

```

    Q(cnt)=Y(lo);
end
% End of Nelder-Mead algorithm
%Determine size of simplex
snorm=0;
for j=1:n+1
    s=norm(V(j)-V(lo));
    if(s>=snorm)
        snorm=s;
    end
end
Q=Q';
V0=V(lo,1:n);
y0=Y(lo);
dV=snorm;
dy=abs(Y(hi)-Y(lo));
if (show==1)
    disp(P);
    disp(Q);
end

```

Exercises for Nelder-Mead and Powell's Methods

- Use Theorem 8.5 to find the local minimum of each of the following functions.
 - $f(x, y) = x^3 + y^3 - 3x - 3y + 5$
 - $f(x, y) = x^2 + y^2 + x - 2y - xy + 1$
 - $f(x, y) = x^2y + xy^2 - 3xy$
 - $f(x, y) = (x - y)/(x^2 + y^2 + 2)$
 - $f(x, y) = 100(y - x^2)^2 + (1 - x)^2$
(Rosenbrock's parabolic valley, circa 1960)
- Let $B = (2, -3)$, $G = (1, 1)$, and $W = (5, 2)$. Find the points M , R , and E and sketch the triangles that are involved.
- Let $B = (-1, 2)$, $G = (-2, -5)$, and $W = (3, 1)$. Find the points M , R , and E and sketch the triangles that are involved.
- Let $B = (0, 0, 0)$, $G = (1, 1, 0)$, $P = (0, 0, 1)$, and $W = (1, 0, 0)$.
 - Sketch the tetrahedron $BGPW$.
 - Find $M = (B + G + P)/3$.
 - Find $R = 2M - W$ and sketch the tetrahedron $BGPR$.
 - Find $E = 2R - M$ and sketch the tetrahedron $BGPE$.

5. Let $\mathbf{B} = (0, 0, 0)$, $\mathbf{G} = (0, 2, 0)$, $\mathbf{P} = (0, 1, 1)$, and $\mathbf{W} = (2, 1, 0)$. Follow the instructions in Exercise 4.
6. Follow the process in Example 8.7 and find \mathbf{X}_1 for $f(x, y) = x^3 + y^3 - 3x - 3y + 5$. Use the initial point $\mathbf{P}_0 = (1/2, 1/3)$.
7. Follow the process in Example 8.7 and find \mathbf{X}_1 for $f(x, y) = x^2y + xy^2 - 3xy$. Use the initial point $\mathbf{P}_0 = (1/2, 1/3)$.
8. Give a vector proof that $\mathbf{M} = (\mathbf{B} + \mathbf{G})/2$ is the midpoint of the line segment joining the points \mathbf{B} and \mathbf{G} .
9. Give a vector proof of equation (7).
10. Give a vector proof of equation (8).
11. Give a vector proof that the medians of any triangle intersect at a point that is two-thirds of the distance from each vertex to the midpoint of the opposite side.

Algorithms and Programs

1. Use Program 8.4 to find the minimum of each of the functions in Exercise 1 with an accuracy of eight decimal places. Use the following starting vertices:
 - (a) $(1, 2)$, $(2, 0)$, and $(2, 2)$
 - (b) $(0, 0)$, $(2, 0)$, and $(2, 1)$
 - (c) $(0, 0)$, $(2, 0)$, and $(2, 1)$
 - (d) $(0, 0)$, $(0, 1)$, and $(1, 1)$
 - (e) $(0, 0)$, $(1, 0)$, and $(0, 2)$
2. Use Program 8.4 to find the local minimum of each of the following functions with an accuracy of eight decimal places.
 - (a) $f(x, y, z) = 2x^2 + 2y^2 + z^2 - 2xy + yz - 7y - 4z$
Start with $(1, 1, 1)$, $(0, 1, 0)$, $(1, 0, 1)$, and $(0, 0, 1)$.
 - (b) $f(x, y, z, u) = 2(x^2 + y^2 + z^2 + u^2) - x(y + z - u) + yz - 3x - 8y - 5z - 9u$
Start the search near $(1, 1, 1, 1)$.
 - (c) $f(x, y, z, u) = xyz u + \frac{1}{x} + \frac{1}{y} + \frac{1}{z} + \frac{1}{u}$
Start the search near $(0.7, 0.7, 0.7, 0.7)$.
3. Write a MATLAB program to implement Powell's method.
4. Use the program for Powell's method (Problem 3) to find the local minimum of each of functions in Problem 1 with an accuracy of seven decimal places. Use a starting value near one of the given vertices.
5. Use the program for Powell's method (Problem 3) to find the local minimum of each of functions in Problem 2 with an accuracy of seven decimal places. Use the starting values or start near a vertex given in Problem 2.

6. Find the point on the surface $z = x^2 + y^2$ that is closest to the point $(2, 3, 1)$ with an accuracy of seven decimal places.
7. A company has five factories A, B, C, D, and E, located at the points $(10, 10)$, $(30, 50)$, $(16.667, 29)$, $(0.555, 29.888)$, and $(22.2221, 49.988)$, respectively, in the xy -plane. Assume that the distance between two points represents the driving distance, in miles, between the factories. The company plans to build a warehouse at some point in the plane. It is anticipated that during an average week there will be 10, 18, 20, 14, and 25 deliveries made to factories A, B, C, D, and E, respectively. Ideally, to minimize the weekly mileage of delivery vehicles, where should the warehouse be located?
8. In Problem 7, where should the warehouse be located if, due to zoning restrictions, it must be located at a point on the curve $y = x^2$?

8.3 Gradient and Newton's Methods

Now we turn to the minimization of a function $f(\mathbf{X})$ of N variables, where $\mathbf{X} = (x_1, x_2, \dots, x_N)$ and the partial derivatives of f are accessible.

Steepest Descent or Gradient Method

Definition 8.4. Let $z = f(\mathbf{X})$ be a function of \mathbf{X} such that $\partial f(\mathbf{X})/\partial x_k$ exists for $k = 1, 2, \dots, N$. The *gradient* of f , denoted by $\nabla f(\mathbf{X})$, is the vector

$$(1) \quad \nabla f(\mathbf{X}) = \left(\frac{\partial f(\mathbf{X})}{\partial x_1}, \frac{\partial f(\mathbf{X})}{\partial x_2}, \dots, \frac{\partial f(\mathbf{X})}{\partial x_N} \right). \quad \blacktriangle$$

Example 8.8. Find the gradient of $f(x, y) = \frac{x - y}{x^2 + y^2 + 2}$ at the point $(-3, -2)$.

Substituting $x = -3$ and $y = -2$ into

$$f_x(x, y) = \frac{-x^2 + 2xy + y^2 + 2}{(x^2 + y^2 + 2)^2} \quad \text{and} \quad f_y(x, y) = \frac{-x^2 - 2xy + y^2 - 2}{(x^2 + y^2 + 2)^2}$$

yields

$$\nabla f(-3, -2) = (f_x(-3, -2), f_y(-3, -2)) = \left(\frac{9}{225}, -\frac{19}{225} \right). \quad \blacksquare$$

Recall that the gradient vector in (1) points locally in the direction of the greatest rate of increase of $f(\mathbf{X})$. Hence $-\nabla f(\mathbf{X})$ points locally in the direction of greatest decrease. Start at the point \mathbf{P}_0 and search along the line through \mathbf{P}_0 in the direction $\mathbf{S}_0 = -\nabla f(\mathbf{P}_0)/\|\nabla f(\mathbf{P}_0)\|$. You will arrive at a point \mathbf{P}_1 , where a local minimum occurs when the point \mathbf{X} is constrained to lie on the line $\mathbf{X} = \mathbf{P}_0 + \gamma \mathbf{S}_0$. Since

```

h2=abs(hmin-2*h);
if(h0<h),h=h0;end
if(h1<h),h=h1;end
if(h2<h),h=h2;end
if(h==0),h=hmin;end
if(h<delta),cond=1;end
%Termination test for minimization
e0=abs(y0-ymin);
e1=abs(y1-ymin);
e2=abs(y2-ymin);
if(e0~=0&e0<err),err=e0;end
if(e1~=0&e1<err),err=e1;end
if(e2~=0&e2<err),err=e2;end
if(e0==0&e1==0&e2==0),err=0;end
if(err<epsilon),cond=2;end
if(cond==2&h<delta),cond=3;end
end
cnt=cnt+1;
P(cnt+1,:)= [Pmin ymin];
P0=Pmin;
y0=ymin;
end
if(show==1)
    disp(P);
end

```

Exercises for Gradient and Newton's Methods

- Find the gradient of each function at the given point.
 - $f(x, y) = x^2 + y^3 - 3x - 3y + 5$ at $(-1, 2)$
 - $f(x, y) = 100(y - x^2)^2 + (1 - x)^2$ at $(1/2, 4/3)$
(Rosenbrock's parabolic valley, circa 1960)
 - $f(x, y, z) = \cos(xy) - \sin(xz)$ at $(0, \pi, \pi/2)$
- Use the gradient method to find P_1 and P_2 for the functions and initial points in Exercise 1.
- Find the Hessian matrix for the functions and initial points in Exercise 1.
- Calculate the second-degree Taylor polynomial for the functions in Exercise 1, centered at the given initial points.
- Use formula (10) to find P_1 and P_2 for the functions and initial points in Exercise 1.
- Use the modified Newton's method to find P_1 for the functions and initial points in Exercise 1.

7. Verify that formula (3) is true for the function in Example 8.10.
8. Establish formula (7) for the case $N = 2$ (i.e., $z = f(x_1, x_2)$).
9. Derive formula (8) from formula (7).

Algorithms and Programs

1. Use Program 8.5 to find the minimum of each of the functions in Exercise 1(a) and 1(b) with an accuracy of eight decimal places. Use the initial point $P_0 = (0.3, 0.4)$.
2. In Program 8.5 the x - and y -coordinates of the iterations are stored in the first two columns of the matrix P , respectively. Modify Program 8.5 so that it will plot the x - and y -coordinates of the iterations on the same coordinate system. *Hint.* Incorporate the command `plot(P(:,1), P(:,2), 'r')` into your program. Use this program on the functions in Exercise 1(a) and 1(b). Use the initial point $P_0 = (-0.2, 0.3)$.
3. Write a MATLAB program for Newton's method (formula (10)). Use the program to find the minimum of each of the functions in Exercise 1(a) and 1(b) with an accuracy of eight decimal places. Use the initial point $P_0 = (0.3, 0.4)$.
4. Write a MATLAB program for the modified Newton's method.
5. Use the program for the modified Newton's method (Problem 4) to find the local minimum of each of the following functions with an accuracy of eight decimal places.
 - (a) $f(x, y, z) = 2x^2 + 2y^2 + z^2 - 2xy + yz - 7y - 4z$ with $P_0 = (0.5, 0.4, 0.5)$
 - (b) $f(x, y, z, u) = 2(x^2 + y^2 + z^2 + u^2) - x(y + z - u) + yz - 3x - 8y - 5z - 9u$ with $P_0 = (1, 1, 1, 1)$
 - (c) $f(x, y, z, u) = xyz u + \frac{1}{x} + \frac{1}{y} + \frac{1}{z} + \frac{1}{u}$ with $P_0 = (0.7, 0.7, 0.7, 0.7)$
6. Use Program 8.5 to find the local minimum of each of the functions in Problem 5 with an accuracy of eight decimal places. Use a starting value near one of the given vertices.
7. Find the point, with an accuracy of seven decimal places, on the surface $z = x^2 + y^2$ that is closest to the point $(2, 3, 1)$.
8. A company has five factories, A, B, C, D, and E, located at the points $(10, 10)$, $(30, 50)$, $(16.667, 29)$, $(0.555, 29.888)$, and $(22, 2221, 49.988)$, respectively, in the xy -plane. Assume that the distance between two points represents the driving distance, in miles, between the factories. The company plans to build a warehouse at some point in the plane. It is anticipated that during an average week there will be 10, 18, 20, 14, and 25 deliveries made to factories A, B, C, D, and E, respectively. Ideally, to minimize the weekly mileage of delivery vehicles, where in the xy -plane should the warehouse be located?
9. In Problem 8, where should the warehouse be located if due to zoning restrictions, it must be located at a point on the curve $y = x^2$?

```

h=abs(h);
h0=abs(hmin);
h1=abs(hmin-h);
h2=abs(hmin-2*h);

%Determine magnitude of next h
if(h0<h),h=h0;end
if(h1<h),h=h1;end
if(h2<h),h=h2;end
if(h==0),h=hmin;end
if(h<delta),cond=1;end
if (abs(h)>big|abs(pmin)>big),cond=5;end

%Termination test for minimization
e0=abs(y0-ymin);
e1=abs(y1-ymin);
e2=abs(y2-ymin);
if(e0~=0 & e0<err),err=e0;end
if(e1~=0 & e1<err),err=e1;end
if(e2~=0 & 2<err),err=e2;end
if(e0~=0 & e1==0 & e2==0),error=0;end
if(err<epsilon),cond=2;end
p0=pmin;
k=k+1;
P(k)=p0;
end
if(cond==2&&h<delta),cond=3;end
end
p=p0;
dp=h;
yp=feval(f,p);
dy=err;

```

Exercises for Minimization of a Function of One Variable

1. Use Theorem 8.1 to determine where each of the following functions is increasing and where it is decreasing.
 - (a) $f(x) = 2x^3 - 9x^2 + 12x - 5$
 - (b) $f(x) = x/(x + 1)$
 - (c) $f(x) = (x + 1)/x$
 - (d) $f(x) = x^x$

2. Use Definition 8.3 to show that the following functions are unimodal on the given intervals.
- $f(x) = x^2 - 2x + 1; [0, 4]$
 - $f(x) = \cos(x); [0, 4]$
 - $f(x) = x^x; [0.1, 10]$
 - $f(x) = -x(3-x)^{5/3}; [0, 3]$
3. Use Theorems 8.3 and 8.4, if possible, to find all local minima and maxima of each of the following functions on the given interval.
- $f(x) = 4x^3 - 8x^2 - 11x + 5; [0, 2]$
 - $f(x) = x + 3/x^2; [0.5, 3]$
 - $f(x) = (x + 2.5)/(4 - x^2); [-1.9, 1.9]$
 - $f(x) = e^x/x^2; [0.5, 3]$
 - $f(x) = -\sin(x) - \sin(3x)/3; [0, 2]$
 - $f(x) = -2\sin(x) + \sin(2x) - 2\sin(3x)/3; [1, 3]$
4. Find the point on the parabola $y = x^2$ that is closest to the point $(3, 1)$.
5. Find the point on the curve $y = \sin(x)$ that is closest to the point $(2, 1)$.
6. Find the point(s) on the circle $x^2 + y^2 = 25$ that is farthest from the chord AB if $A = (3, 4)$ and $B = (-1, \sqrt{24})$.
7. Use the golden ratio search and five-digit rounding arithmetic to find $[a_k, b_k]$ for $k = 0, 1, 2$, for each of the following functions. *Note.* Each function is unimodal on the given interval.
- $f(x) = e^x + 2x + \frac{x^2}{2}; [-2.4, -1.6]$
 - $f(x) = -\sin(x) - x + \frac{x^2}{2}; [0.8, 1.6]$
 - $f(x) = \frac{x^2}{2} - 4x - x \cos(x); [0.5, 2.5]$
 - $f(x) = x^3 - 5x^2 + 23; [1, 5]$
8. Use the Fibonacci search and five-digit rounding arithmetic to find $[a_k, b_k]$ for $k = 0, 1, 2$, for each of the functions in Exercise 7. In each case assume that F_{10} is the smallest Fibonacci number satisfying a given tolerance ϵ .
9. Carry out two iterations of the quadratic approximation method, using five-digit rounding arithmetic, for each of the functions in Exercise 7.
10. Use the cubic search method and five-digit rounding arithmetic to find p_1 and p_2 for each of the functions in Exercise 7.
11. The golden ratio search is applied to a function on the given interval. Determine the length of the k th subinterval.
- $[0, 1], k = 4$
 - $[-2.3, -1.6], k = 5$
 - $[-4.6, 3.5], k = 10$

12. For each interval and value of ϵ find the smallest Fibonacci number F_n satisfying inequality (7).
- (a) $[-0.1, 3.4]$, $\epsilon = 10^{-4}$
 (b) $[-2.3, 5.3]$, $\epsilon = 10^{-6}$
 (c) $[3.33, 3.99]$, $\epsilon = 10^{-8}$

13. Algebraically establish the identity

$$1 - \frac{F_{n-k-1}}{F_{n-k}} = \frac{F_{n-k-2}}{F_{n-k}}.$$

14. Establish formulas (19), (20), and (21).
 15. Establish formula (22).
 16. Establish formula (23).
 17. *Dichotomous search method.* The dichotomous search is another bracketing method for determining the minimum of a unimodal function f on a closed interval $[a_0, b_0]$ without using derivatives. The values c_0 and d_0 are placed symmetrically at a distance ϵ from the midpoint of the interval, $(a_0 + b_0)/2$. Depending on the values of $f(c_0)$ and $f(d_0)$ a new subinterval is obtained. The process is then repeated by determining c_1 and d_1 .

Input: ϵ , the distinguishability constant; and tol , the length of the final subinterval. While $b_k - a_k \geq tol$, let

$$c_k = \frac{a_k + b_k}{2} - \epsilon \quad \text{and} \quad d_k = \frac{a_k + b_k}{2} + \epsilon.$$

If $f(c_k) < f(d_k)$, let $a_{k+1} = a_k$ and $b_{k+1} = d_k$. Otherwise, let $a_{k+1} = c_k$ and $b_{k+1} = b_k$. Let $k = k + 1$ and continue loop.

- (a) Use the dichotomous search and five-digit rounding arithmetic to find $[a_1, b_1]$ and $[a_2, b_2]$ for the function $f(x) = e^x + 2x + x^2/2$ on the interval $[-2.4, -1.6]$. Use the distinguishability constant $\epsilon = 0.1$.
 (b) Show that the length of the k th subinterval is given by

$$b_k - a_k = \frac{1}{2^k}(b_0 - a_0) + 2\epsilon \left(1 - \frac{1}{2^k}\right)$$

- (c) For the function in part (a) determine the value of k such that $b_k - a_k < 10^{-4}$, where $\epsilon = 10^{-6}$.

18. *Cubic bracketing search method.* Assume that f is unimodal and differentiable on the interval $[a_0, b_0]$. Again, we consider a search method that explicitly uses f' . We seek the abscissa of the minimum, p_{\min} , of a cubic polynomial that agrees with f and f' at the endpoints a_0 and b_0 . Let

$$P(x) = \alpha(x - a_0)^3 + \beta(x - a_0)^2 + \gamma(x - a_0) + \rho,$$

where $P(a_0) = f(a_0)$, $P(b_0) = f(b_0)$, $P'(a_0) = f'(a_0)$, and $P'(b_0) = f'(b_0)$. If $f(p_{\min}) > 0$, then set $b_1 = p_{\min}$ and $a_1 = a_0$; else set $a_1 = p_{\min}$ and $b_1 = b_0$.

Continue the iteration process until the length of the k th subinterval is less than the desired error: $b_k - a_k < \epsilon$. As with the cubic search introduced in the text, it remains to find explicit formulas for the coefficients α , β , γ , and ρ .

- (a) Show that $p_{\min} = a_0 + \frac{-\beta + \sqrt{\beta^2 - 3\alpha\gamma}}{3\alpha}$.
- (b) Show that $\rho = P(a_0) = f(a_0)$ and $\gamma = P'(a_0) = f'(a_0)$.
- (c) Show that $\alpha = \frac{G - 2D}{b_0 - a_0}$ and $\beta = 3D - G$, where $F = \frac{f(b_0) - f(a_0)}{b_0 - a_0}$,
 $D = \frac{F - \gamma}{b_0 - a_0}$ and $G = \frac{f'(b_0) - f'(a_0)}{b_0 - a_0}$.
- (d) Use the cubic bracketing search and five-digit rounding arithmetic to find $[a_1, b_1]$ and $[a_2, b_2]$ for the function $f(x) = e^x + 2x + x^2/2$ on the interval $[a_0, b_0] = [-2.4, -1.6]$.

Algorithms and Programs

- Use Program 8.1 to find the local minimum of each of the functions in Exercise 7 with an accuracy of six decimal places.
- Use Program 8.2 to find the local minimum of each of the functions in Exercise 7 with an accuracy of six decimal places.
- Use Program 8.3 to find the local minimum of each of the functions in Exercise 7 with an accuracy of six decimal places. Start with the midpoint of the given interval.
- Use Program 8.1 and/or 8.3 to find all local maxima, with an accuracy of six decimal places, of the function $f(x) = \cos^2(x) - \sin(x)$ on the interval $[0, 2\pi]$
- Use Program 8.1 and/or 8.3 to find all the local maxima and minima, with an accuracy of six decimal places of the following function in the interval $[0, 2]$.

$$f(x) = \frac{x^3 + x^2 - 12x - 12}{2x^6 - 3x^5 - 4x^4 + 9x^2 + 12x - 18}$$

- Write a MATLAB program for the cubic approximation method presented in Section 8.1. Use the program to find the local minimum of each of the functions in Exercise 7 with an accuracy of six decimal places.
- Write a MATLAB program for the dichotomous search method in Exercise 17. Use the program to find the local minimum of each of the functions in Exercise 7 with an accuracy of six decimal places.
- Use Program 8.1 and/or 8.3 to find all the local maxima and minima with an accuracy of six decimal places, of the:
 - extrapolated cubic spline that passes through $(0.0, 0.0)$, $(1.0, 0.5)$, $(2.0, 2.0)$, and $(3.0, 1.5)$.
 - parabolically terminated cubic spline that passes through $(0.0, 0.0)$, $(1.0, 0.5)$, $(2.0, 2.0)$, and $(3.0, 1.5)$.

9. Use Program 8.1 and/or 8.3 to find all the local maxima and minima with an accuracy of six decimal places, of the trigonometric polynomial $T_7(x)$ from Section 5.4, Algorithms and Programs, Problem 5(b).

8.2 Nelder-Mead and Powell's Methods

The definitions in Section 8.1 extend naturally to functions of several variables. Suppose that $f(x_1, x_2, \dots, x_N)$ is defined in the region

$$(1) \quad R = \left\{ (x_1, x_2, \dots, x_N) : \sum_{k=1}^N (x_k - p_k)^2 < r^2 \right\}.$$

The function $f(x_1, x_2, \dots, x_N)$ has a local minimum at the point (p_1, p_2, \dots, p_N) provided that

$$(2) \quad f(p_1, p_2, \dots, p_N) \leq f(x_1, x_2, \dots, x_N)$$

for each point $(x_1, x_2, \dots, x_N) \in R$. The function $f(x_1, x_2, \dots, x_N)$ has a local maximum at the point (p_1, p_2, \dots, p_N) provided that

$$(3) \quad f(p_1, p_2, \dots, p_N) \geq f(x_1, x_2, \dots, x_N)$$

or each point $(x_1, x_2, \dots, x_N) \in R$.

The introduction of minimization methods for multivariable functions will be simplified by considering functions of two independent variables, $f(x, y)$. The graph of a function of two independent variables can be interpreted geometrically as a surface (see Figure 8.1). The second partial derivative test for an extreme value of a function $f(x, y)$ is an extension of Theorem 8.4.

Theorem 8.5 (Second Partial 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 have a local extremum at (p, q) .
- (iv) If $f_{xx}(p, q)f_{yy}(p, q) - f_{xy}^2(p, q) = 0$, then this test is inconclusive.