I3344
Numerical Simulation & Modeling

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Tentative Syllabus

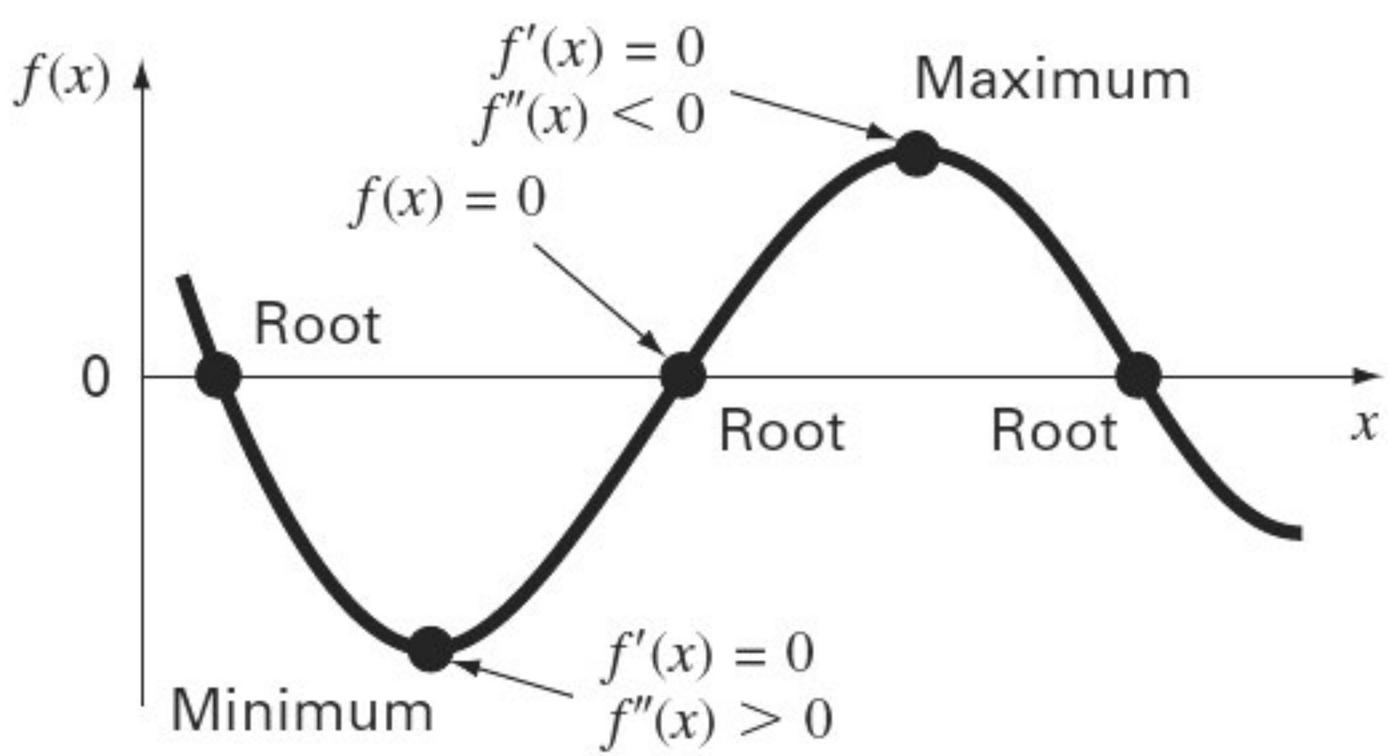
- ✓ Interpolation and extrapolation
  - ✓ Linear: linear regression y = ax + b; correlation, standard deviation, etc.
  - ✓ Non-linear: k nearest neighbors (KNN)
  - ✓ Validation of two models: k-fold cross validation method.
- ✓ Solving a linear equation
  - ✓ Direct methods: Gauss and LU
  - ✓ Iterative methods: Jacobi and Gauss-Seidel
- ✓ Derivation
  - ✓ Finite difference method (FDM): Euler and Runge-kutta
- ✓ Integration: surface estimation
  - ✓ Finite Element Method (FEM).
  - ✓ Monte Carlo method.
  - ✓ Comparison of two methods.
- ✓ Non-linear problems
  - ✓ Bisection method
- **Optimization**
- Introduction to the notion of parallel computing and underlying algorithms

Outline

- Introduction
- Golden Section Search
- Newton Method

Introduction

- **Root location** and **optimization** are **related** in the sense that both involve guessing and searching for a point on a function.
    - **Root location**: searching for zeros of a function
    - **Optimization**: searching for the minimum or the maximum.



Mathematical Background

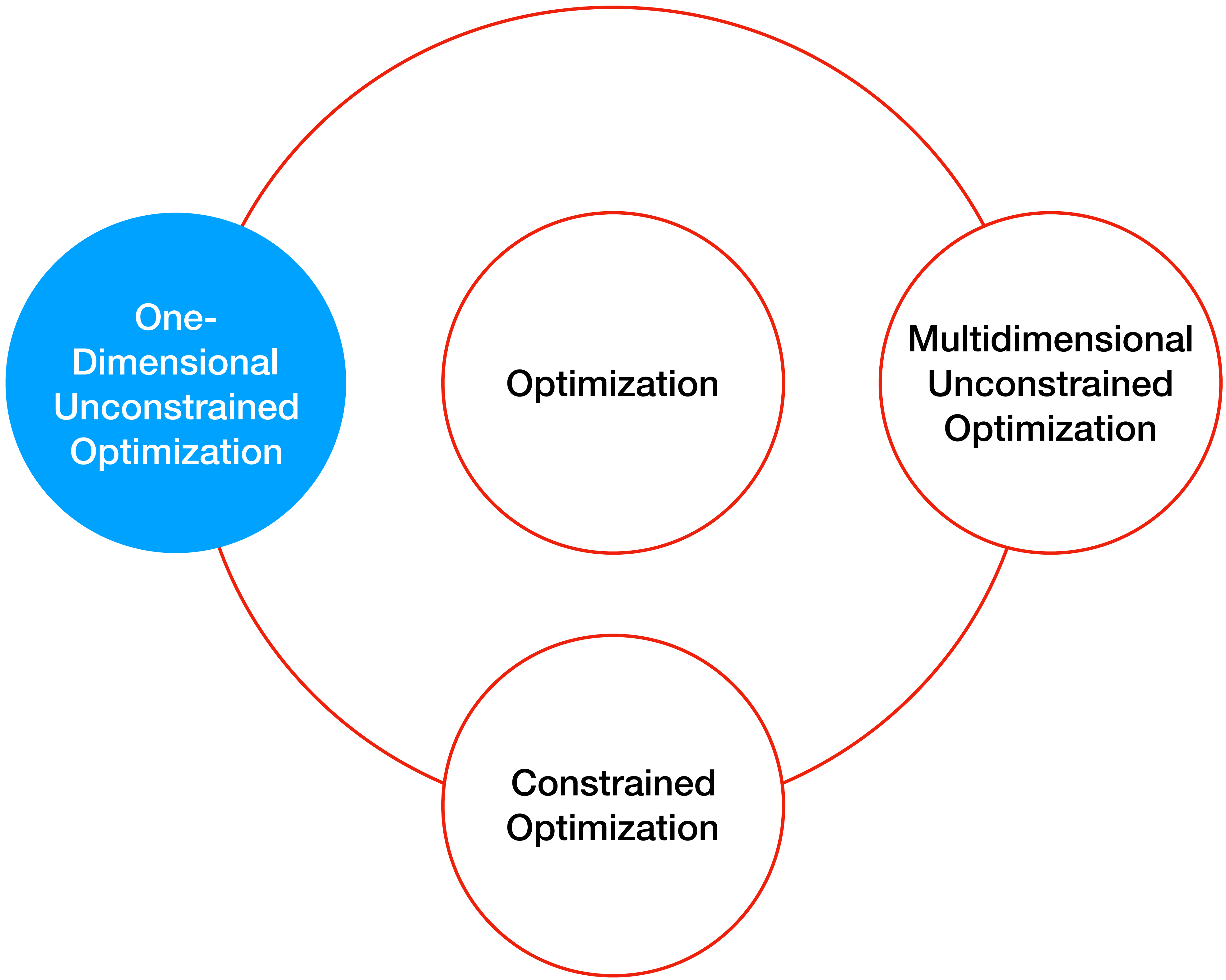
- An optimization or mathematical programming problem generally be stated as:

Find x, which <u>minimizes</u> or <u>maximizes</u> f(x) subject to

$$d_i(\boldsymbol{x}) \leq a_i \qquad i = 1, 2, \ldots, m$$
$$e_i(\boldsymbol{x}) = b_i \qquad i = 1, 2, \ldots, p$$

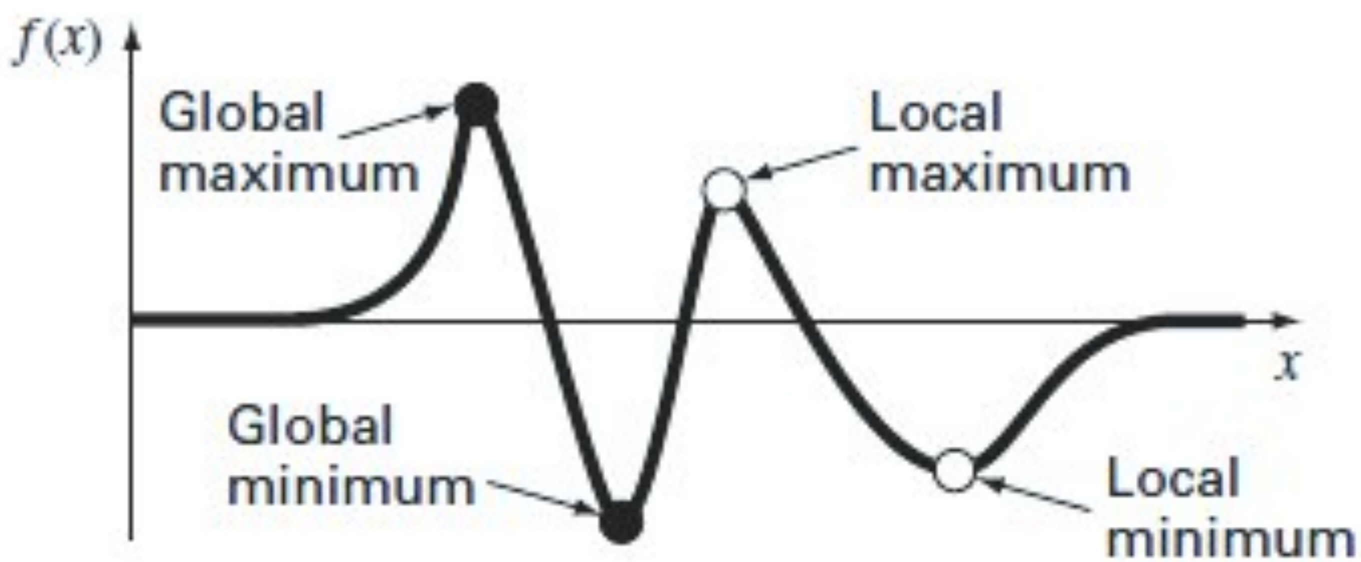
- *x is an n-dimensional design vector*
- *$f(x)$ is the objective function*
- *$d_i(x)$ are inequality constraints*
- *$e_i(x)$ are equality constraints*
- *a_i and b_i are constants*

Introduction (cont’d)



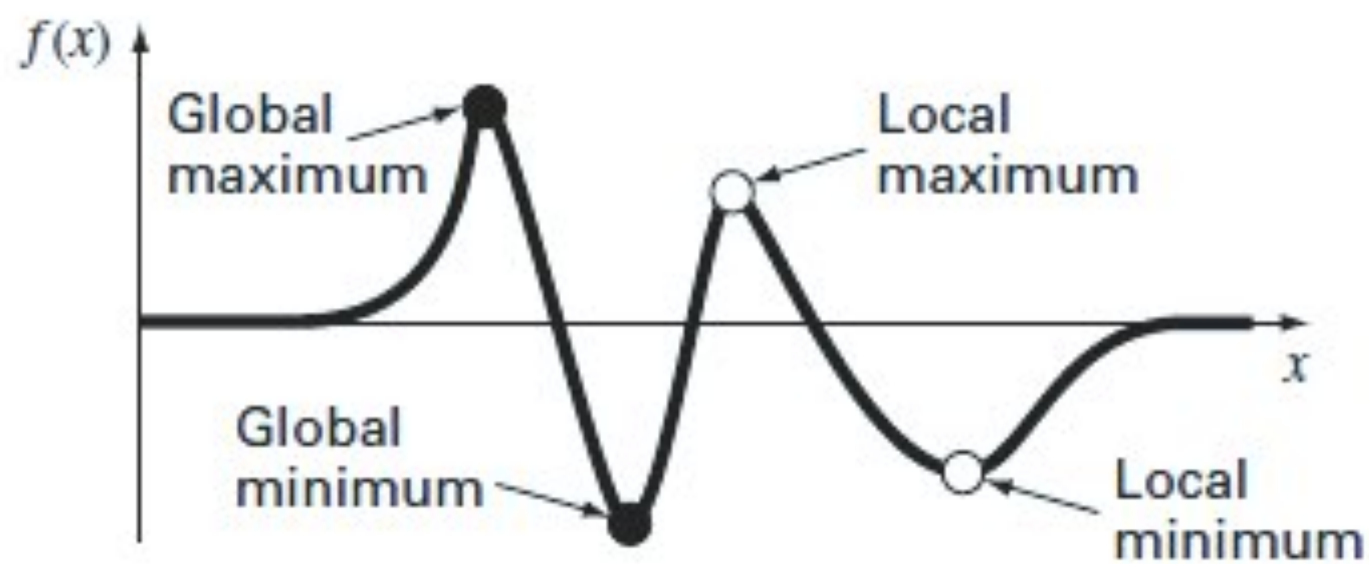
Introduction (cont'd)

- **Multimodal** cases: Both **local** and **global optima** can occur for a single function



Introduction (cont'd)

- How to **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 <u>largest of the optima</u> as global**.
  - **Perturbing the starting point associated to a local optima** to see if the routine returns a better point or the same local optima.



Golden-Section Search

- A unimodal function has a **single maximum (resp. minimum) in the a given interval**. For a unimodal function:
  - **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**.
  - 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.

Golden-Section Search (cont'd)

$$\ell_0 = \ell_1 + \ell_2$$

- the sum of the two sub lengths l_1 and l_2 must equal the original interval length.

$$\frac{\ell_1}{\ell_0} = \frac{\ell_2}{\ell_1}$$

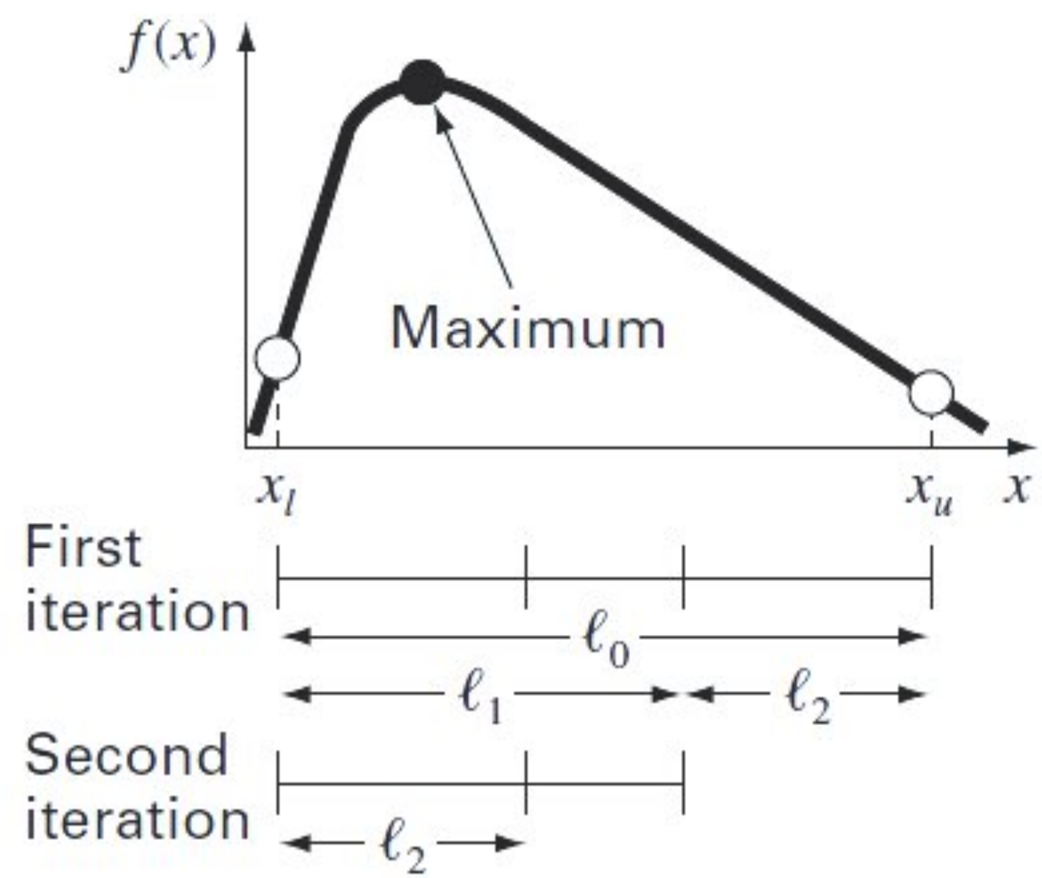
- the ratio of the length must be equal

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

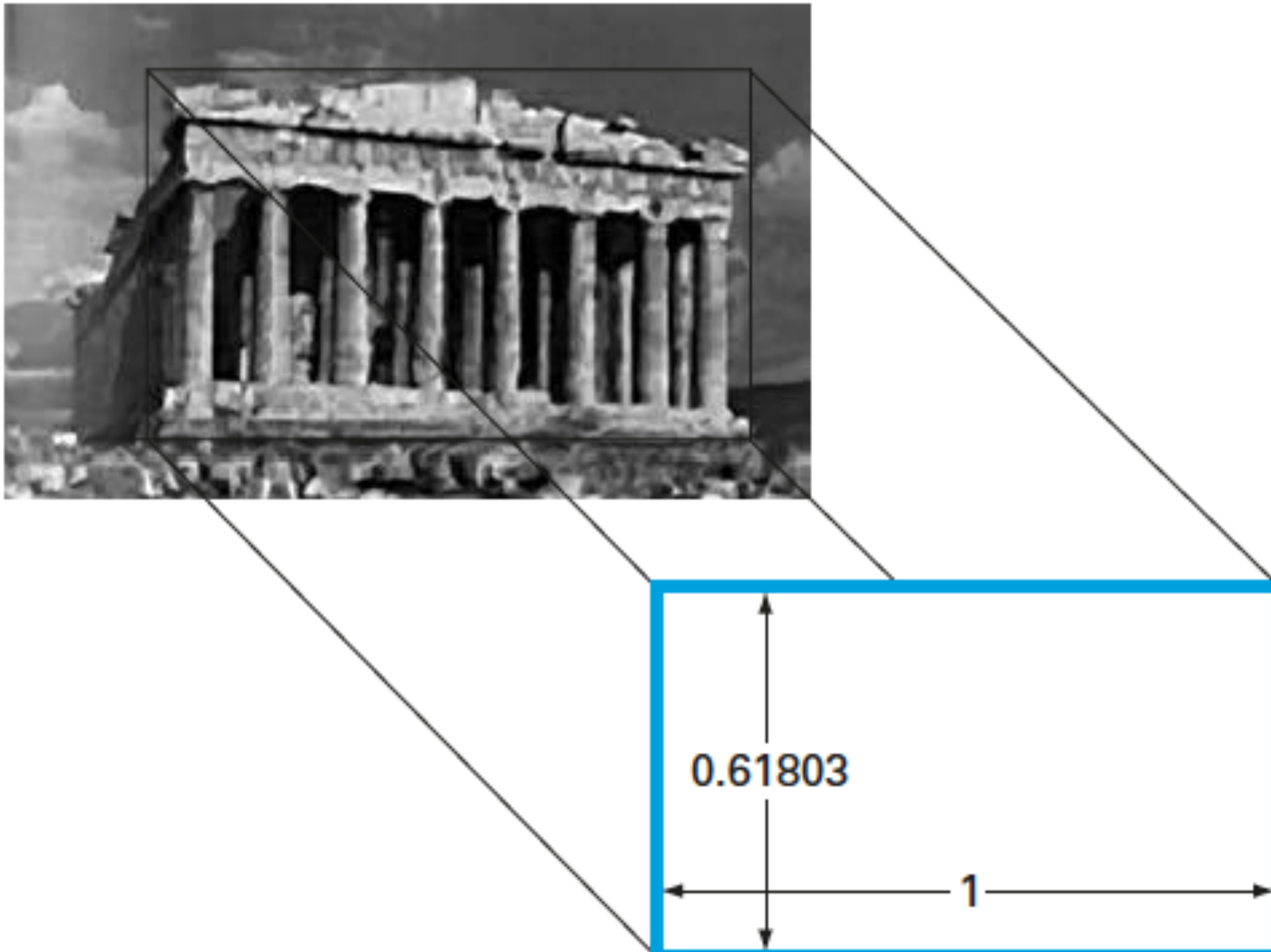
$$1 + R = \frac{1}{R} \qquad R^2 + R - 1 = 0$$

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

Golden Ratio



Golden Ratio (History)



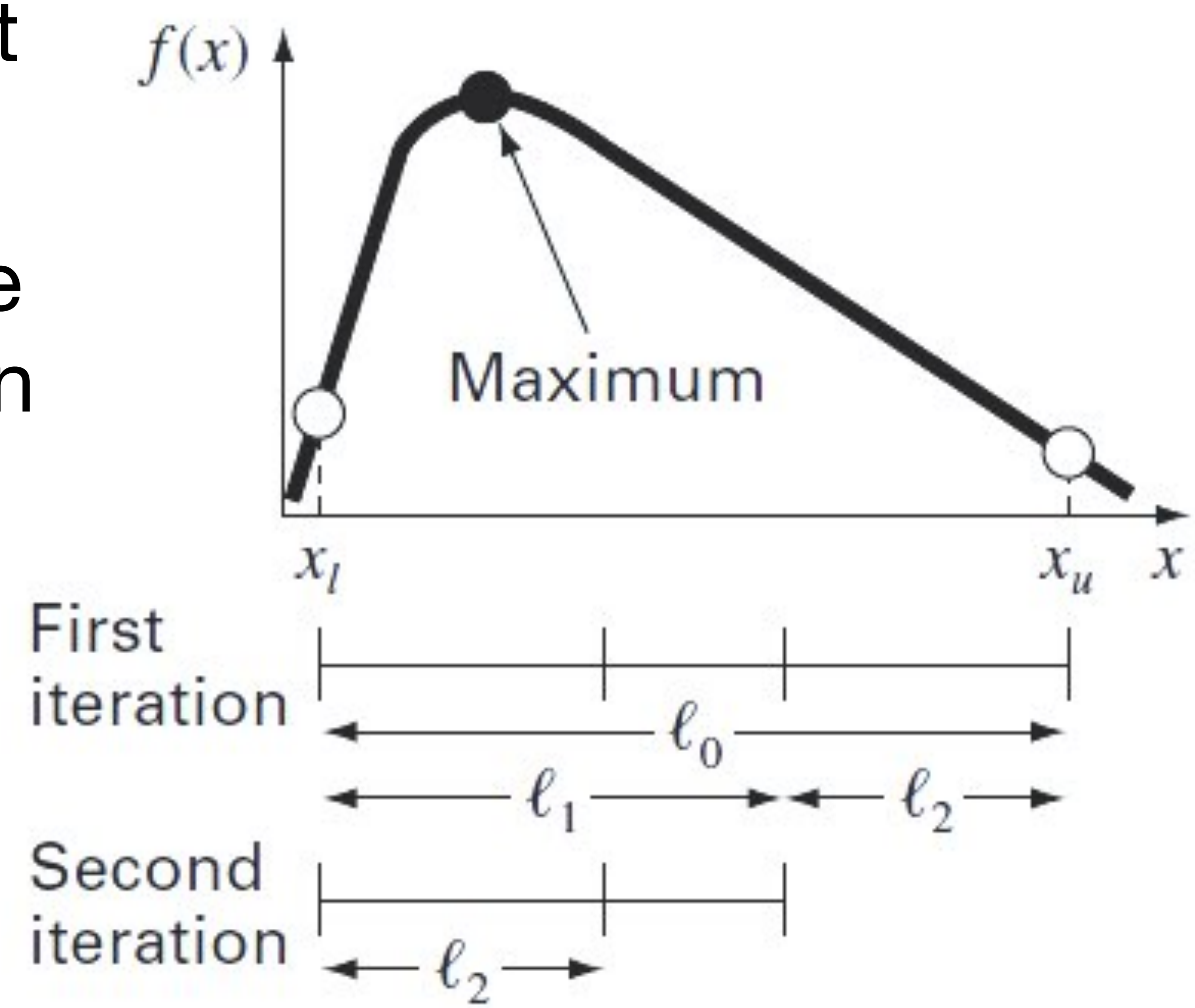
Golden-Section Search (cont’d)

- The method starts with two initial guesses, x_l and x_u, that bracket one local extremum of f(x)
- 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 (cont'd)

- If $f(x_1)>f(x_2)$

  => the domain of x to the left of x_2 from x_l to x_2 does not contain the maximum

  => can be eliminated => new $x_l = x_2$

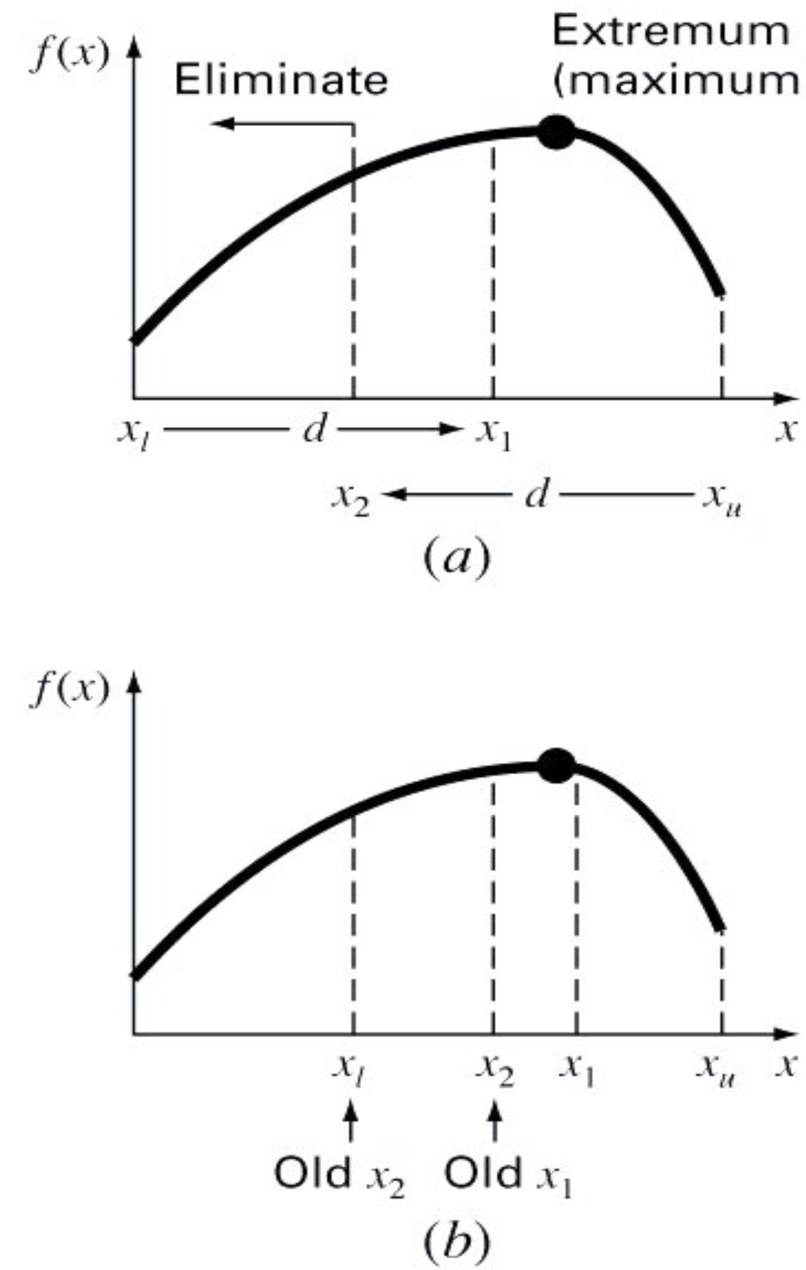
- If $f(x_2)>f(x_1)$

  => the domain of x to the right of x_1 from x_l to x_2, would have been eliminated => new $x_u = x_1$

- New x_1 is determined as before

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

- Stop condition: $|x_u - x_l| < \varepsilon$, max = $(x_l + x_u)/2$



Exercise

- *Use the golden-section search to find the maximum of the following function within the interval x_l=0 and x_u=4.*

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

- *Note*

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

$$x_1 = x_l + d$$

$$x_2 = x_u - d$$

Exercise - Solution

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

$$d = \frac{\sqrt{5}-1}{2}(4-0) = 2.472$$

$$x_1 = 0 + 2.472 = 2.472$$

$$x_2 = 4 - 2.472 = 1.528$$

$$f(x_2) = f(1.528) = 2\sin(1.528) - \frac{1.528^2}{10} = 1.765$$

$$f(x_1) = f(2.472) = 0.63$$

- Because $f(x_2) > f(x_1)$, the maximum is in the interval defined by x_l, x_2, and x_1.
- For the new interval
  - LB remains $x_l = 0$, x_1 becomes the UB => $x_u = 2.472$.
  - Former x_2 value becomes the new x_1, that is, $x_1 = 1.528$.

$$d = \frac{\sqrt{5}-1}{2}(2.472-0) = 1.528$$

$$x_2 = 2.4721 - 1.528 = 0.944$$

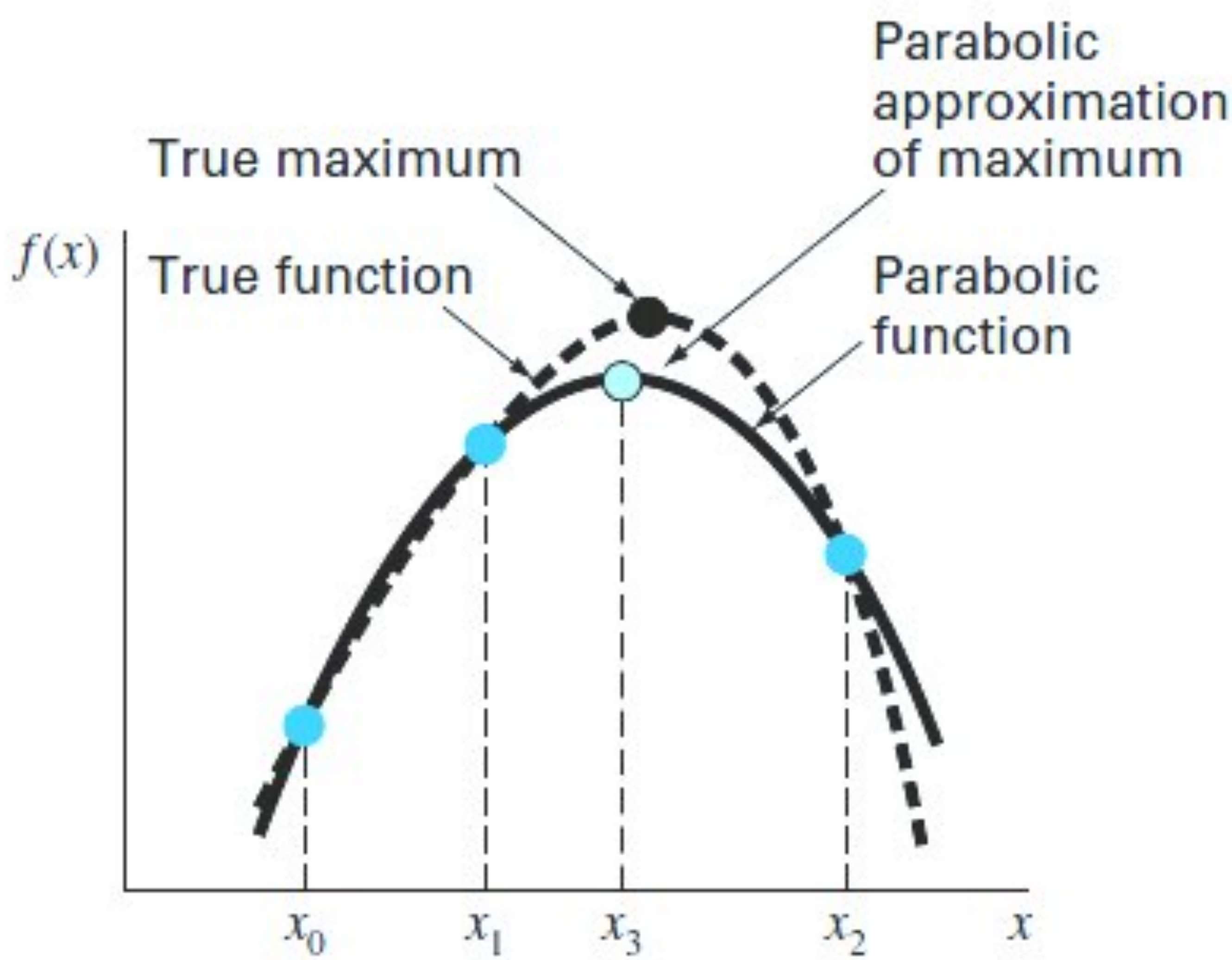
Exercise - Solution (cont'd)

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

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

Quadratic Interpolation

- Parabolic interpolation takes advantage of the fact that a **second-order polynomial** often provides a **good approximation** to the shape of f(x) **near an optimum**



Quadratic Interpolation (cont'd)

- There is <u>**only one**</u> **quadratic polynomial or parabola connecting three points.**
- if we have **three points that jointly bracket an optimum**, we can **fit a parabola to the points.**
- Then we can **differentiate it**, **set the result equal to zero**, and **solve for an estimate of the optimal x.**
- It can be shown through some algebraic manipulations that the result is

$$x_3 = \frac{f(x_0)(x_1^2 - x_2^2) + f(x_1)(x_2^2 - x_0^2) + f(x_2)(x_0^2 - x_1^2)}{2f(x_0)(x_1 - x_2) + 2f(x_1)(x_2 - x_0) + 2f(x_2)(x_0 - x_1)}$$

- $\mathbf{x_0}$**,** $\mathbf{x_1}$**, and** $\mathbf{x_2}$ are the <u>initial guesses</u>, and $\mathbf{x_3}$ is the <u>value of x</u> that corresponds to the <u>maximum value of the parabolic fit</u> to the guesses
- and so on (same as golden section search)

Exercise

- Use parabolic interpolation to approximate the maximum of the following function with initial guesses of $x_0=0$, $x_1=1$, and $x_2=4$.

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

- Note:

$$x_3 = \frac{f(x_0)(x_1^2 - x_2^2) + f(x_1)(x_2^2 - x_0^2) + f(x_2)(x_0^2 - x_1^2)}{2f(x_0)(x_1 - x_2) + 2f(x_1)(x_2 - x_0) + 2f(x_2)(x_0 - x_1)}$$

Exercise - Solution

$$x_0 = 0 \qquad f(x_0) = 0$$
$$x_1 = 1 \qquad f(x_1) = 1.5829$$
$$x_2 = 4 \qquad f(x_2) = -3.1136$$

$$x_3 = \frac{0(1^2 - 4^2) + 1.5829(4^2 - 0^2) + (-3.1136)(0^2 - 1^2)}{2(0)(1 - 4) + 2(1.5829)(4 - 0) + 2(-3.1136)(0 - 1)} = 1.5055$$

Because the function value for the new point is higher than for the intermediate point (x_1) and the new x value is to the right of the intermediate point, the lower guess (x_0) is discarded. Therefore, for the next iteration

$$x_0 = 1 \qquad f(x_0) = 1.5829$$
$$x_1 = 1.5055 \qquad f(x_1) = 1.7691$$
$$x_2 = 4 \qquad f(x_2) = -3.1136$$

$$x_3 = \frac{1.5829(1.5055^2 - 4^2) + 1.7691(4^2 - 1^2) + (-3.1136)(1^2 - 1.5055^2)}{2(1.5829)(1.5055 - 4) + 2(1.7691)(4 - 1) + 2(-3.1136)(1 - 1.5055)}$$
$$= 1.4903 \qquad f(1.4903) = 1.7714.$$

Exercise - Solution

Quadratic

i	x_0	$f(x_0)$	x_1	$f(x_1)$	x_2	$f(x_2)$	x_3	$f(x_3)$
1	0.0000	0.0000	1.0000	1.5829	4.0000	−3.1136	1.5055	1.7691
2	1.0000	1.5829	1.5055	1.7691	4.0000	−3.1136	1.4903	1.7714
3	1.0000	1.5829	1.4903	1.7714	1.5055	1.7691	1.4256	1.7757
4	1.0000	1.5829	1.4256	1.7757	1.4903	1.7714	1.4266	1.7757
5	1.4256	1.7757	1.4266	1.7757	1.4903	1.7714	1.4275	1.7757

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
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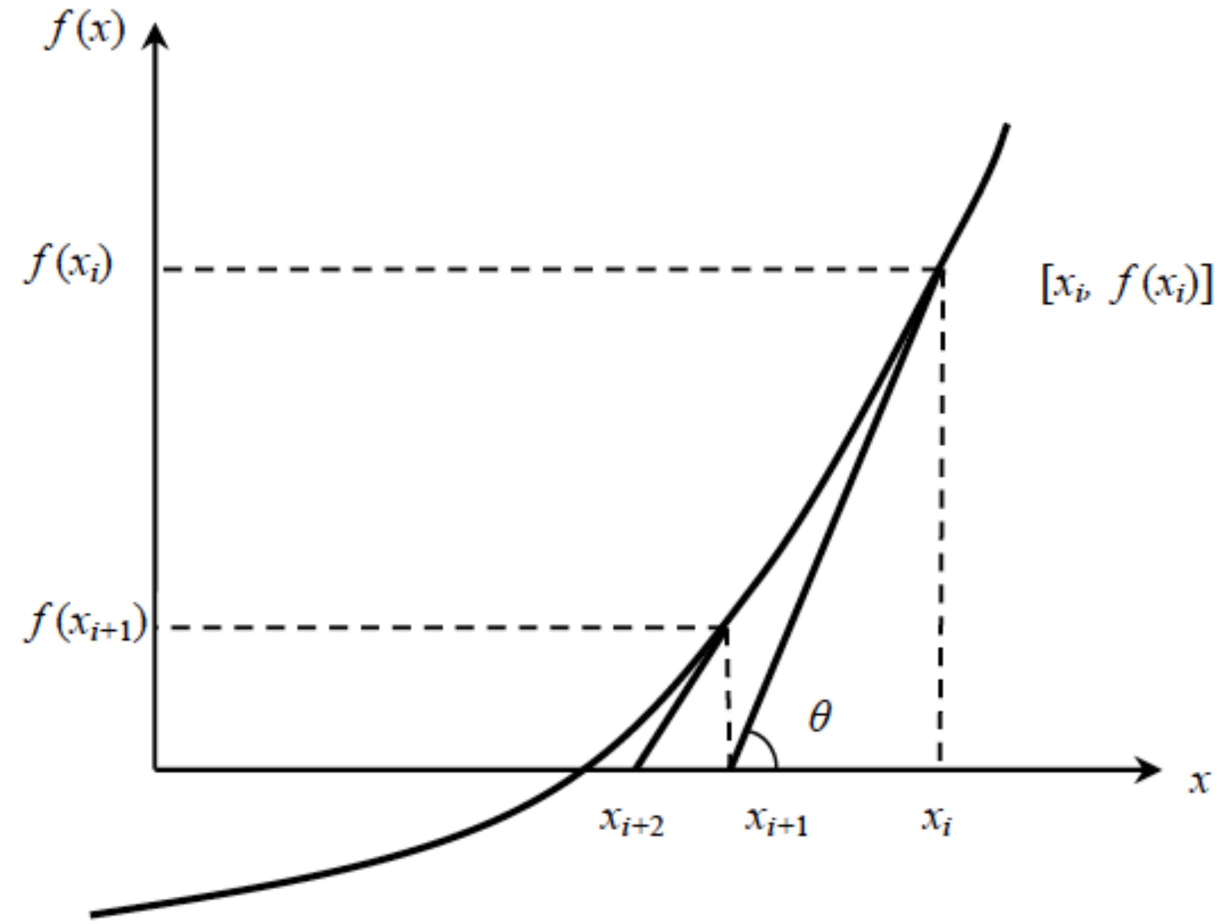
Newton's Method

- Based on the Newton- Raphson method to find the root of an equation
- The Newton-Raphson method is based on the principle that *if the initial guess of the root of f(x) = 0 is at x_i, then if one draws the tangent to the curve at $f(x_i)$, the point x_{i+1} where the tangent crosses the x-axis is an improved estimate of the root*



$$f'(x_i) = \tan\theta = \frac{f(x_i) - 0}{x_i - x_{i+1}} \Rightarrow x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Newton’s Method (cont’d)

- Consider a new function g(x)=f'(x).
- The optimal value x* satisfies: f'(x*)=g(x*)=0
- We can use the following as a technique to the extremum of f(x).

- Start with an initi

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

the iterations until finding $f'(x_k) = 0$ (ıe)

Exercise

- Use Newton's method to approximate the maximum of the following function with initial guesses of x_0=2.5

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

- Note:

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

Exercise - Solution

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

$$f'(x) = 2 \cos x - \frac{x}{5}$$

$$f''(x) = -2 \sin x - \frac{1}{5}$$

$$x_{i+1} = x_i - \frac{2 \cos x_i - x_i/5}{-2 \sin x_i - 1/5}$$

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

Exercise

Employ the following methods to find the maximum of

$f(x) = 4x - 1.8x^2 + 1.2x^3 - 0.3x^4$

(a) Golden-section search ($x_l = -2$, $x_u = 4$, $\varepsilon_s = 1\%$).

(b) Parabolic interpolation ($x_0=1.75$, $x_1=2$, $x_2=2.5$, iter. = 4).

(c) Newton's method ($x_0 = 3$, $\varepsilon_s=1\%$).