

2.2. Algorithms for unconstrained multivariable optimization

joining B and W (Figure 2.23). Similar to M , the midpoint S can be calculated from:

$$S = \frac{B + W}{2} \quad (2.105)$$

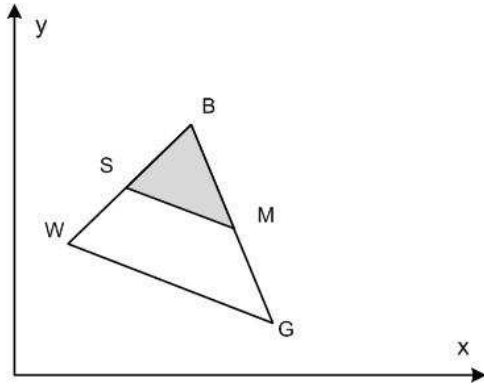


Figure 2.23: Shrinking toward B

The algorithm must terminate in a finite number of steps or iterations. The stop criterion can be one or all of the following:

- The simplex becomes sufficiently small, or the vertices are within a given tolerance ε
- The function does not change for successive iterations.
- The number of iterations or function evaluations exceeds a maximum value allowed.

For the two-dimensional case, the details are summarized in Algorithm 11, (Mathews and Fink, 2004).

Example 2.5 Use the Nelder-Mead algorithm to find the minimum of:

$$f(x, y) = (x - 10)^2 + (y - 10)^2 \quad (2.106)$$

We calculate the first steps and illustrate them graphically.

Algorithm 11 Nelder-Mead method

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Define function  $f(x, y)$  and tolerance  $\varepsilon$ 
Select 3 initial vertices  $V_1, V_2, V_3$ 
while stop criterion not fulfilled do
  Compute  $f(V_1), f(V_2), f(V_3)$  and set the labels  $B, G, W$ 
  Compute  $M = (B + G)/2$  and  $R = 2M - W$ 
  if  $f(R) < f(W)$  then
    Compute  $E = 2R - M, f(E)$ 
    if  $f(E) < f(R)$  then
      Replace  $W$  with  $E$ 
    else
      Replace  $W$  with  $R$ 
    end if
  else
    Compute  $C_1$  and  $C_2$  and choose  $C$ 
    if  $f(C) < f(W)$  then
      Replace  $W$  with  $C$ 
    else
      Compute  $S$  and  $f(S)$ 
      Replace  $W$  with  $S$ 
      Replace  $G$  with  $M$ 
    end if
  end if
end while
```

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First iteration Start with three vertices conveniently chosen at the origin and on the axes (Figure 2.24):

$$V_1 = (0, 0), \quad V_2 = (2, 0), \quad V_3 = (0, 6) \quad (2.107)$$

and calculate the function values $f(x, y)$ at these points:

$$f(0, 0) = 200, \quad f(2, 0) = 164, \quad f(0, 6) = 116 \quad (2.108)$$

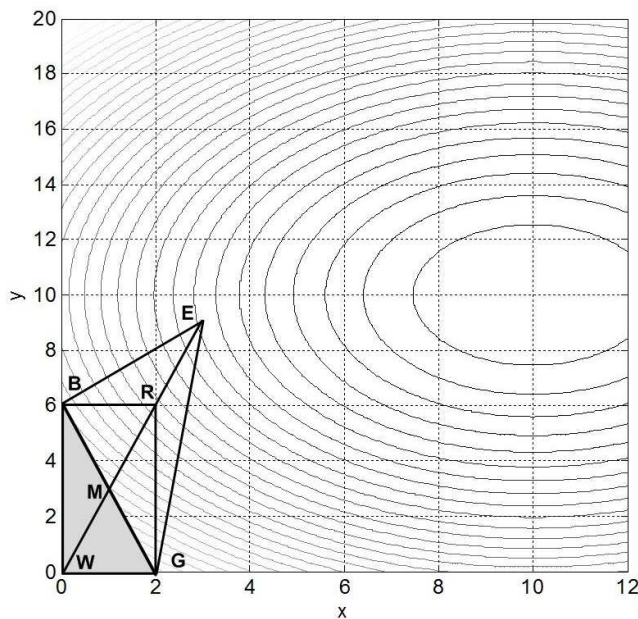


Figure 2.24: The first sequence of triangles

Since $f(0, 6) < f(2, 0) < f(0, 0)$, the vertices will be assigned the names:

$$B = (0, 6), \quad G = (2, 0), \quad W = (0, 0) \quad (2.109)$$

The midpoint of BG is:

$$M = \frac{B + G}{2} = (1, 3) \quad (2.110)$$

and the reflected point:

$$R = 2M - W = (2, 6) \quad (2.111)$$

The function value at R , $f(R) = f(2, 6) = 80 < f(G) < f(B)$ and the extended point E will be calculated from:

$$E = 2R - M = (3, 9) \quad (2.112)$$

The new triangle is $\triangle BGE$.

Second iteration Since the function value at E is $f(3, 9) = 50 < f(G) < f(B)$, the vertices labels for the current stage are (Figure 2.25):

$$B = (3, 9), \quad G = (0, 6), \quad W = (2, 0) \quad (2.113)$$

The new midpoint of BG and the reflected point R are:

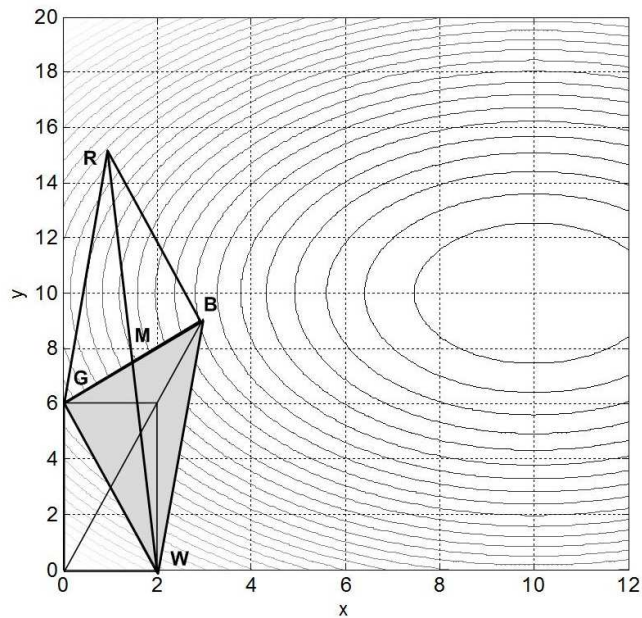


Figure 2.25: The second sequence of triangles

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$$M = \frac{B + G}{2} = (1.5, 7.5), \quad R = 2M - W = (1, 15) \quad (2.114)$$

The value of f at the reflected point is: $f(1, 15) = 106$. It is less than $f(G) = f(0, 6) = 116$ but greater than $f(B) = f(3, 9) = 50$. Therefore, the extended point will not be calculated and the new triangle is $\triangle RGB$.

Third iteration Because $f(3, 9) < f(1, 15) < f(0, 6)$, the new labels are (Figure 2.26):

$$B = (3, 9), \quad G = (1, 15), \quad W = (0, 6) \quad (2.115)$$

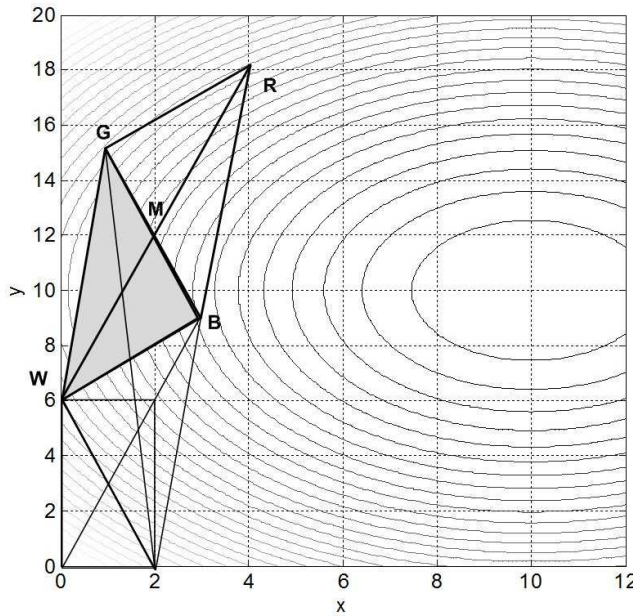


Figure 2.26: The third sequence of triangles

A new midpoint and a reflected point are calculated:

$$M = \frac{B + G}{2} = (2, 12), \quad R = 2M - W = (4, 18) \quad (2.116)$$

and the function takes at R the value $f(R) = f(4, 18) = 100$. This is again less than the value at G but it is not less than the value at B , thus the point R will be a vertex of the next triangle $\triangle RGB$.

Fourth iteration Because $f(3, 9) < f(4, 18) < f(1, 15)$, the new labels are (Fig-

ure 2.27):

$$B = (3, 9), \quad G = (4, 18), \quad W = (1, 15) \quad (2.117)$$

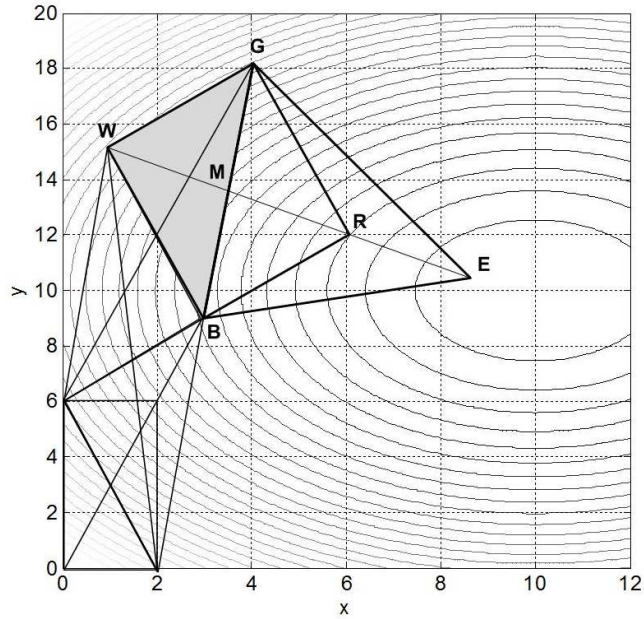


Figure 2.27: The fourth sequence of triangles

The midpoint of BG and R result as:

$$M = \frac{B + G}{2} = (3.5, 13.5), \quad R = 2M - W = (6, 12) \quad (2.118)$$

Because $f(R) = f(6, 12) = 20 < f(B)$, we shall build the extended point E :

$$E = 2R - M = (8.5, 10.5) \quad (2.119)$$

The function takes here the value $f(E) = f(8.5, 10.5) = 2.5$, thus the new triangle is $\triangle GBE$.

The calculations continue until the function values at the vertices have almost equal values (with some allowable tolerance ε). It will still take a large number of steps until the procedure will reach the minimum point $(10, 10)$ where the function

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value is 0, but the steps performed above show that the function is decreasing at each iteration.

2.2.6.2 Rosenbrock method

The main drawback of the Nelder-Mead method is that general convergence properties have not been proven. An alternative for a derivative-free algorithm is the method of Rosenbrock whose global convergence to a local optima is assured.

This zero-order method solves the unconstrained optimization problem of minimizing a nonlinear function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, (Rosenbrock, 1960). Starting at an initial point \mathbf{x}_0 , the method explores locally along n orthogonal directions seeking for a better solution. The first set of directions is usually composed of the base vectors of an n -dimensional coordinate system. During the iterative process, this set is recalculated such that the first vector to point into the direction of the maximum function decrease.

Example 2.6 Consider the orthogonal coordinate system $x_1 - x_2$ shown in Figure 2.28. A set of normalized vectors in the direction of the axes is $(\mathbf{d}_1, \mathbf{d}_2)$ given

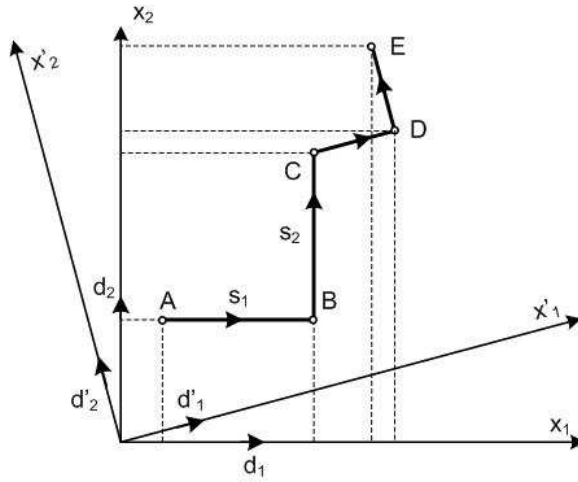


Figure 2.28: Rotation of a coordinate system

by:

$$\mathbf{d}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{d}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (2.120)$$