2h^2}.$$

Solving $Q'(x) = 0$ in the form $Q'(p_0 + h_{\min}) = 0$ yields

$$(16) \qquad \begin{aligned} 0 = {} & \frac{y_0(2(p_0 + h_{\min}) - p_1 - p_2)}{2h^2} - \frac{y_1(4(p_0 + h_{\min}) - 2p_0 - 2p_2)}{2h^2} \\ & + \frac{y_2(2(p_0 + h_{\min}) - p_0 - p_1)}{2h^2}. \end{aligned}$$

Multiply each term in (16) by $2h^2$ and collect terms involving $h_{\min}$:

$$\begin{aligned} -h_{min}(2y_0 - 4y_1 + 2y_2) &= y_0(2p_0 - p_1 - p_2) \\ &\quad - y_1(4p_0 - 2p_0 - 2p_2) + y_2(2p_0 - p_0 - p_1) \\ &= y_0(-3h) - y_1(-4h) + y_2(-h). \end{aligned}$$

This last quantity is easily solved for $h_{\min}$:

$$(17) \qquad h_{\min} = \frac{h(4y_1 - 3y_0 - y_2)}{4y_1 - 2y_0 - 2y_2}.$$

The value $p_{\min} = p_0 + h_{\min}$ is a better approximation to p than p_0. Hence we can replace p_0 with $p_{\min}$ and repeat the two processes outlined above to determine a new h and a new $h_{\min}$. Continue the iteration until the desired accuracy is achieved. The details are outlined in Program 8.3.