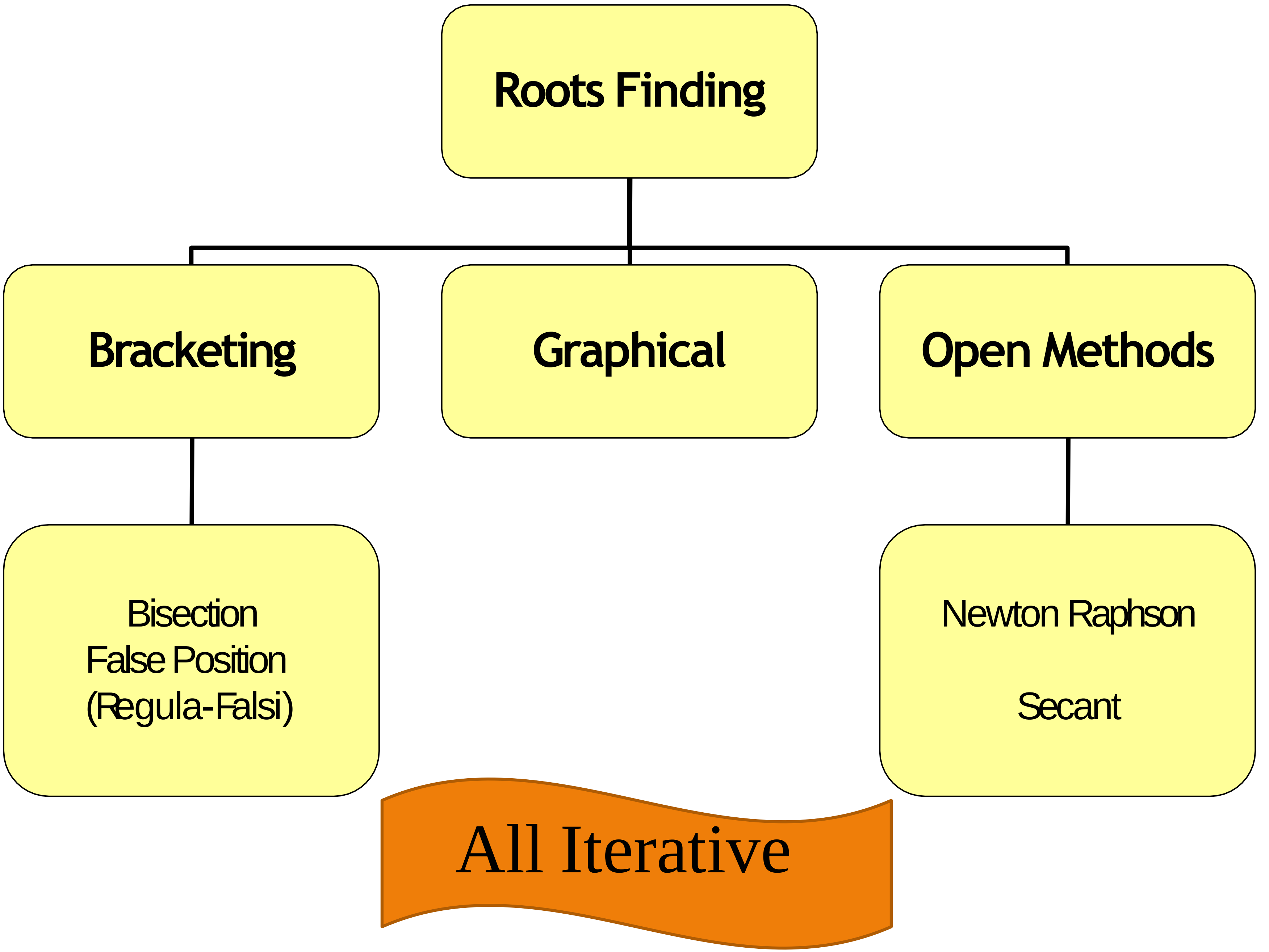
FUNDAMENTAL MATHEMATICS FOR ROBOTICS

Numerical Methods

Arbtip Dheeravongkit

Roots of Equations


Roots Finding
Bracketing
Graphical
Open Methods
Bisection
False Position
(Regula-Falsi)
Newton Raphson
Secant
All Iterative

Root Finding

Open Methods

Simple Fixed-Pointed Iteration

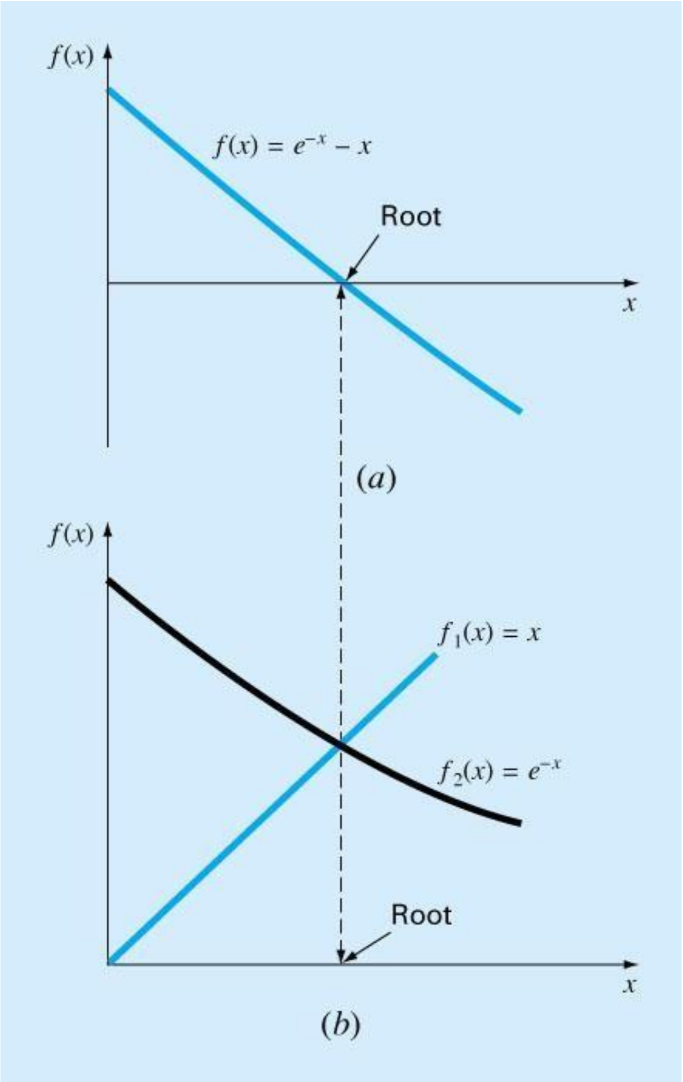
- Rearrange the function so that x is on the left-hand side of the equation

$$x = g(x)$$

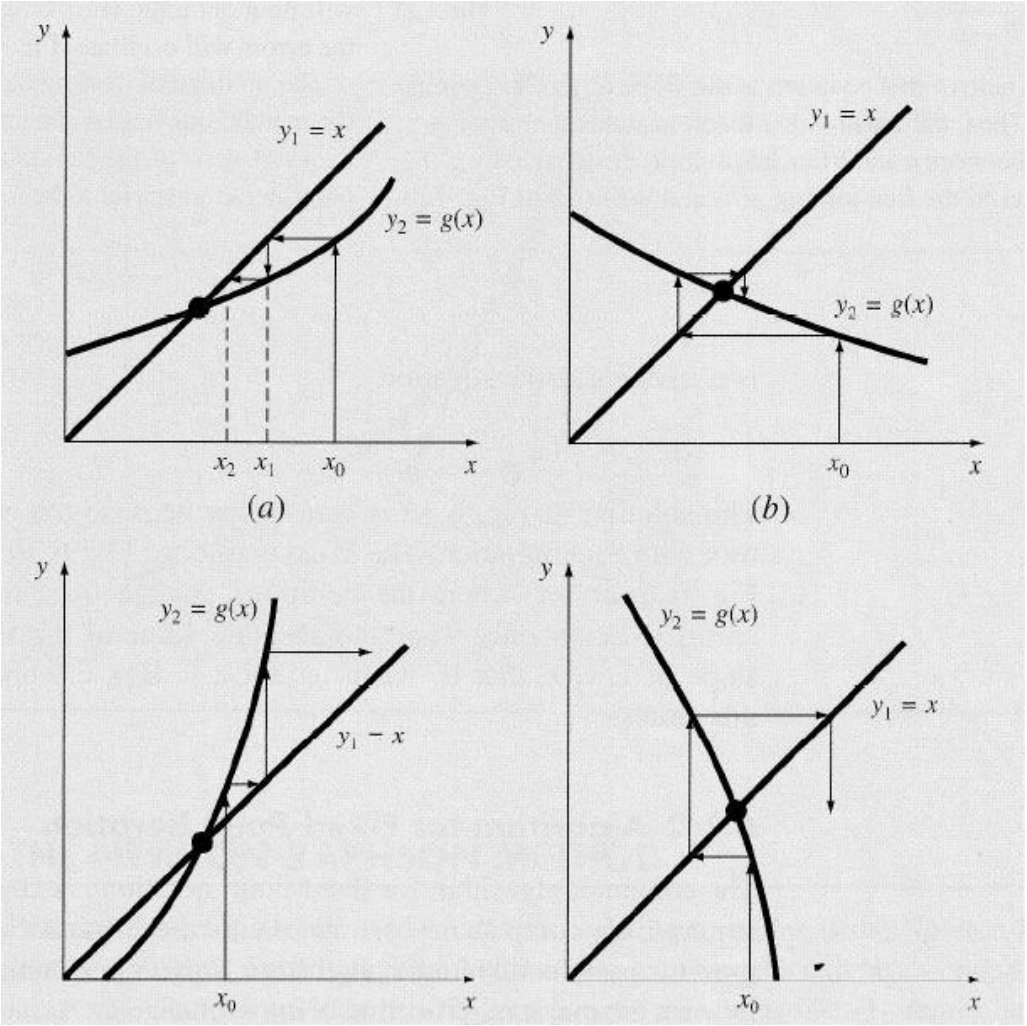
- Example
  - $x^2 - 2x + 3 = 0$
  - $\sin(x) = 0$
- Predict new value of x as a function of old value of x
  - $x_{i+1} = g(x_i)$
- While bracketing methods are "convergent", Fixed-point method may sometimes "diverge".
  - Depends on the initial guess and how the function behaves

Simple Fixed-Point Iteration Convergence

- x=g(x) can be expressed as a pair of equations:
  - y1=x
  - y2=g(x) (component equations)
- Plot them separately.



Simple Fixed-Point Iteration Convergence



Converge when $|g'(x)| < 1$ OR when the slope of g(x) is less than the slope of the line f(x)=x

Simple Fixed-Point Iteration

- Proof

If converge, the error is roughly proportional to and less than the error of the previous step

Newton-Raphson Method

- The most widely used method
- Based on Taylor series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + f''(x_i)\frac{\Delta x^2}{2!} + O\Delta x^3$$

The root is the value of x_{i+1} when $f(x_{i+1}) = 0$

Rearranging,

Solve for

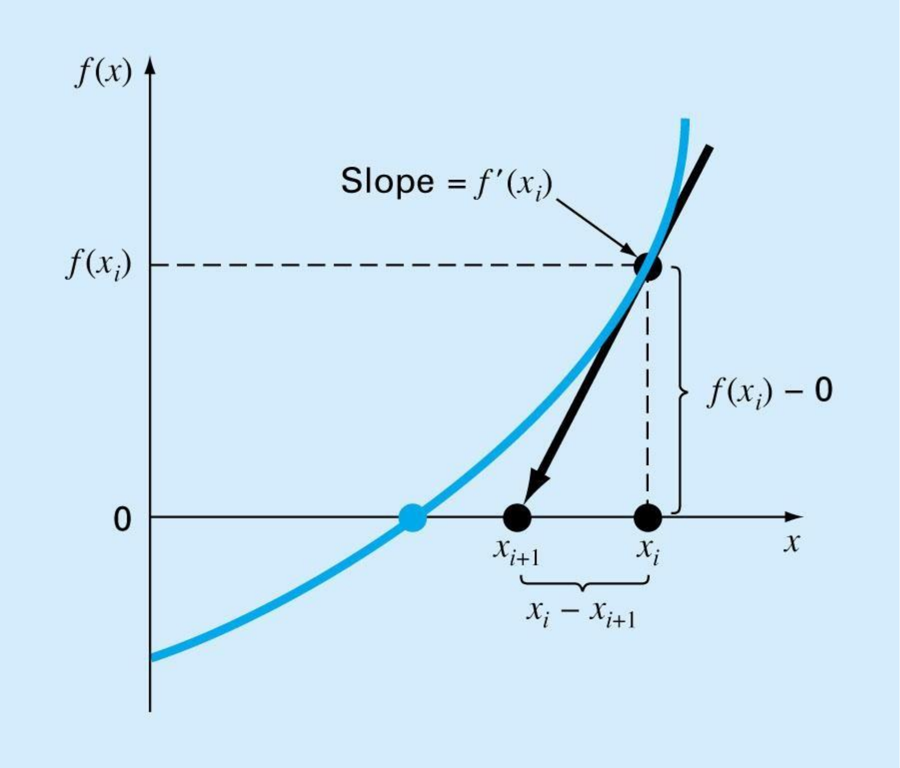
$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

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

Newton-Raphson formula

Newton-Raphson Method

- A convenient method for functions whose derivatives can be evaluated analytically.
- It may not be convenient for functions whose derivatives cannot be evaluated analytically.



Newton-Raphson Method

- Example
  Estimate the root of $f(x) = e^{-x} - x$
  Initial guess $x_0 = 0$

i	x_i	ε_t (%)
0	0	100
1	0.500000000	11.8
2	0.566311003	0.147
3	0.567143165	0.0000220
4	0.567143290	$< 10^{-8}$

Newton-Raphson Method

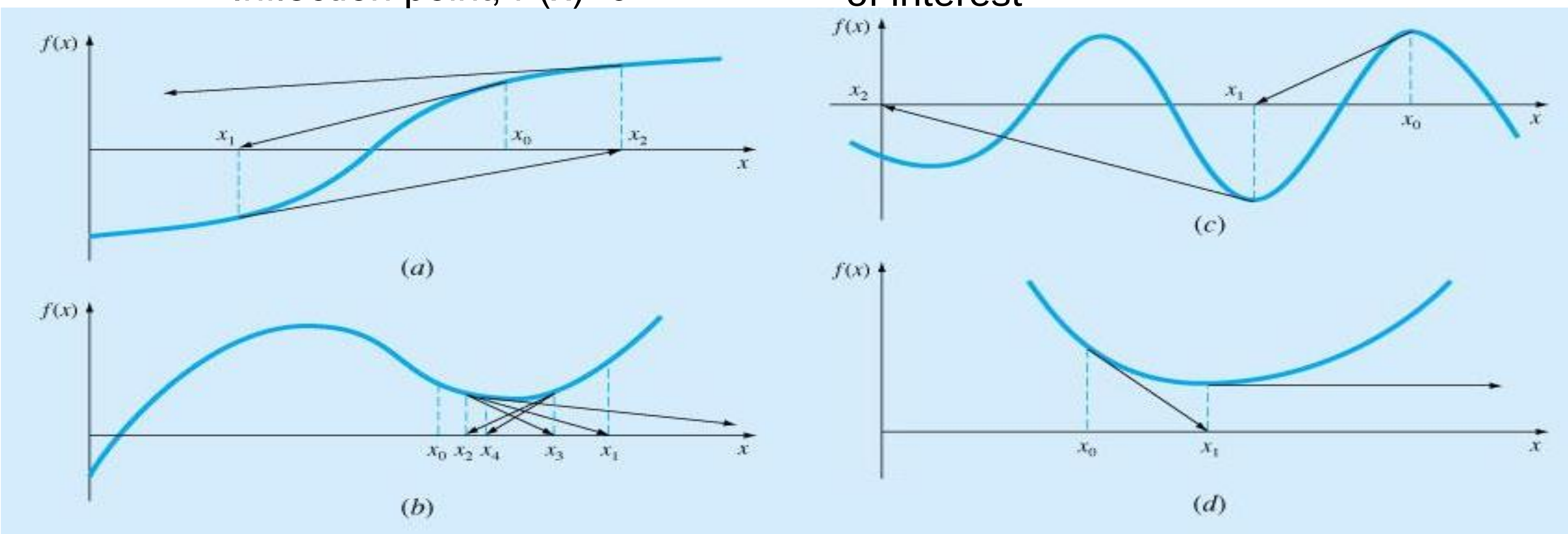
- Proof: Quadratic convergence $E_{t,i+1} \cong \dfrac{-f''(x_r)}{2f'(x_r)} E_{t,i}^2$

Newton-Raphson Method Convergence

- Pitfalls of NR

Inflection point, f“(x)=0

Near zero slope → move away from area of interest



Oscillate around local minimum or maximum

Zero slope → Truly a disaster

Newton-Raphson Method Convergence

- Convergence depends on the accuracy of the initial guess
- Take an initial guess that is “sufficiently” close to the root
- For some function, no guess will work!
  - Good computer program should be able to recognize slow convergence or divergence
    - A plotting routine should be included
    - At the end of computation, substitute the final estimated root to the original function to see whether the result is close to zero (Oscillating convergence)
    - Include an upper limit on the number of iterations
    - Alert user and take account of the possibility that $f'(x)$ might equal to zero

The Secant Method

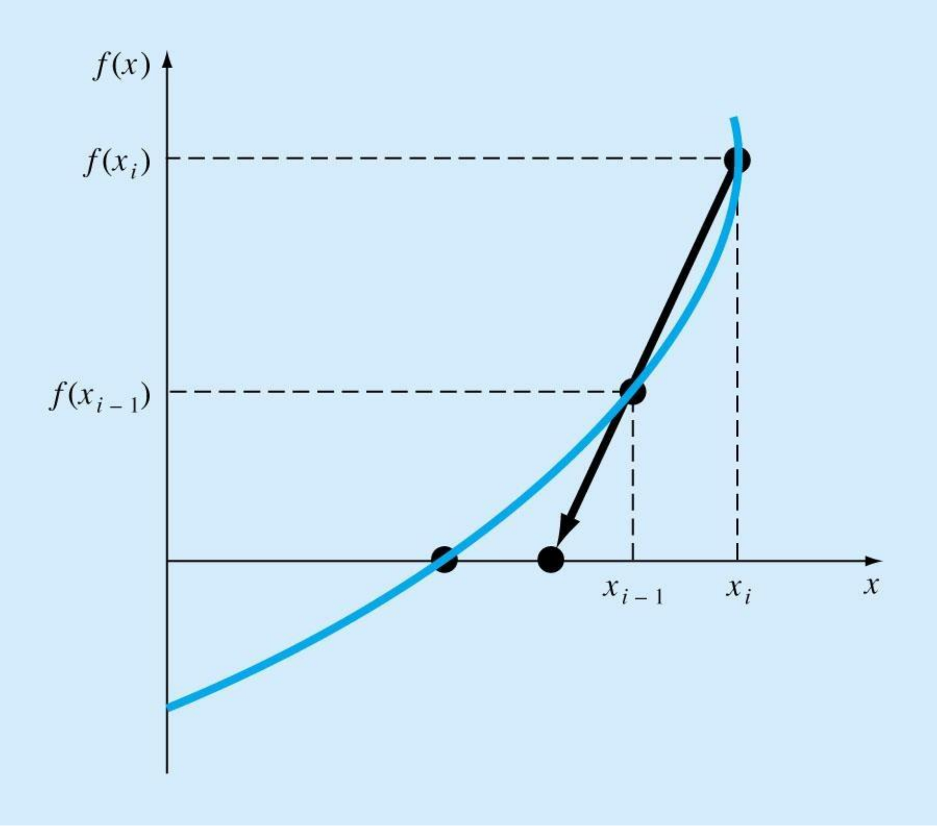
- Useful for functions whose derivatives are difficult to evaluate
- Approximate derivative by a backward finite divided difference

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

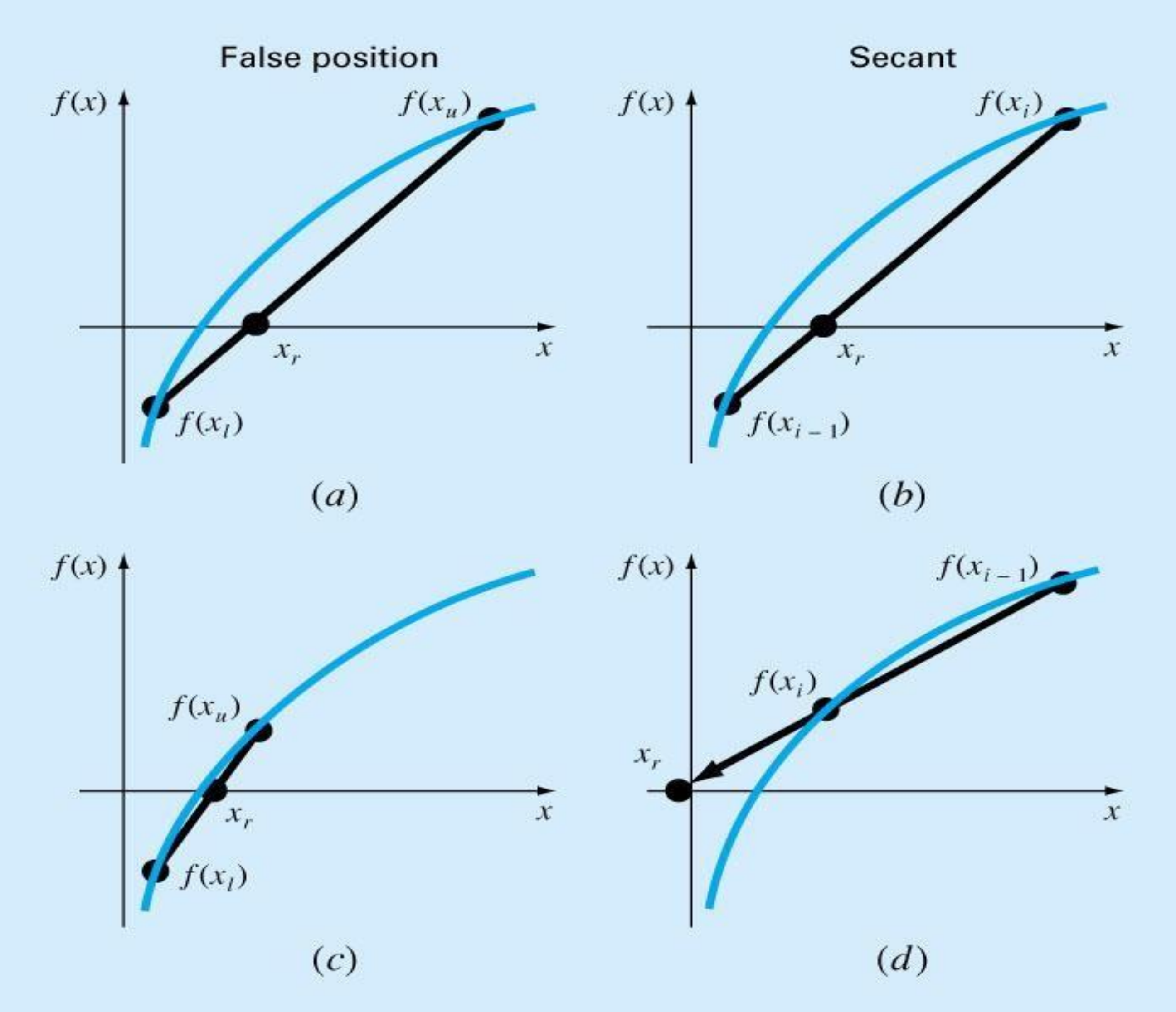
$$x_{i+1} = x_i - f(x_i)\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \qquad i = 1,2,3,\ldots$$

The Secant Method

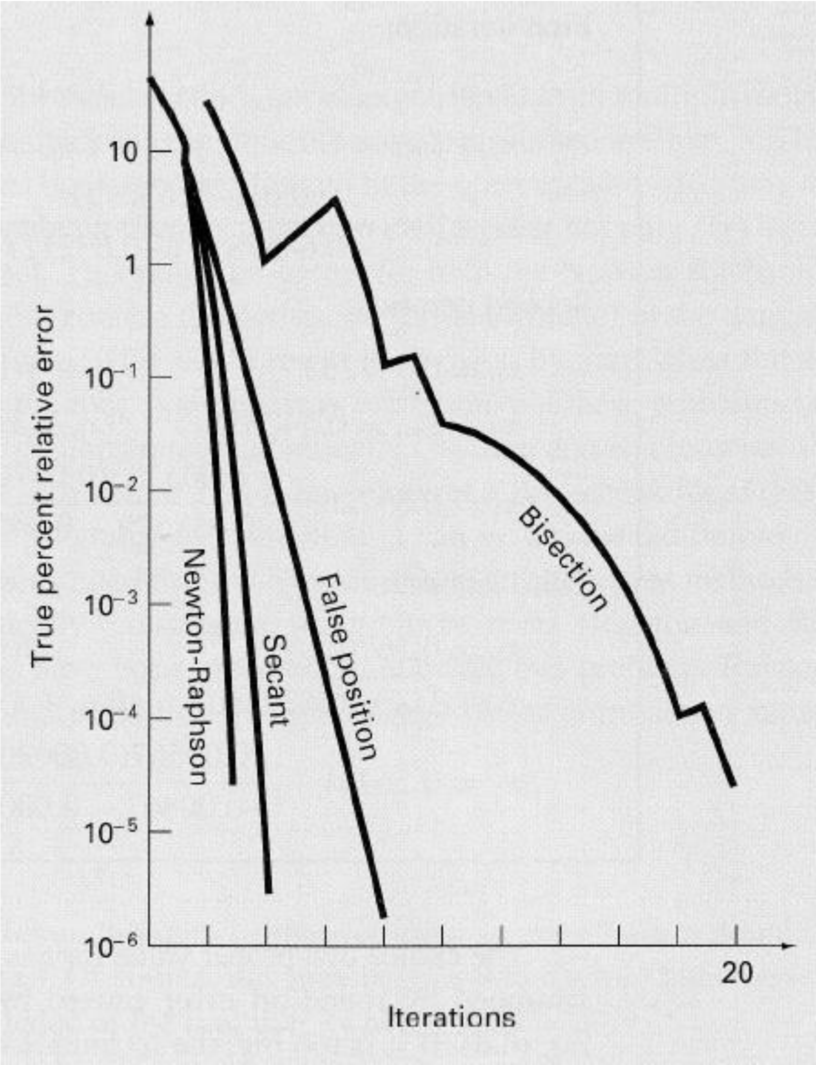
- Requires two initial estimates of x , e.g, x_o, x_1. However, because f(x) is not required to change signs between estimates, it is not classified as a "bracketing" method.
- Convergence is not guaranteed.



The Secant Method VS False-Position

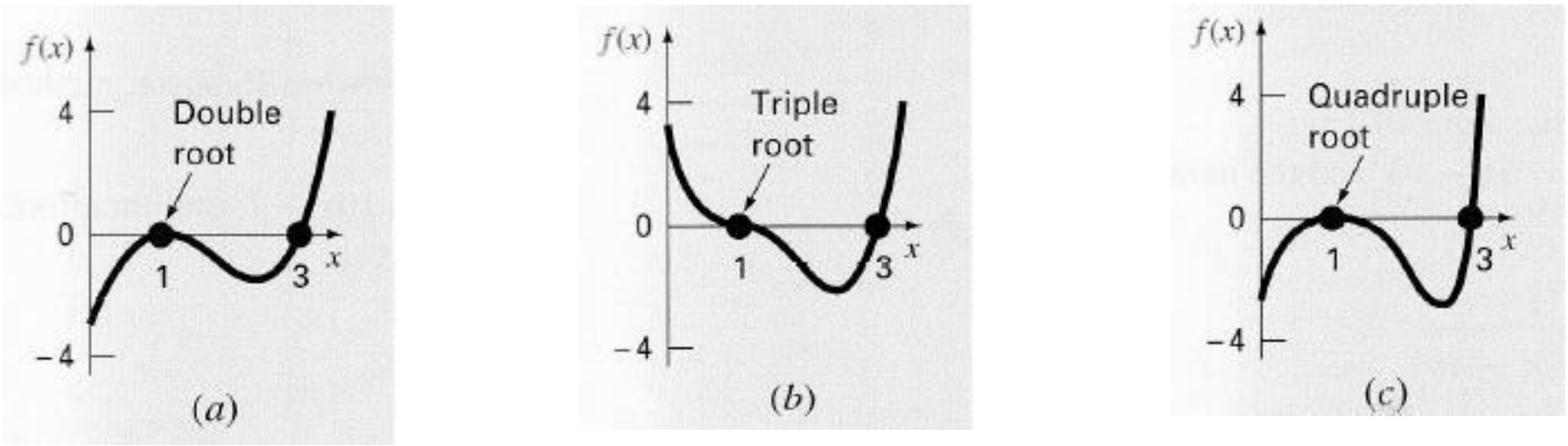


The Secant Method
Comparing true percent relative error



Determine the roots of $f(x)=e^{-x}-x$

Multiple Roots



- Odd multiple roots cross the axis, whereas even ones do not

Multiple Roots

- For even multiple roots, function does not change sign
  - Cannot use bracketing methods
  - Can only use open methods that may diverge
- f'(x) goes to zero at the root
  - Division by zero problem for Newton-Raphson and secant methods
  - f(x) will always reach zero before f'(x) (Ralston and Rabinowitz, 1978) → incorporate zero check for f(x) in computer program
- NR and secant methods are linearly convergent for multiple roots
  - Modified Newton-Raphson for quadratic convergence

$$u(x) = \frac{f(x)}{f'(x)} \qquad u'(x) = \frac{f'(x)f'(x) - f(x)f''(x)}{[f'(x)]^2}$$

$$x_{i+1} = x_i - \frac{u(x_i)}{u'(x_i)} \qquad x_{i+1} = x_i - \frac{f(x_i)f'(x_i)}{[f'(x_i)]^2 - f(x_i)f''(x_i)}$$

Multiple Roots

- Example

$$f(x) = (x-3)(x-1)^2 = x^3 - 5x^2 + 7x - 3$$

$$f'(x_i) = 3x^2 - 10x + 7$$

$$x_{i+1} = x_i - \frac{x_i^3 - 5x_i^2 + 7x_i - 3}{3x_i^2 - 10x_i + 7}$$

which can be solved iteratively for

i	x_i	ε_t (%)
0	0	100
1	0.4285714	57
2	0.6857143	31
3	0.8328654	17
4	0.9133290	8.7
5	0.9557833	4.4
6	0.9776551	2.2

$$x_{i+1} = x_i - \frac{(x_i^3 - 5x_i^2 + 7x_i - 3)(3x_i^2 - 10x_i + 7)}{(3x_i^2 - 10x_i + 7)^2 - (x_i^3 - 5x_i^2 + 7x_i - 3)(6x_i - 10)}$$

which can be solved for

i	x_i	ε_t (%)
0	0	100
1	1.105263	11
2	1.003082	0.31
3	1.000002	0.00024

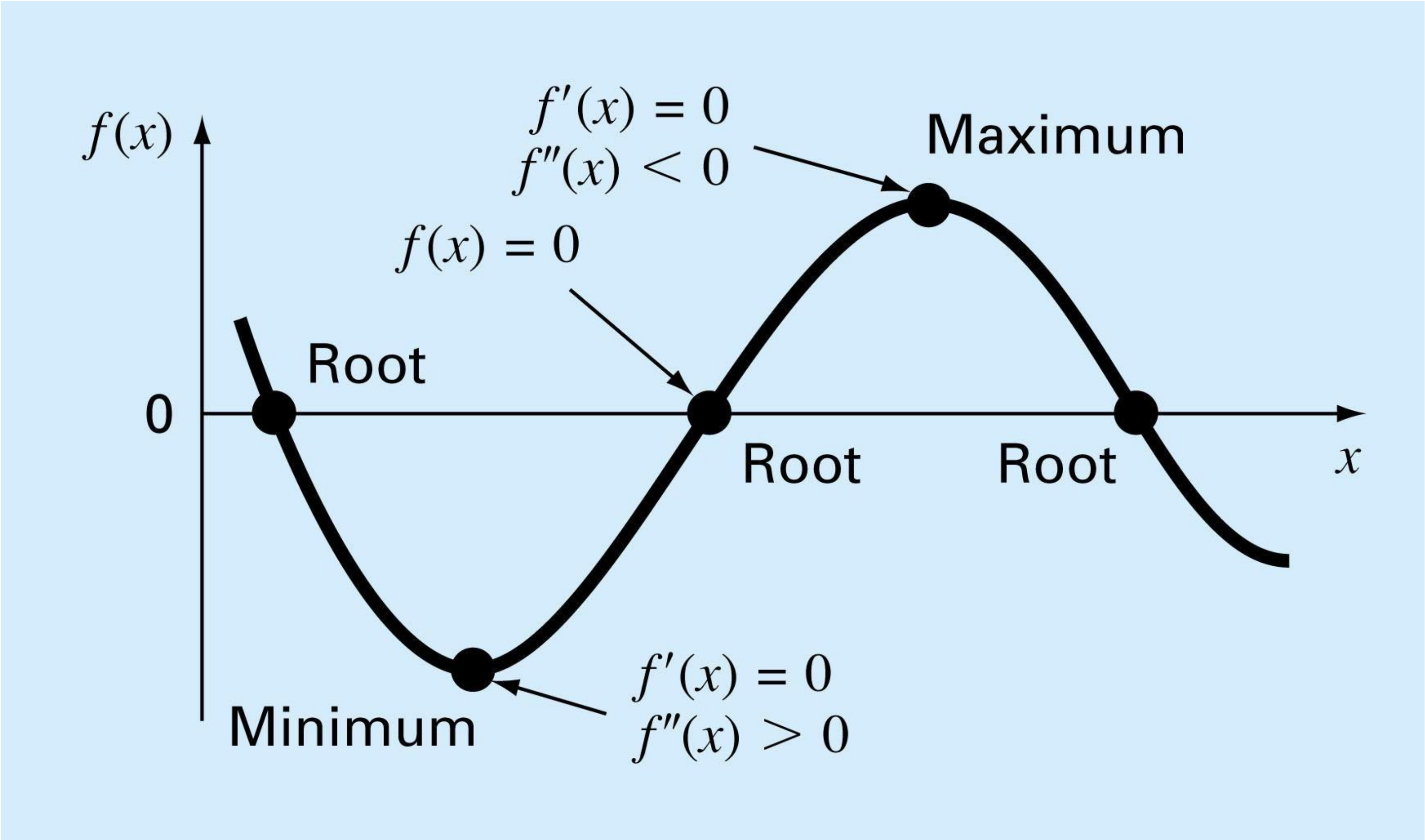
i	Standard	ε_t (%)	Modified	ε_t (%)
0	4	33	4	33
1	3.4	13	2.636364	12
2	3.1	3.3	2.820225	6.0
3	3.008696	0.29	2.961728	1.3
4	3.000075	0.0025	2.998479	0.051
5	3.000000	2×10^{-7}	2.999998	7.7×10^{-5}

Optimization

Optimization

- 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.

Optimization



Mathematical Background

- An optimization or mathematical programming problem generally be stated as:
  Find x, which minimizes or maximizes f(x) subject to

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

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

  - 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
  - a_i and b_i are constants

Optimization

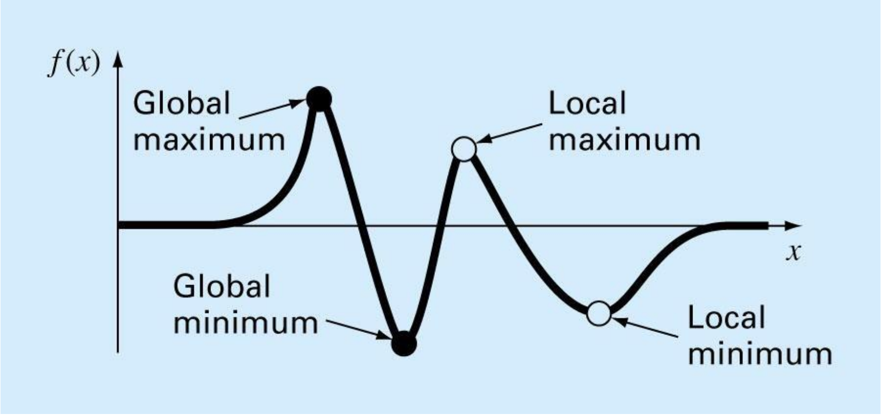
- Optimization problems can be classified on the basis of the form of f(x):
  - If f(x) and the constraints are linear, we have linear programming.
  - If f(x) is nonlinear or quadratic and/or the constraints are nonlinear, we have nonlinear programming.
- When equations(*) are included, we have a constrained optimization problem; otherwise, it is unconstrained optimization problem.

Optimization

One-Dimensional Unconstrained

One-Dimensional Unconstrained Optimization

- 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.

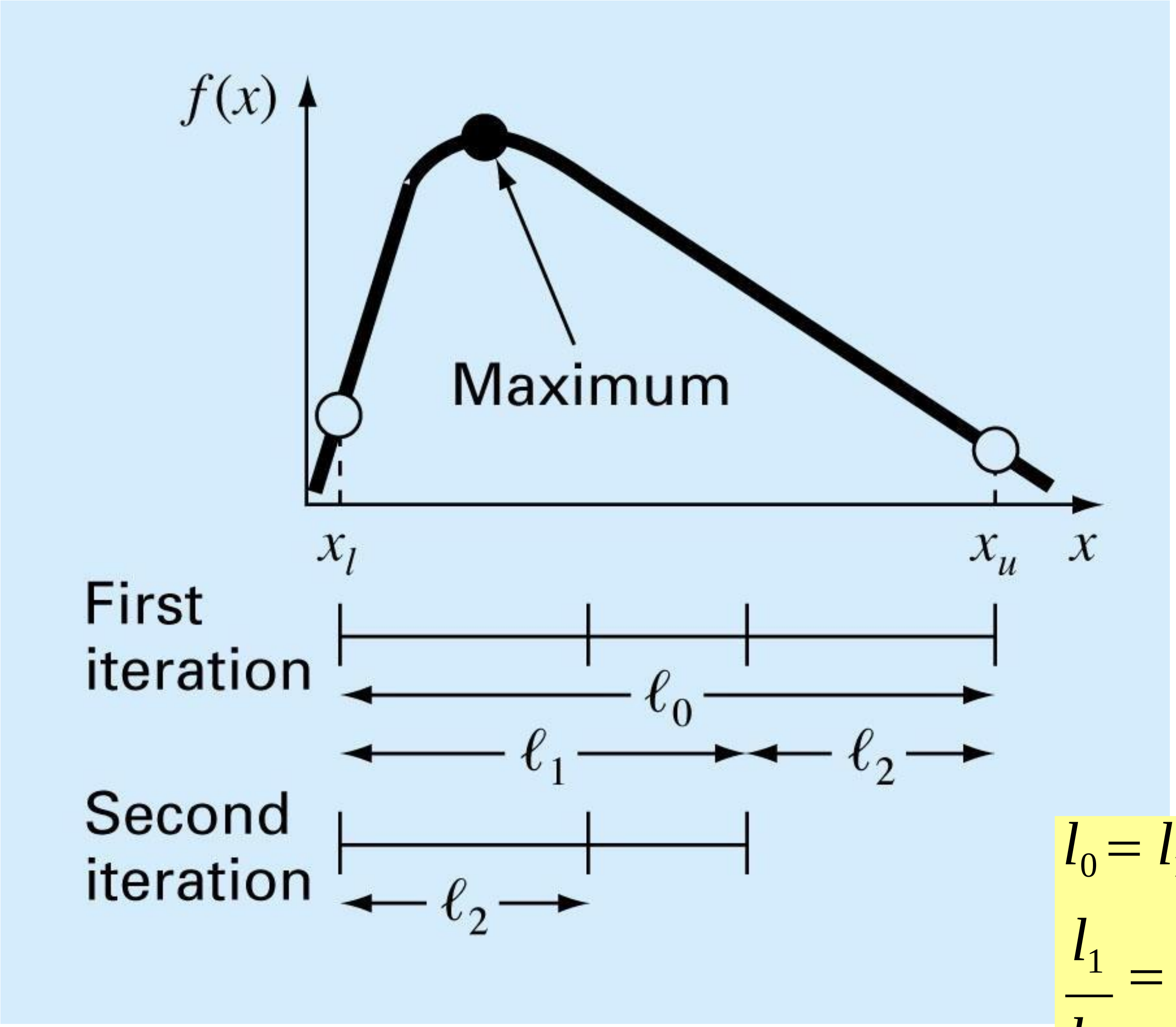


Global and Local Optimums

- How do we distinguish global and local optimums?
  - 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.



$$l_0 = l_1 + l_2$$

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

Golden-Section Search

$$l_0 = l_1 + l_2$$

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

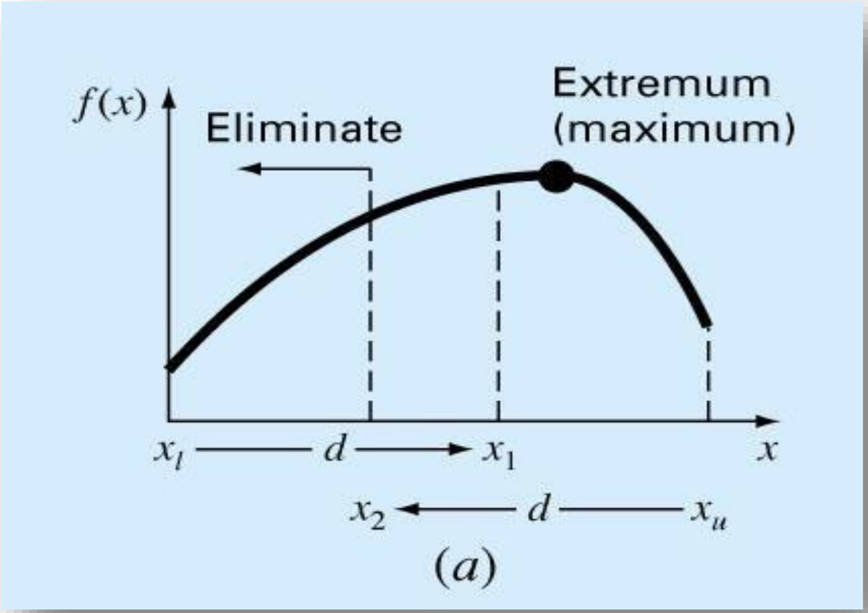
$$\frac{l_1}{l_1 + l_2} = \frac{l_2}{l_1} \qquad R = \frac{l_2}{l_1}$$

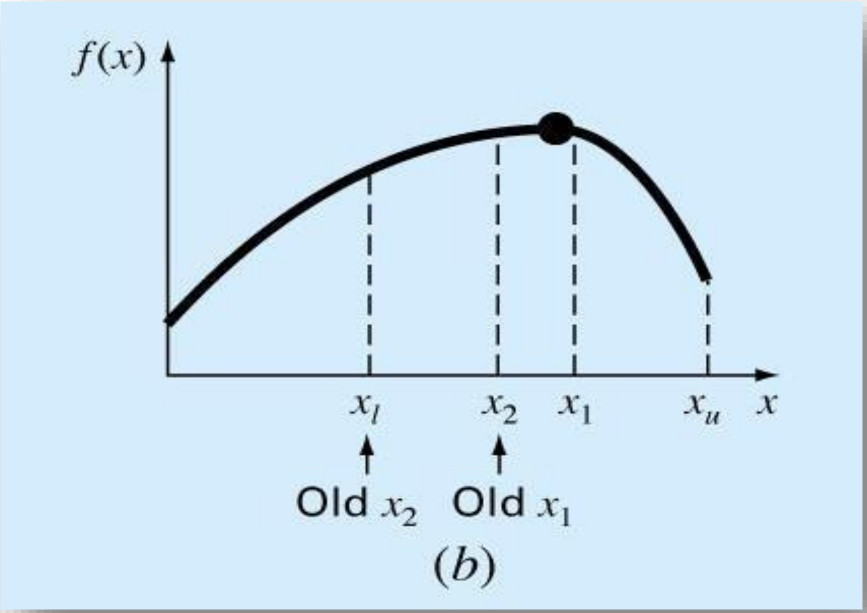
$$1 + R = \frac{1}{R} \qquad R^2 + R - 1 = 0$$

$$R = \frac{-1 + \sqrt{1 - 4(-1)}}{2} = \frac{\sqrt{5} - 1}{2} = 0.61803$$

Golden Ratio

Golden-Section Search





Golden-Section Search

- Bracketing Method
  - 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

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

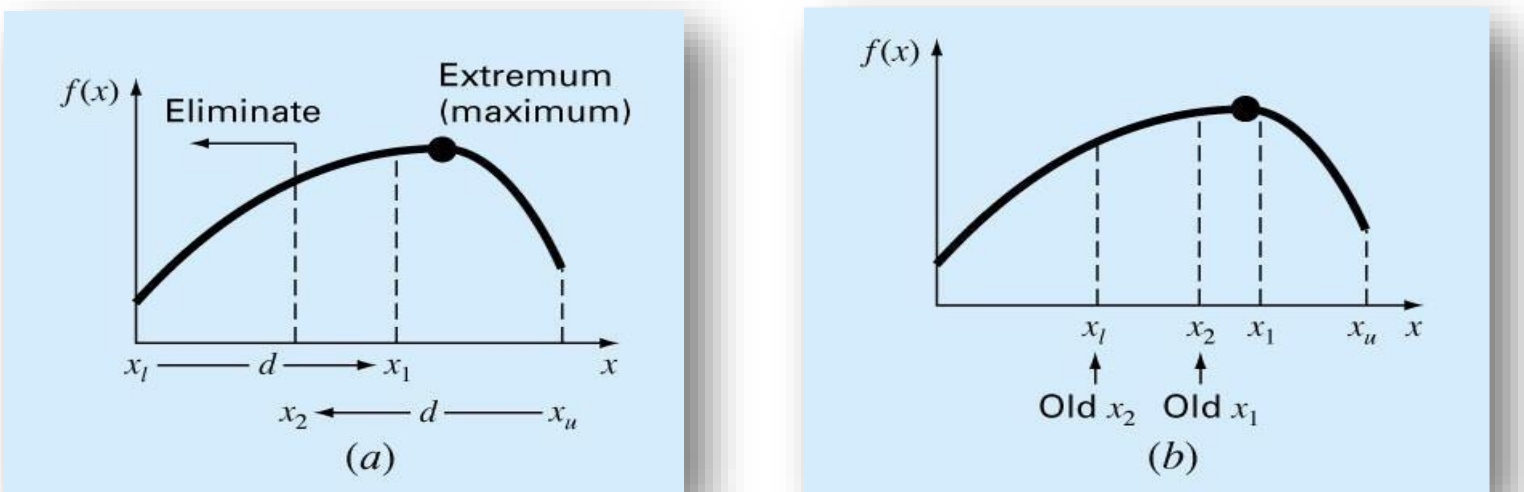
$$x_1 = x_l + d$$

$$x_2 = x_u - d$$

  - The function is evaluated at these two interior points

Golden-Section Search

- 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 x1 is determined as before



Golden-Section Search

- 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

Golden-Section Search

- Example

$$f(x) = 2\sin x - \frac{x^2}{10}, \; x_l = 0, \; x_u = 4$$

Golden-Section Search

i	x_l	$f(x_l)$	x_2	$f(x_2)$	x_1	$f(x_1)$	x_u	$f(x_u)$	d
1	0	0	1.5279	1.7647	2.4721	0.6300	4.0000	−3.1136	2.4721
2	0	0	0.9443	1.5310	1.5279	1.7647	2.4721	0.6300	1.5279
3	0.9443	1.5310	1.5279	1.7647	1.8885	1.5432	2.4721	0.6300	0.9443
4	0.9443	1.5310	1.3050	1.7595	1.5279	1.7647	1.8885	1.5432	0.5836
5	1.3050	1.7595	1.5279	1.7647	1.6656	1.7136	1.8885	1.5432	0.3607
6	1.3050	1.7595	1.4427	1.7755	1.5279	1.7647	1.6656	1.7136	0.2229
7	1.3050	1.7595	1.3901	1.7742	1.4427	1.7755	1.5279	1.7647	0.1378
8	1.3901	1.7742	1.4427	1.7755	1.4752	1.7732	1.5279	1.7647	0.0851

Newton's Method

- An open method
- Similar to Newton-Raphson Method
- Defining a new function g(x)=f'(x)
- Because the optimal value x* satisfies

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

  We can use the following formula to find the extremum of $f(x)$

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

- May be divergent

Newton's Method

- Example

$$f(x) = 2\sin x - \frac{x^2}{10},\ x_0 = 2.5$$

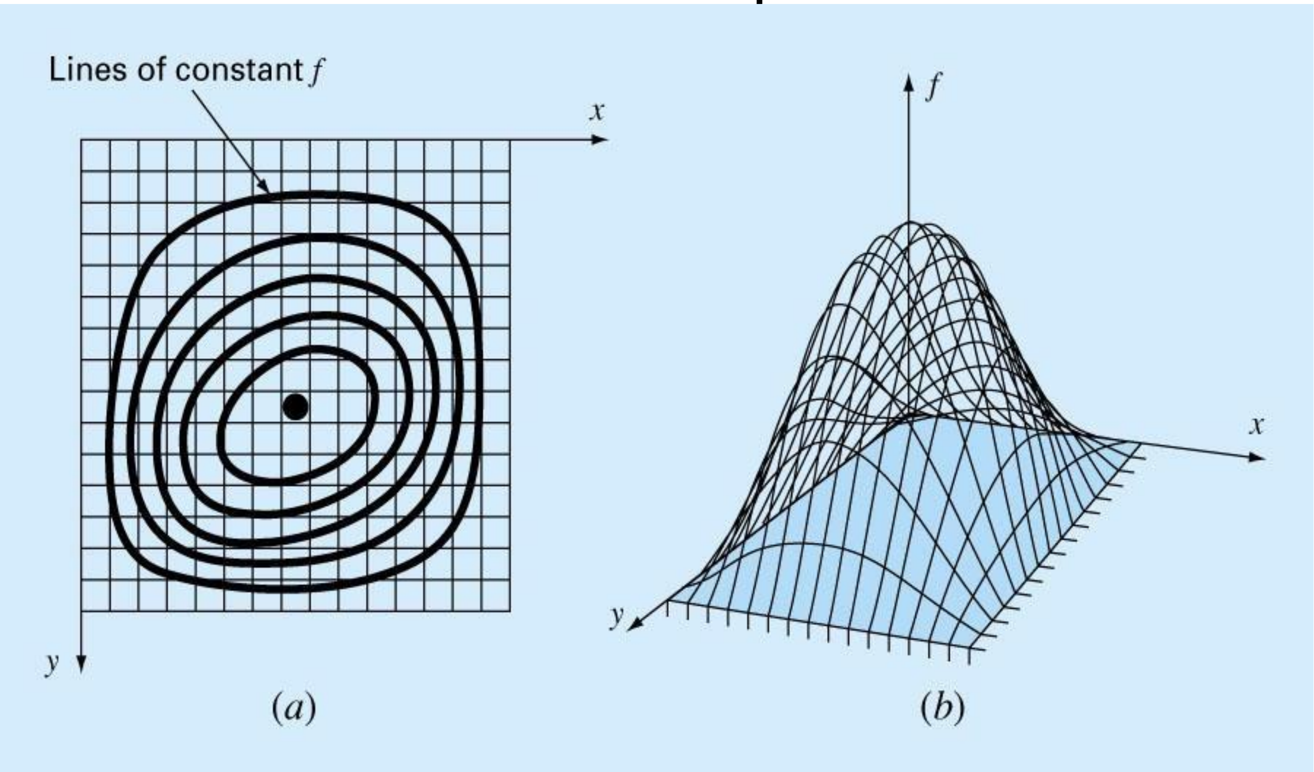
Newton's Method

i	x	$f(x)$	$f'(x)$	$f''(x)$
0	2.5	0.57194	−2.10229	−1.39694
1	0.99508	1.57859	0.88985	−1.87761
2	1.46901	1.77385	−0.09058	−2.18965
3	1.42764	1.77573	−0.00020	−2.17954
4	1.42755	1.77573	0.00000	−2.17952

Thus, within four iterations, the result converges rapidly on the true value.

Optimization

- One-dimensional Unconstrained Optimization
  - Golden-Section Search
  - Newton's Method
- Multidimensional Unconstrained Optimization



Optimization

Multidimensional Unconstrained

Multidimensional Unconstrained Optimization

- Techniques to find minimum and maximum of a function of several variables

- 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

Direct Methods: Random Searches

- 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

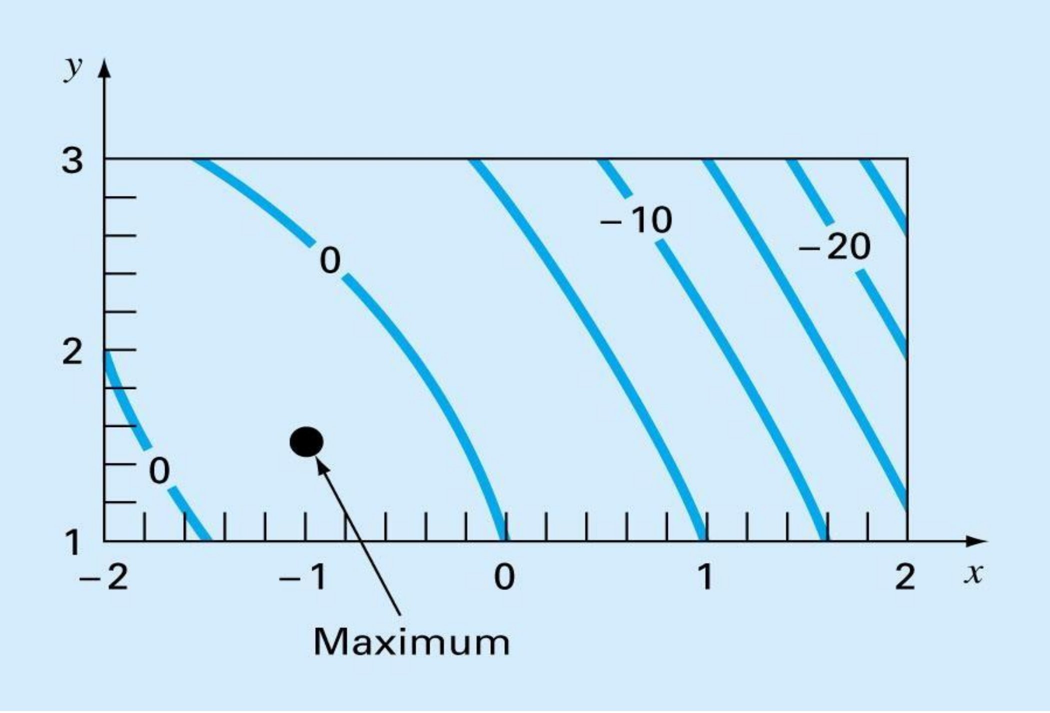
$$f(x, y) = y - x - 2x^2 - 2xy - y^2$$

can be found using a random number generator

Direct Methods: Random Searches

$$0 \le r \le 1 \qquad x = x_l + (x_u - x_l)r \qquad y = y_l + (y_u - y_l)r$$

- Take sufficient number of samples
- Keep track of the maximum value from among random trials



Direct Methods: Random Searches

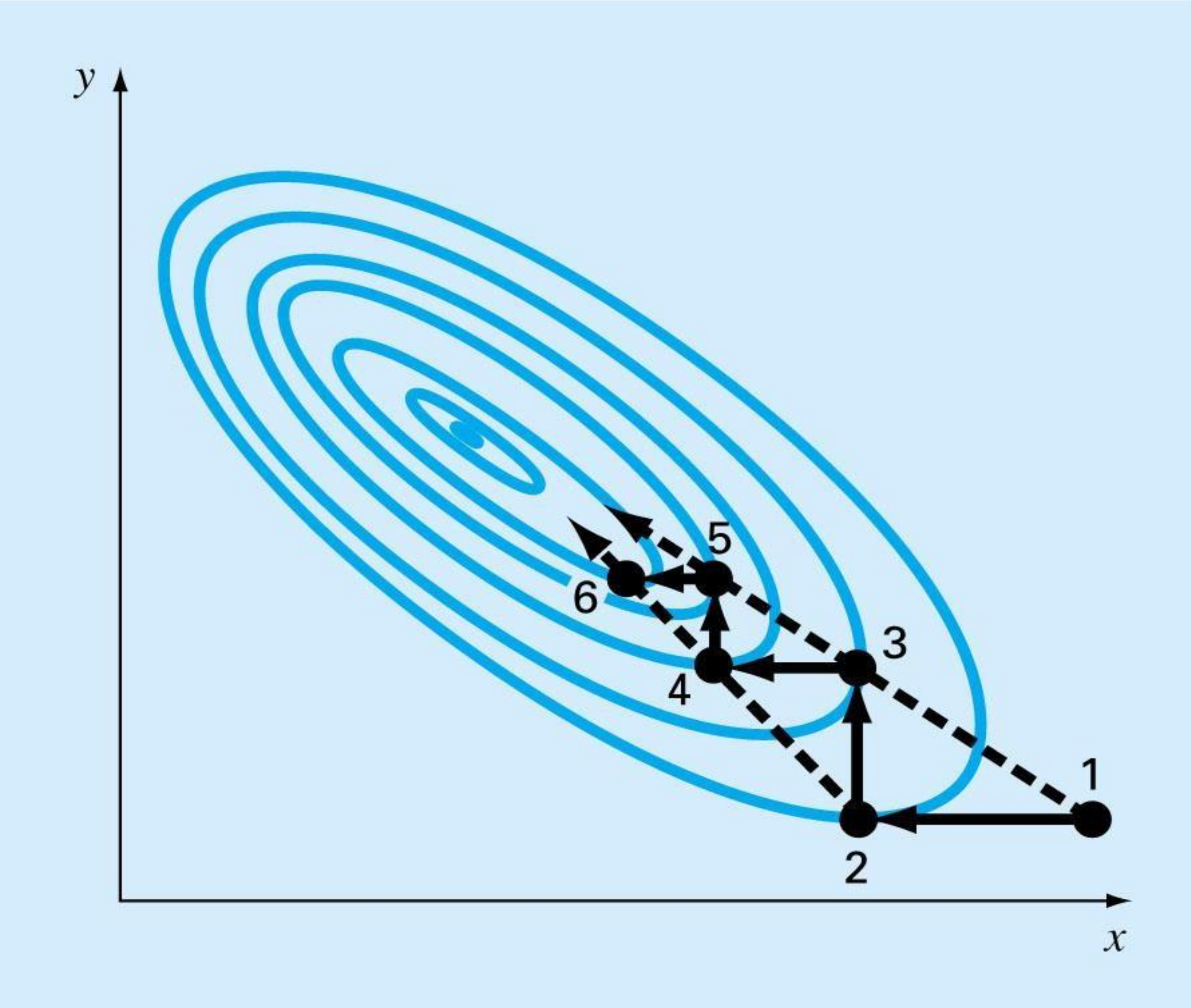
- Advantages
  - Works even for discontinuous and nondifferentiable functions
  - Always find global optimum rather than a local optimum

- 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

Direct Methods:
Univariate and Pattern Searches

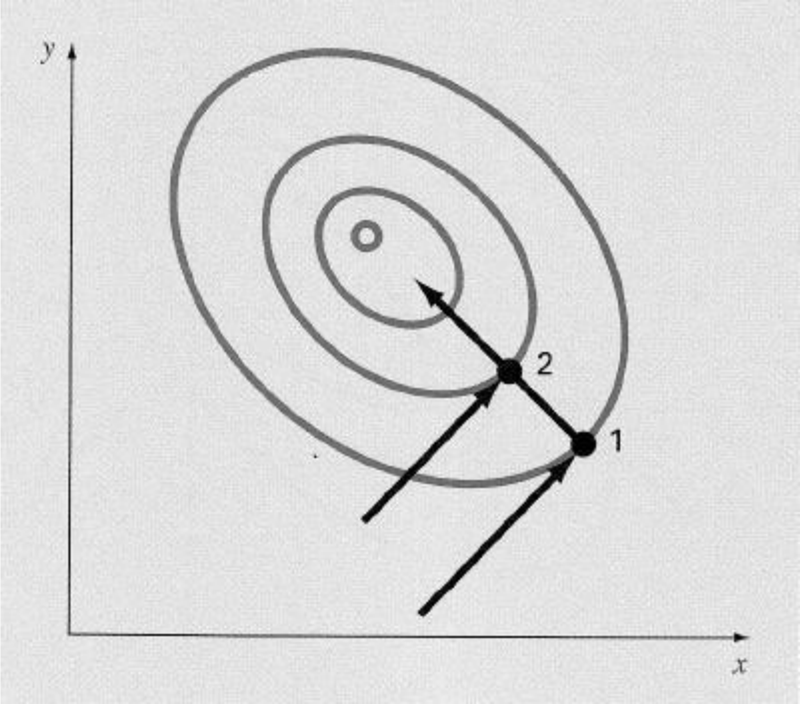
- More efficient than random search and still doesn't require derivative evaluation.

- 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.


y
x
1
2
3
4
5
6

Direct Methods: Powell's Method

- If points 1 and 2 are obtained by one dimensional searches in the same direction but from different starting points
  - The line formed by 1 and 2 will be directed toward the maximum
  - Conjugated Direction



Direct Methods: Powell's Method