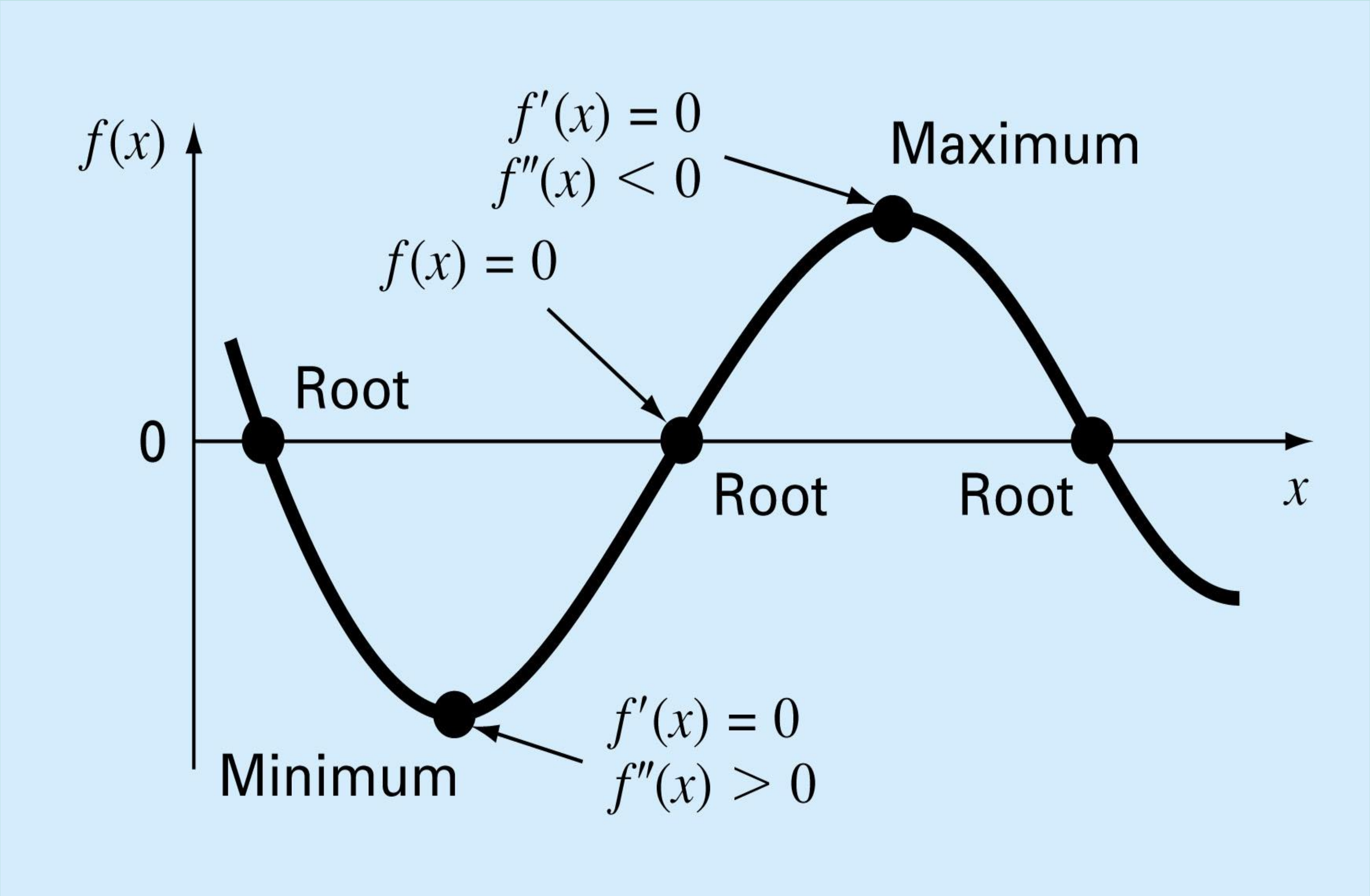
Optimization

Part 4

- Root finding and optimization are related, both involve guessing and searching for a point on a function.
- Fundamental difference is:
  - Root finding is searching for zeros of a function or functions
  - Optimization is finding the minimum or the maximum of a function of several variables.

figure PT4.1



Mathematical Background

- An *optimization* or *mathematical programming* problem generally be stated as:

  Find x, which minimizes or maximizes $f(x)$ subject to

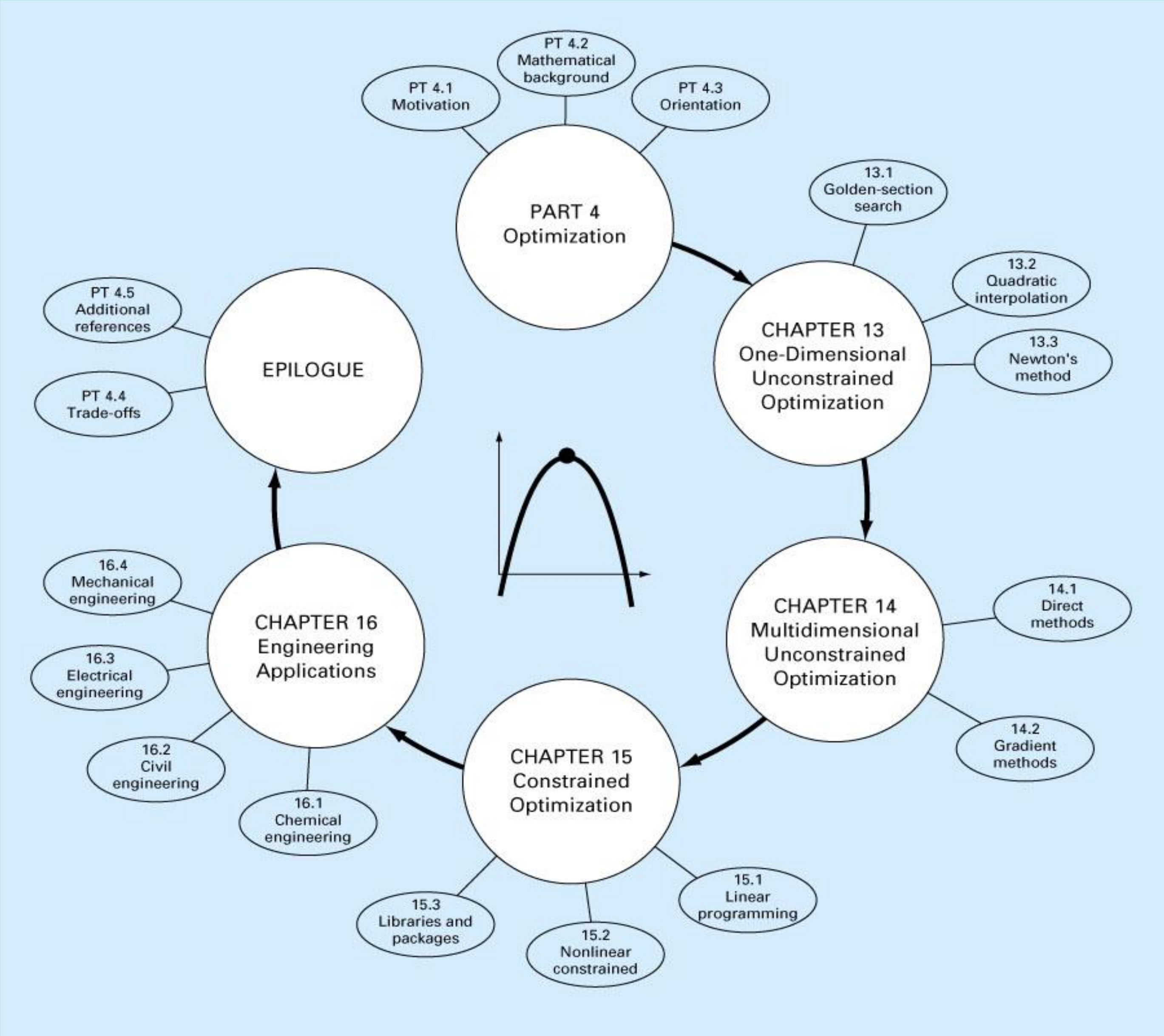
$$d_i(x) \leq a_i \quad i = 1, 2, \ldots, m^*$$

$$e_i(x) = b_i \quad i = 1, 2, \ldots, p^*$$

Where x is an n-dimensional *design vector*, $f(x)$ is the *objective function*, $d_i(x)$ are *inequality constraints*, $e_i(x)$ are *equality constraints*, and a_i and b_i are constants

- Optimization problems can be classified on the basis of the form of *f(x):*
  - If *f(x)* and the constraints are linear, we have linear programming.
  - If *f(x)* is quadratic and the constraints are linear, we have quadratic programming.
  - If *f(x)* is not linear or quadratic and/or the constraints are nonlinear, we have nonlinear programming.
- When equations(*) are included, we have a *constrained optimization* problem; otherwise, it is *unconstrained optimization* problem.

Figure PT4.5



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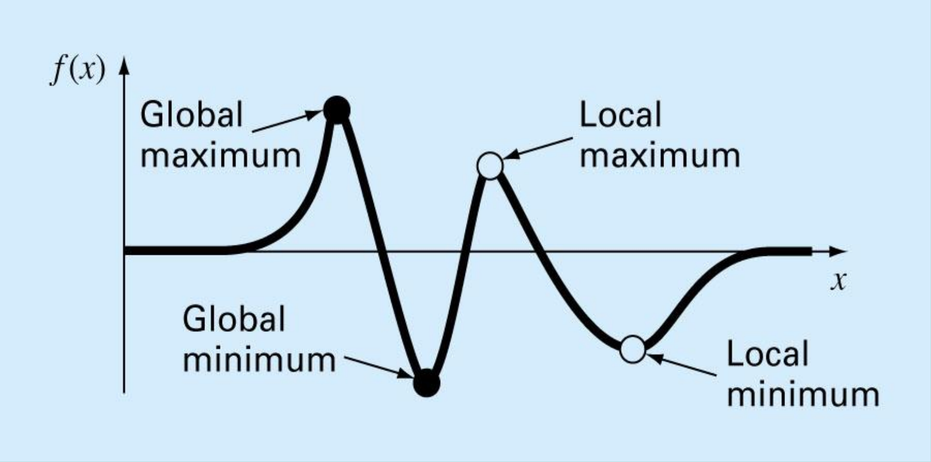
One-Dimensional Unconstrained Optimization

Chapter 13

- In *multimodal* functions, both local and global optima can occur. In almost all cases, we are interested in finding the absolute highest or lowest value of a function.

Figure 13.1



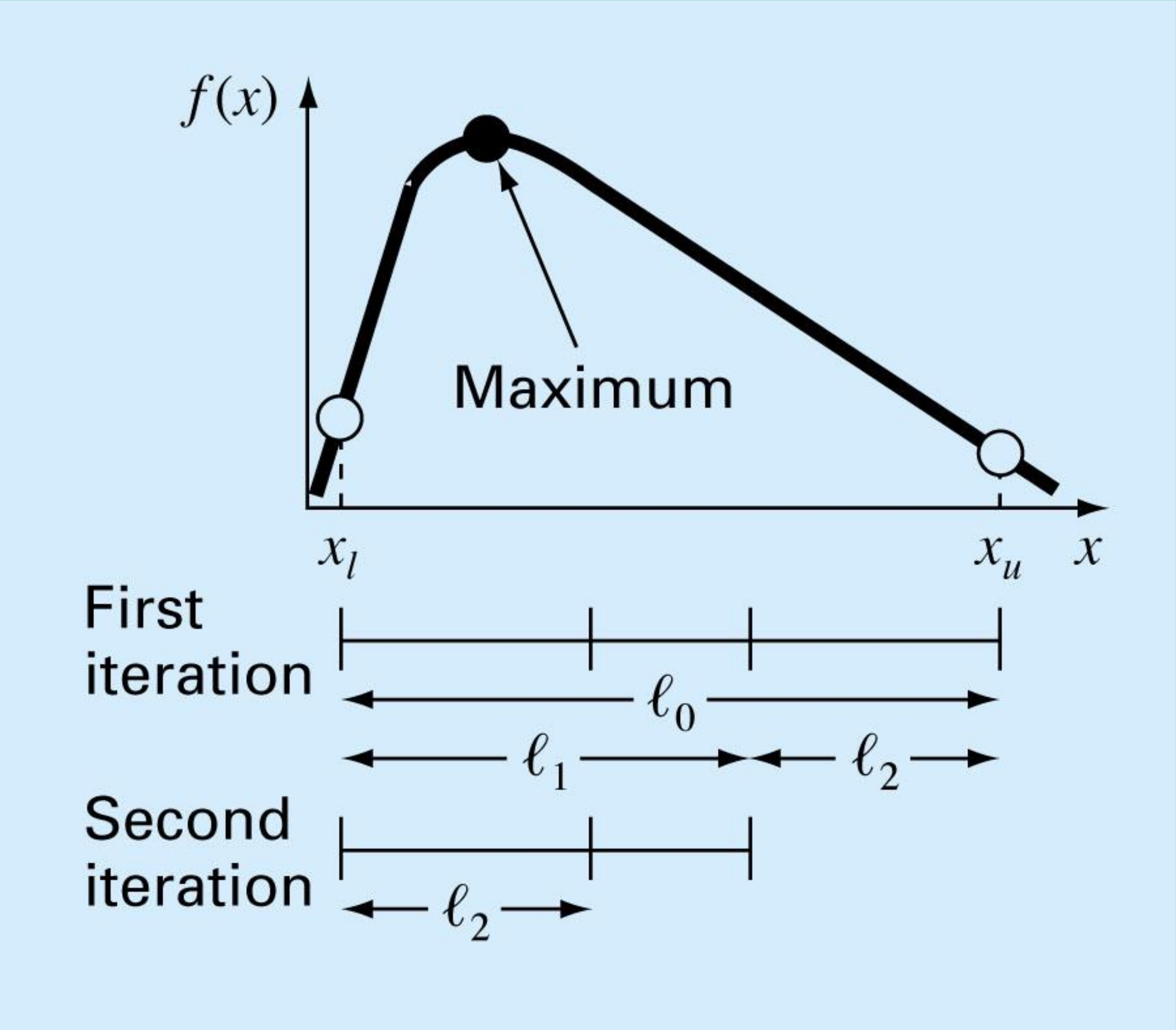
How do we distinguish global optimum from local one?

- By graphing to gain insight into the behavior of the function.
- Using randomly generated starting guesses and picking the largest of the optima as global.
- Perturbing the starting point to see if the routine returns a better point or the same local minimum.

Golden-Section Search

- A *unimodal* function has a single maximum or a minimum in the a given interval. For a *unimodal* function:
  - First pick two points that will bracket your extremum [x_l, x_u].
  - Pick an additional third point within this interval to determine whether a maximum occurred.
  - Then pick a fourth point to determine whether the maximum has occurred within the first three or last three points
  - The key is making this approach efficient by choosing intermediate points wisely thus minimizing the function evaluations by replacing the old values with new values.

Figure 13.2



f(x)
Maximum
x_l
x_u
x
First iteration
ℓ_0
ℓ_1
ℓ_2
Second iteration
ℓ_2

$$l_0 = l_1 + l_2$$
$$\frac{l_1}{l_0} = \frac{l_2}{l_1}$$

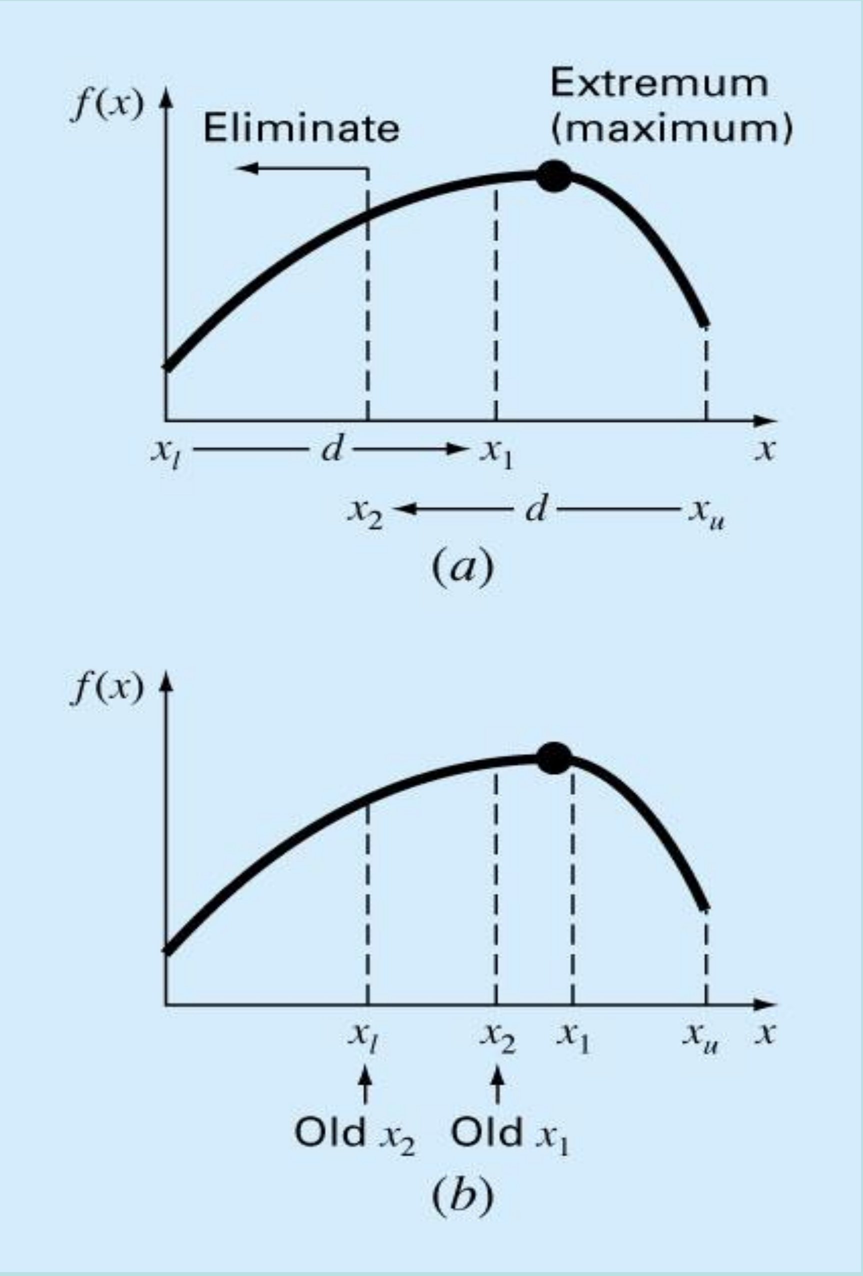
•The first condition specifies that the sum of the two sub lengths l_1 and l_2 must equal the original interval length.

•The second say that the ratio of the length must be equal

$$\frac{l_1}{l_1 + l_2} = \frac{l_2}{l_1} \qquad R = \frac{l_2}{l_1}$$
$$1 + R = \frac{1}{R} \qquad R^2 + R - 1 = 0$$
$$R = \frac{-1 + \sqrt{1 - 4(-1)}}{2} = \frac{\sqrt{5} - 1}{2} = 0.61803$$

Golden Ratio

Figure 13.4



f(x)
Eliminate
Extremum
(maximum)
x_l
d
x_1
x
x_2
d
x_u
(a)
f(x)
x_l
x_2
x_1
x_u
x
Old x_2
Old x_1
(b)

The method starts with two initial guesses, x_l and x_u, that bracket one local extremum of $f(x)$:

- Next two interior points x_1 and x_2 are chosen according to the golden ratio

$$d = \frac{\sqrt{5}-1}{2}(x_u - x_l)$$
$$x_1 = x_l + d$$
$$x_2 = x_u - d$$

- The function is evaluated at these two interior points.

Two results can occur:

- If $f(x_1)>f(x_2)$ then the domain of x to the left of x_2 from x_l to x_2, can be eliminated because it does not contain the maximum. Then, x_2 becomes the new x_l for the next round.

- If $f(x_2)>f(x_1)$, then the domain of x to the right of x_1 from x_l to x_2, would have been eliminated. In this case, x_1 becomes the new x_u for the next round.

- New $x_{1\ i}$s determined as before

$$x_1 = x_l + \frac{\sqrt{5}-1}{2}(x_u - x_l)$$

- The real benefit from the use of golden ratio is because the original x_1 and x_2 were chosen using golden ratio, we do not need to recalculate all the function values for the next iteration.

Newton's Method

- A similar approach to Newton- Raphson method can be used to find an optimum of f(x) by defining a new function g(x)=f'(x). Thus because the same optimal value x* satisfies both

  $f'(x^*)=g(x^*)=0$

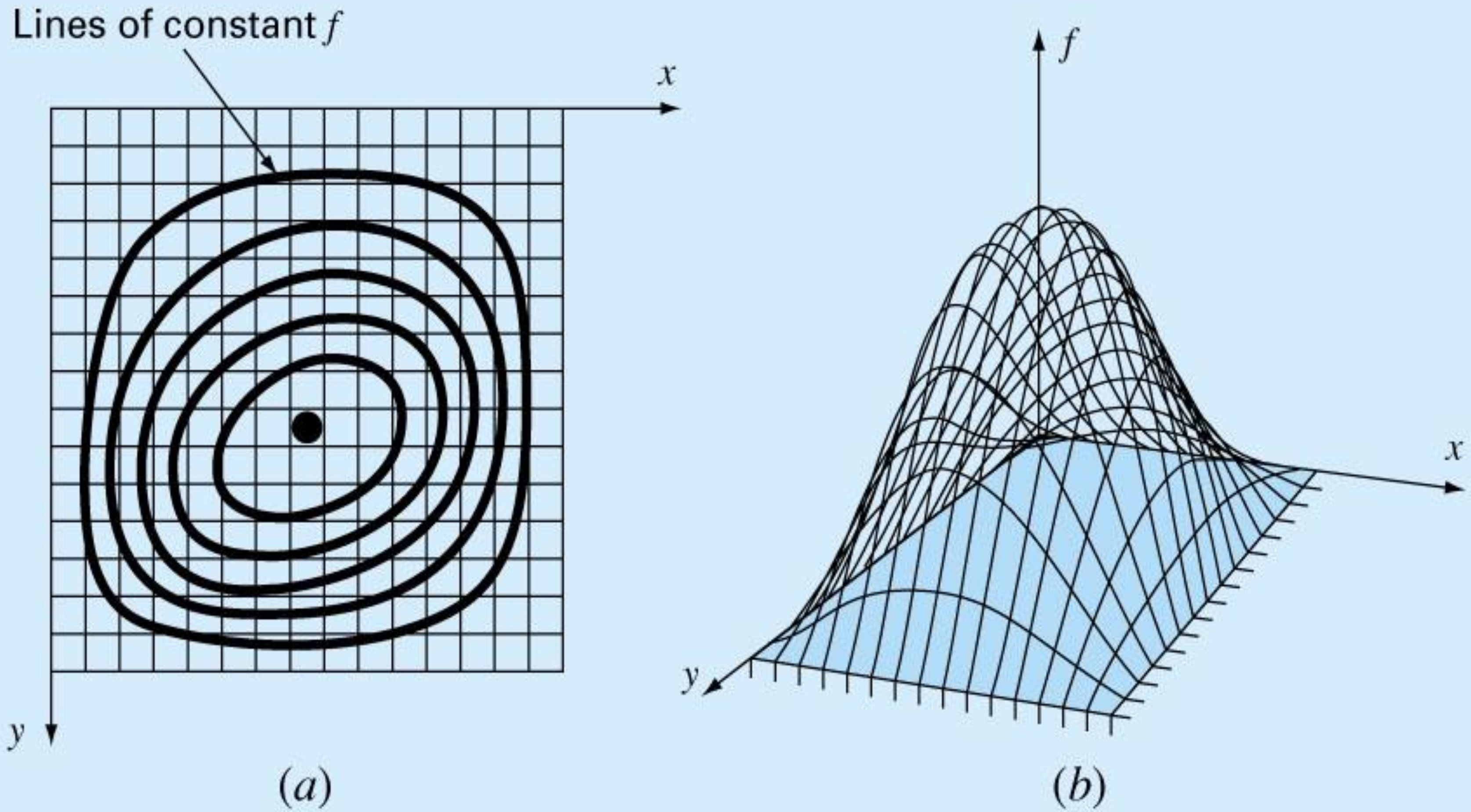
  We can use the following as a technique to the extremum of *f(x)*.

$$x_{i+1} = x_i \frac{f'(x_i)}{f''(x_i)}$$

Multidimensional Unconstrained Optimization
Chapter 14

- Techniques to find minimum and maximum of a function of several variables are described.
- These techniques are classified as:
  - That require derivative evaluation
    - *Gradient* or descent (or *ascent*) methods
  - That do not require derivative evaluation
    - *Non-gradient* or *direct* methods.

Figure 14.1



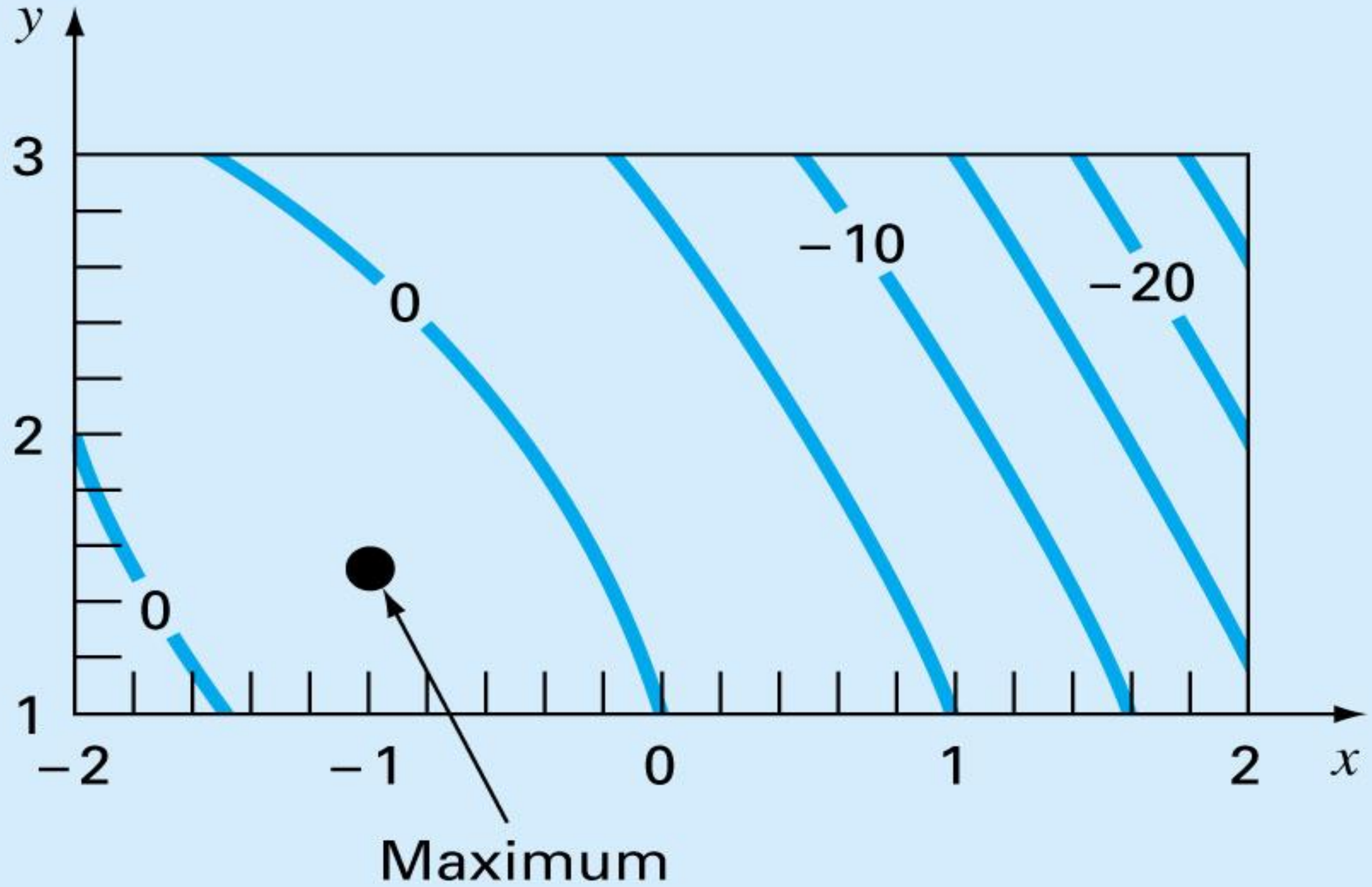
DIRECT METHODS
Random Search

- Based on evaluation of the function randomly at selected values of the independent variables.
- If a sufficient number of samples are conducted, the optimum will be eventually located.
- Example: maximum of a function

$$f(x, y) = y - x - 2x^2 - 2xy - y^2$$

can be found using a random number generator.

Figure 14.2



Advantages/

- Works even for discontinuous and nondifferentiable functions.
- Always finds the global optimum rather than the global minimum.

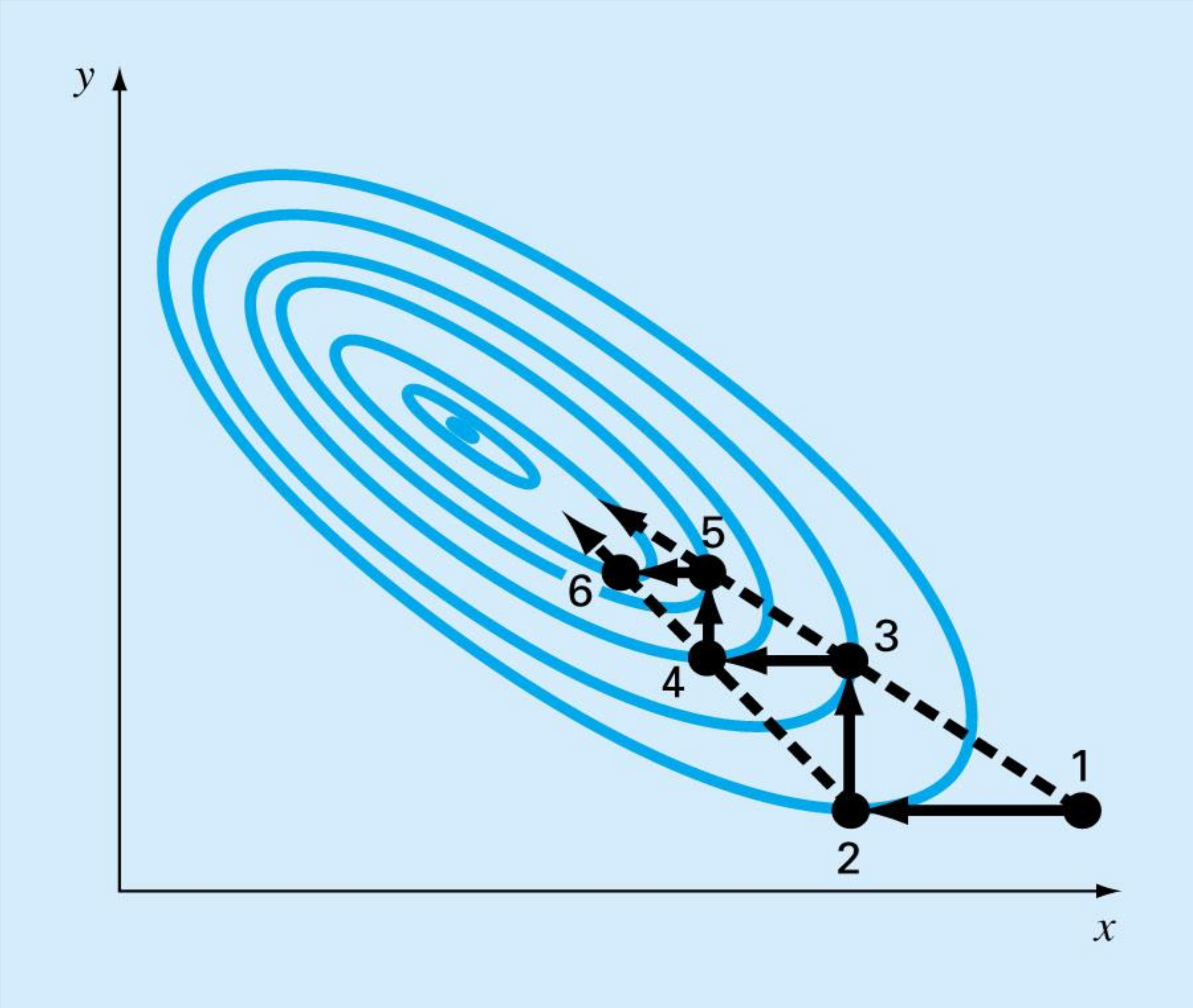
Disadvantages/

- As the number of independent variables grows, the task can become onerous.
- Not efficient, it does not account for the behavior of underlying function.

Univariate and Pattern Searches

- More efficient than random search and still doesn’t require derivative evaluation.
- The basic strategy is:
  - Change one variable at a time while the other variables are held constant.
  - Thus problem is reduced to a sequence of one-dimensional searches that can be solved by variety of methods.
  - The search becomes less efficient as you approach the maximum.

Figure 14.3



- *Pattern directions* can be used to shoot directly along the ridge towards maximum.

Figure 14.4

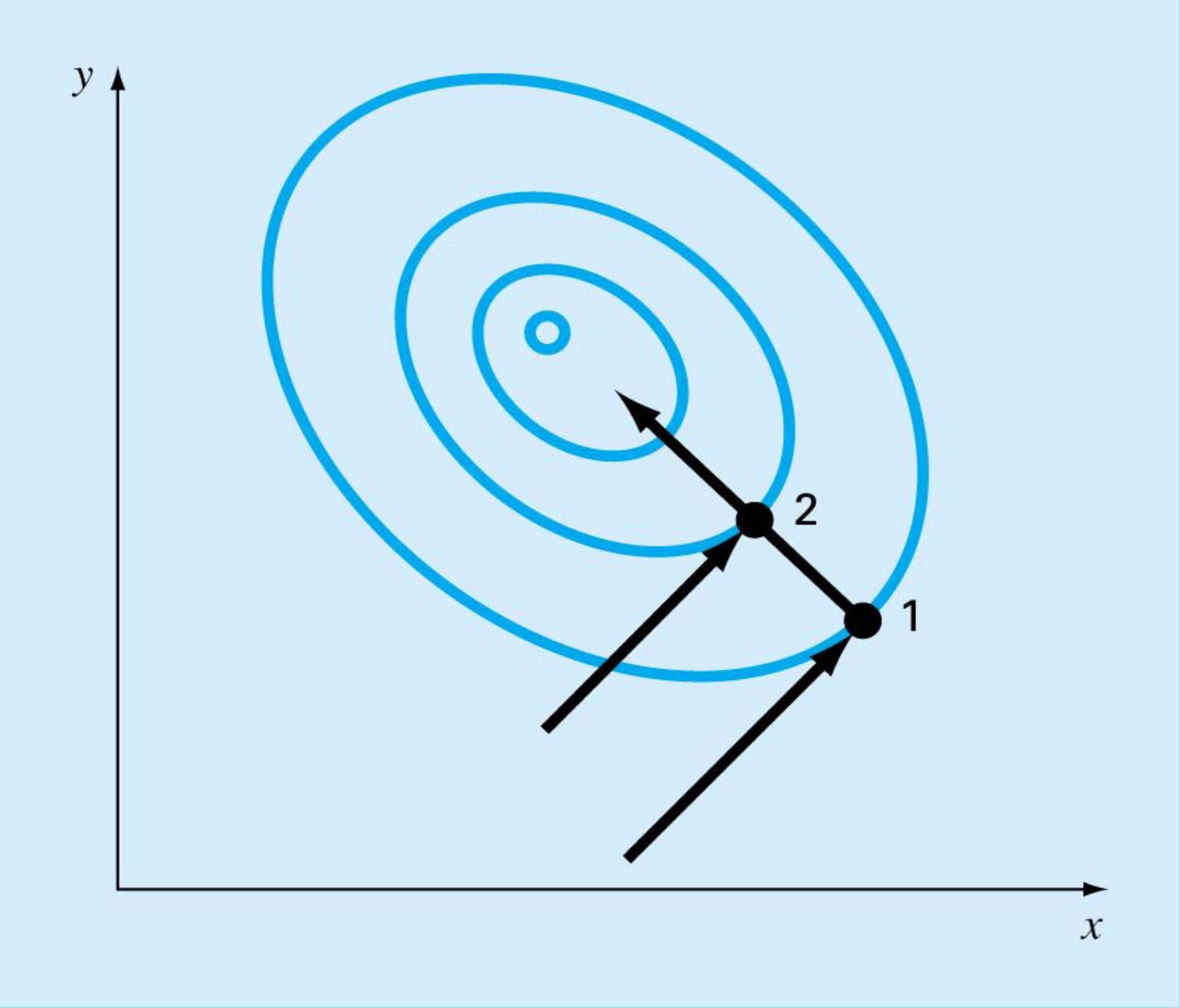
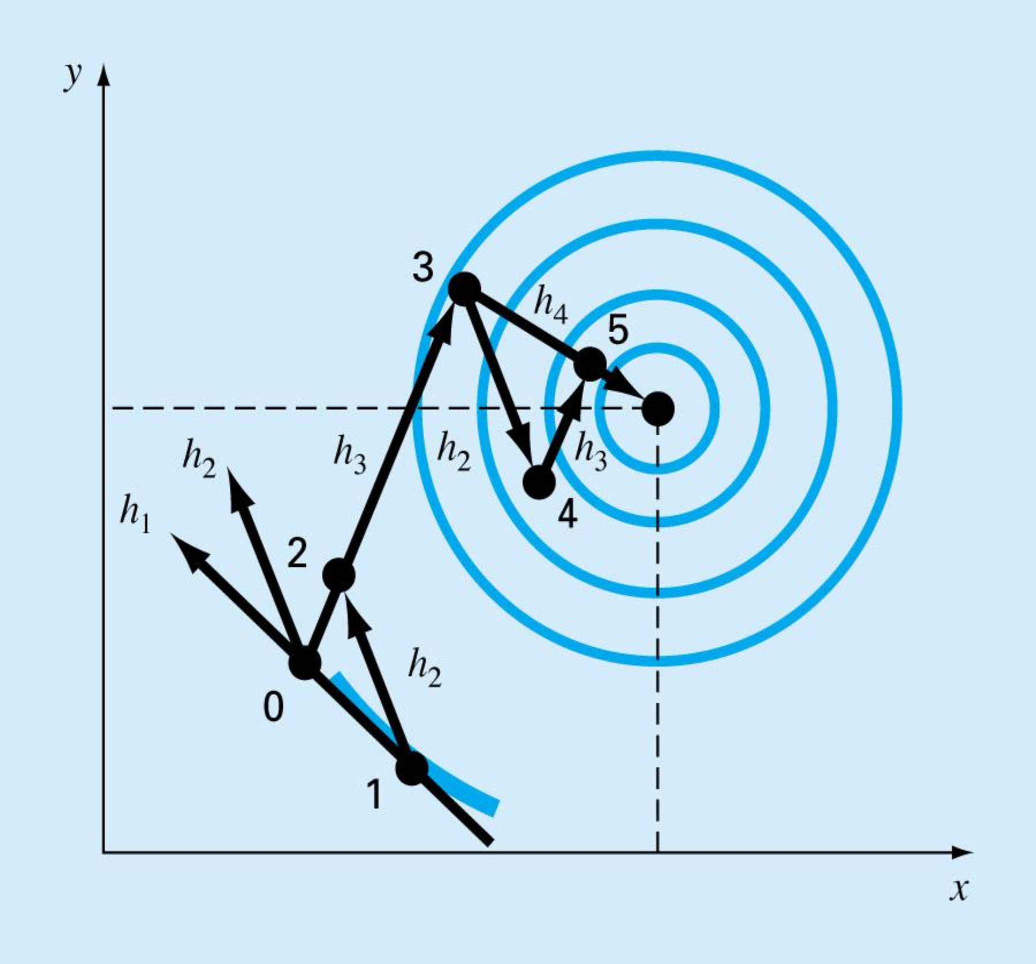


Figure 14.5

- Best known algorithm, *Powell's method*, is based on the observation that if points 1 and 2 are obtained by one-dimensional searches in the same direction but from different starting points, then, the line formed by 1 and 2 will be directed toward the maximum. Such lines are called *conjugate directions*.



GRADIENT METHODS
Gradients and Hessians

The Gradient/

- If *f(x,y)* is a two dimensional function, the *gradient* vector tells us
  - What direction is the steepest ascend?
  - How much we will gain by taking that step?

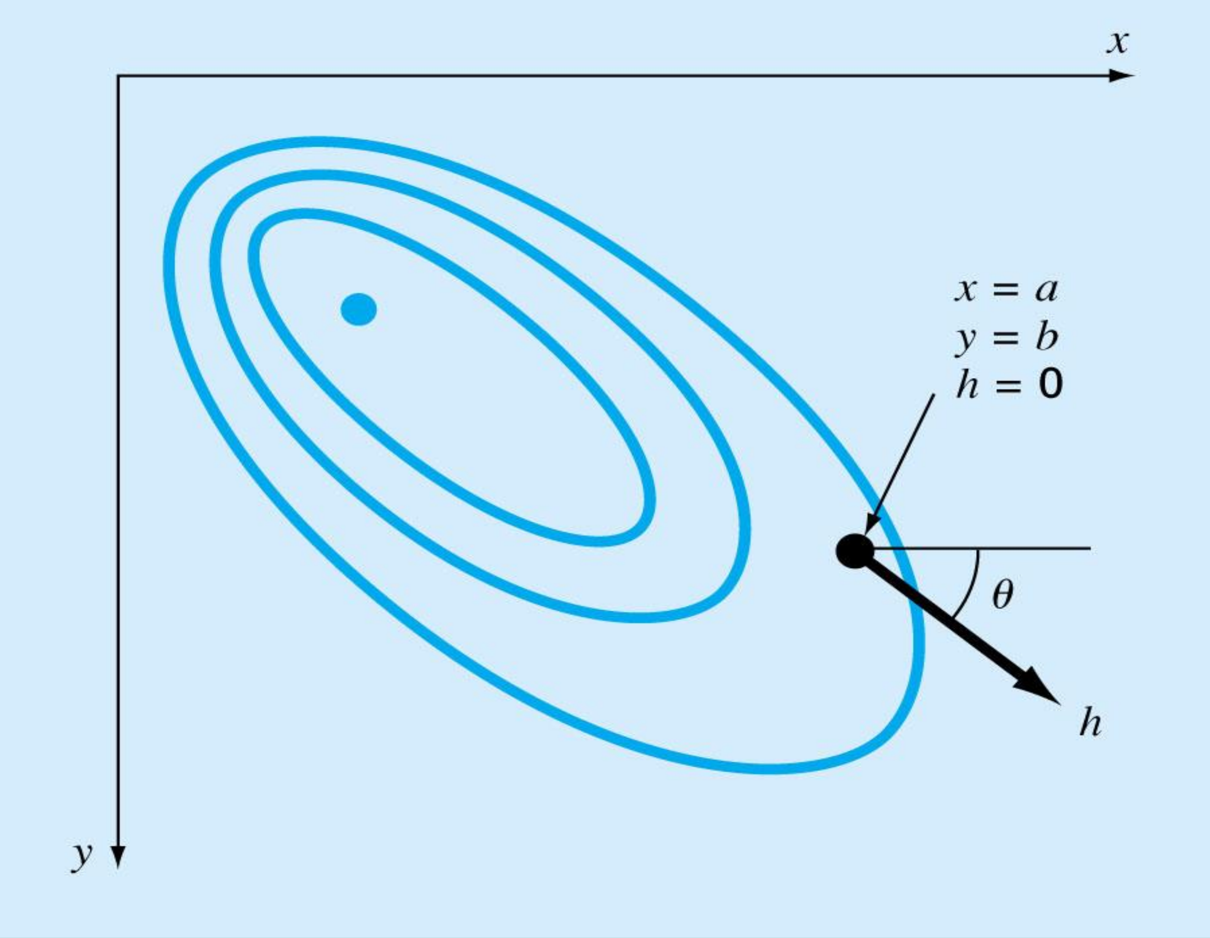
$$\nabla f = \frac{\partial f}{\partial x}\mathrm{i} + \frac{\partial f}{\partial y}\mathrm{j} \qquad \text{or } del\ f$$

Directional derivative of *f(x,y)* at point x=a and **y=b**

Figure 14.6

- For n dimensions

$$\nabla f(x) = \begin{Bmatrix} \dfrac{\partial f}{\partial x_1}(\mathrm{x}) \\ \dfrac{\partial f}{\partial x_2}(\mathrm{x}) \\ \vdots \\ \dfrac{\partial f}{\partial x_n}(\mathrm{x}) \end{Bmatrix}$$



The Hessian/

- For one dimensional functions both first and second derivatives valuable information for searching out optima.
  - First derivative provides (a) the steepest trajectory of the function and (b) tells us that we have reached the maximum.
  - Second derivative tells us that whether we are a maximum or minimum.
- For two dimensional functions whether a maximum or a minimum occurs involves not only the partial derivatives w.r.t. x and y but also the second partials w.r.t. x and y.

Figure 14.7

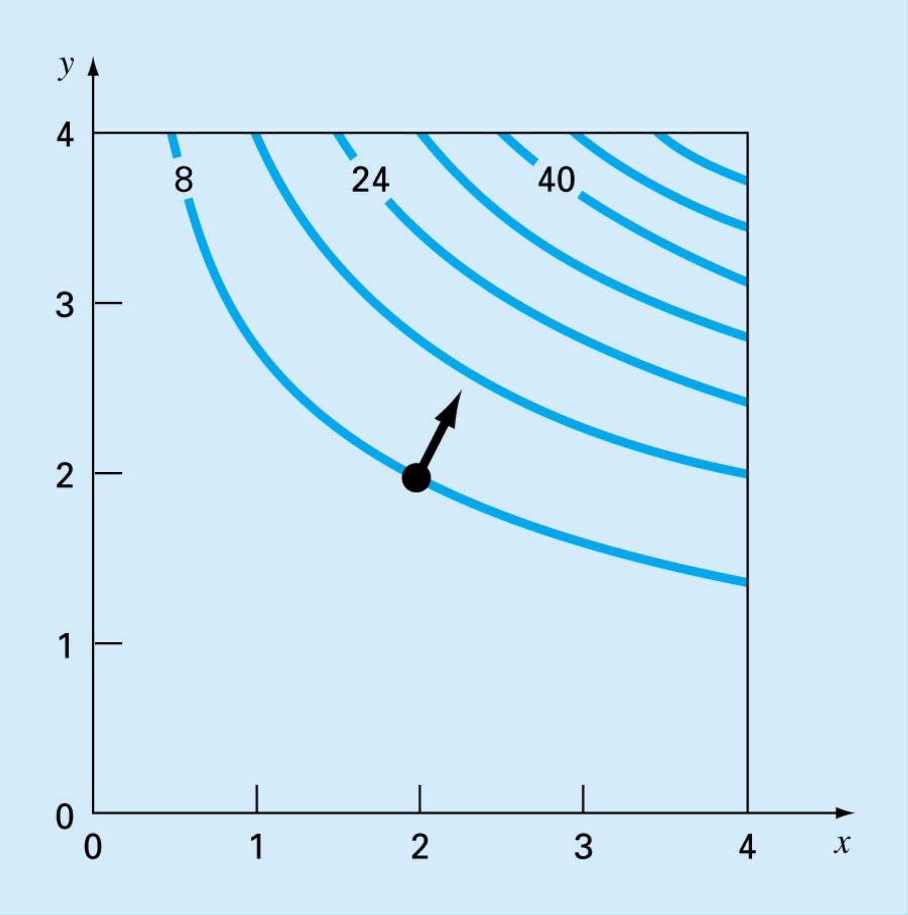
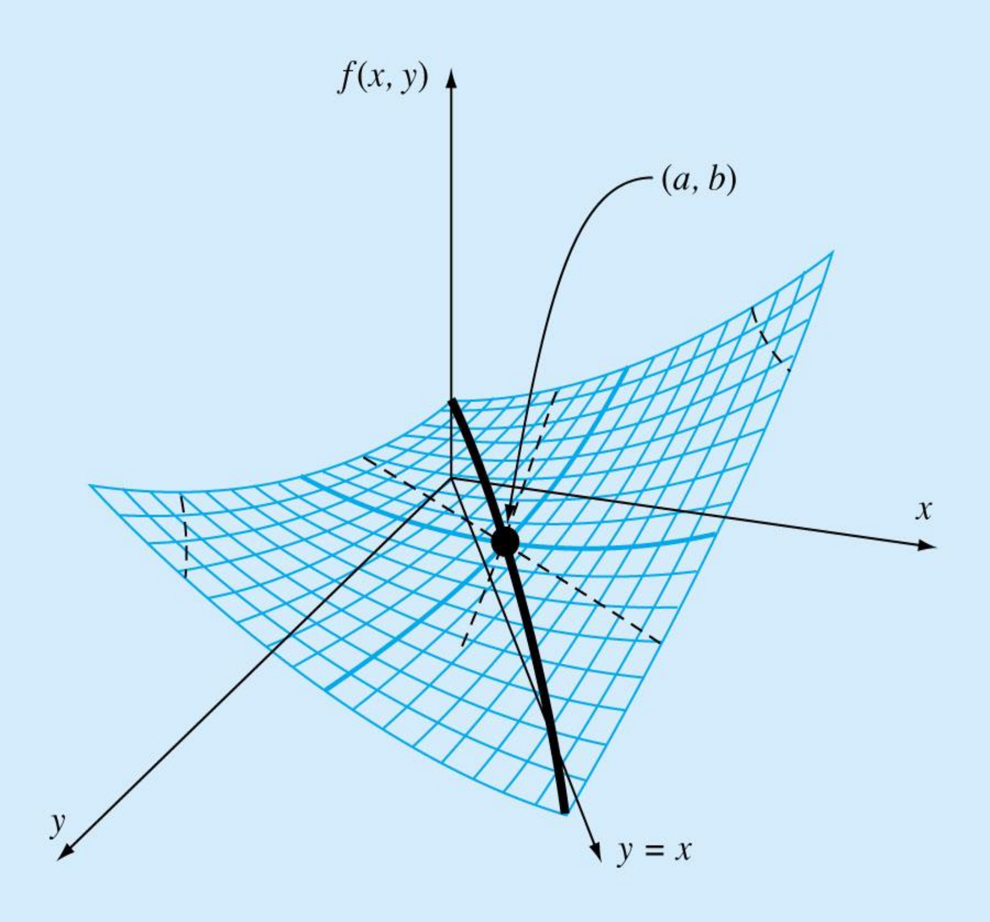


Figure 14.8



- Assuming that the partial derivatives are continuous at and near the point being evaluated

$$\left|H\right| = \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$$

$$\text{If } \left|\text{H}\right| \succ 0 \text{ and } \frac{\partial^2 f}{\partial x^2} \succ 0\text{, then f(x, y) has a local minimum}$$

$$\text{If } \left|\text{H}\right| \succ 0 \text{ and } \frac{\partial^2 f}{\partial x^2} \prec 0\text{, then f(x, y) has a local minimum}$$

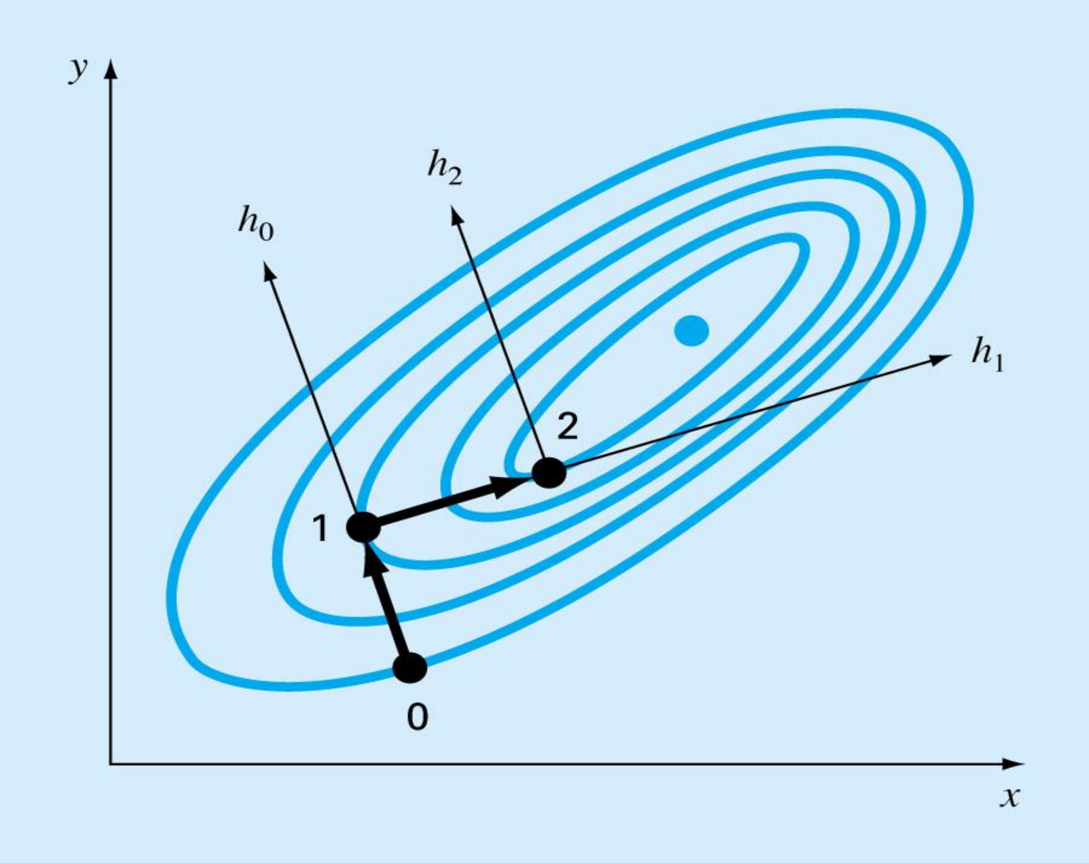
$$\text{If } \left|\text{H}\right| \prec 0\text{, then f(x, y) has a saddle point}$$

The quantity [H] is equal to the determinant of a matrix made up of second derivatives

The Steepest Ascend Method

- Start at an initial point (x_o,y_o), determine the direction of steepest ascend, that is, the gradient. Then search along the direction of the gradient, h_o, until we find maximum. Process is then repeated.

Figure 14.9



- The problem has two parts
  - Determining the "best direction" and
  - Determining the "best value" along that search direction.
- Steepest ascent method uses the gradient approach as its choice for the "best" direction.
- To transform a function of *x* and *y* into a function of *h* along the gradient section:

$$x = x_o + \frac{\partial f}{\partial x} h$$

$$y = y_o + \frac{\partial f}{\partial y} h$$

h is distance along the h axis

Figure 14.10

- If $x_o=1$ and $y_o=2$

$$\nabla f = 3i + 4j$$

$$x = 1 + 3h$$

$$y = 2 + 4h$$