One-Dimensional Unconstrained Optimization

Chapter 13

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Mathematical Background

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

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

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

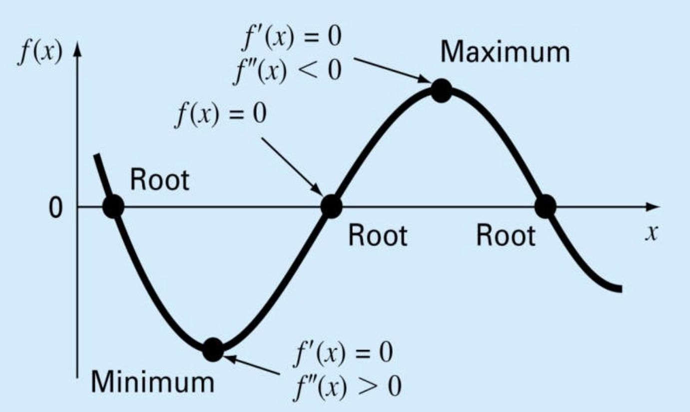
- Optimization problems can be classified on the basis of the form of *f(x):*
  - If *f(x)* and the constraints are linear, we have ***linear programming***.
  - If *f(x)* is quadratic and the constraints are linear, we have ***quadratic programming***.
  - If *f(x)* is not linear or quadratic and/or the constraints are nonlinear, we have ***nonlinear programming***.

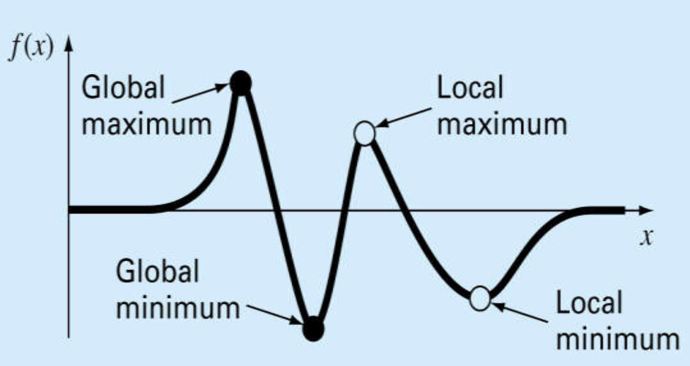
- When equations(*) are included, we have a ***constrained optimization*** problem; otherwise, it is ***unconstrained optimization*** problem.

One-Dimensional Unconstrained Optimization

- **Root finding** and **optimization** are related. Both involve guessing and searching for a point on a function. Difference is:
  - Root finding is searching for zeros of a function
  - Optimization is finding the ***minimum*** or the ***maximum*** of a function of several variables.

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





How do we look for the global optimum?

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

Golden Ratio

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].
- Then, pick two more points within this interval to determine whether a **maximum** has occurred within the *first three* or *last three* points

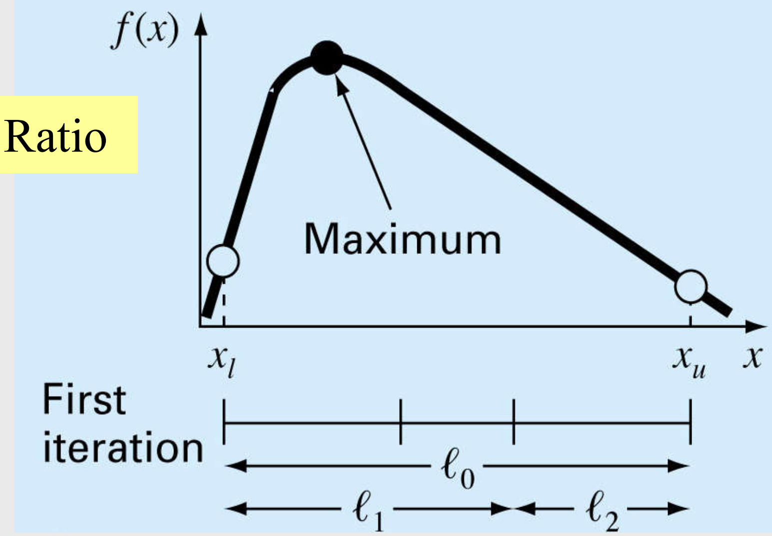
$$l_0 = l_1 + l_2 \quad \text{and} \quad \frac{l_1}{l_0} = \frac{l_2}{l_1}$$

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

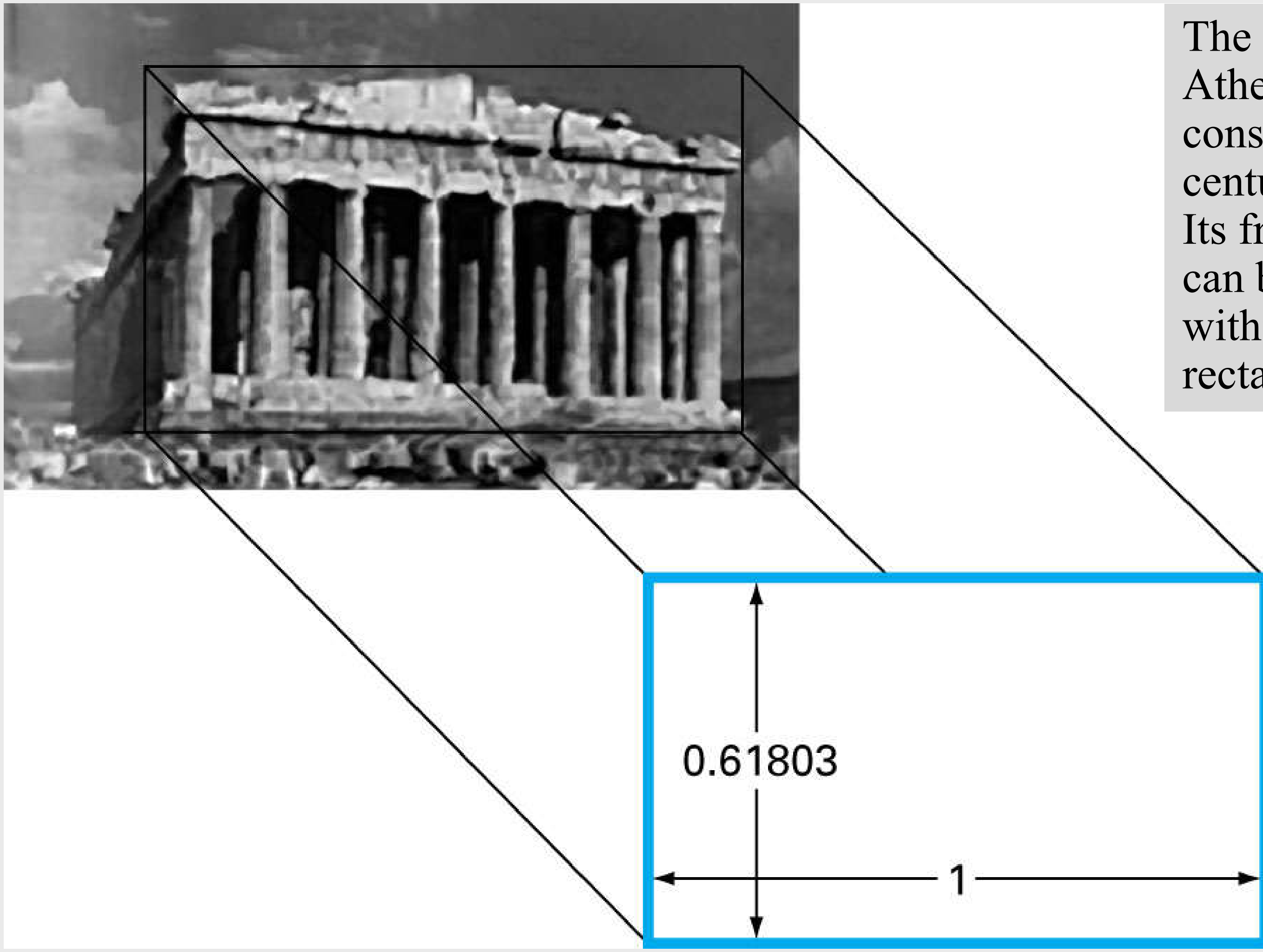
$$1 + R = \frac{1}{R} \qquad R^2 + R - 1 = 0$$

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

Golden Ratio



Golden Ratio



The Parthenon in Athens, Greece was constructed in the 5th century B.C.
Its front dimensions can be fit exactly within a golden rectangle

Golden-Section Search

- Pick two initial guesses, x_l and x_u, that bracket one local extremum of $f(x)$:
- Choose two interior points x_1 and x_2 according to the **golden ratio**

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

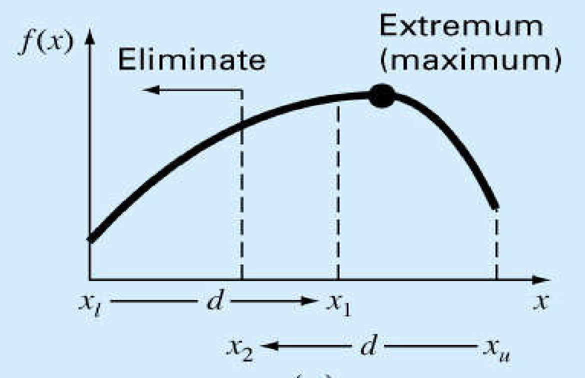
$$x_1 = x_l + d$$

$$x_2 = x_u - d$$

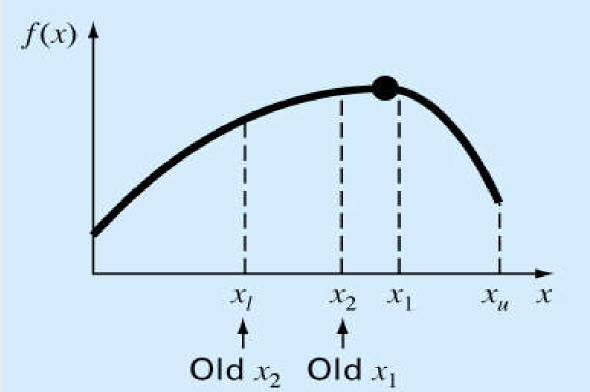
Evaluate the function at x_1 and x_2 :

- If $f(x_1) > f(x_2)$ then the domain of x to the left of x_2 (from x_l to x_2) does not contain the maximum and can be eliminated. Then, x_2 becomes the new x_l
- If $f(x_2) > f(x_1)$, then the domain of x to the right of x_1 (from x_1 to x_u) can be eliminated. In this case, x_1 becomes the new x_u .
- The benefit of using **golden ratio** is that we do not need to recalculate all the function values in the next iteration.

If $f(x_1) > f(x_2)$ then **New** $x_2 \leftarrow x_1$ else **New** $x_1 \leftarrow x_2$



(a)



(b)

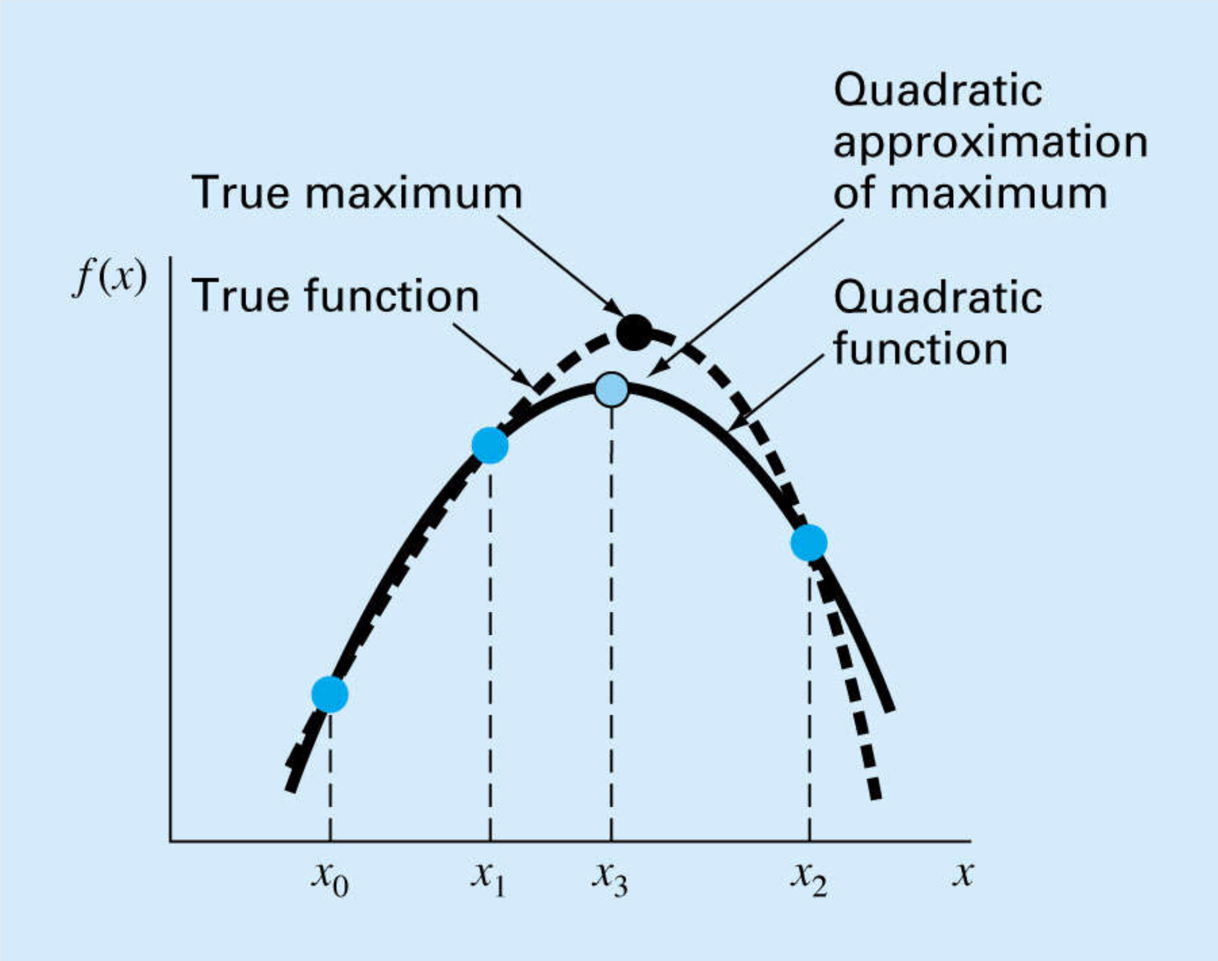
Stopping Criteria

$$|x_u - x_l| < \varepsilon$$

```
FUNCTION Gold (xlow, xhigh, maxit, es, fx)
R = (5^0.5 - 1)/2
xℓ = xlow; xu = xhigh
iter = 1
d  = R * (xu - xℓ)
x1 = xℓ + d; x2 = xu - d
f1 = f(x1)
f2 = f(x2)
IF f1 > f2 THEN                                    IF f1 < f2 THEN
  xopt = x1
  fx = f1
ELSE
  xopt = x2
  fx = f2
END IF
DO
  d = R*d
  IF f1 > f2 THEN                                  IF f1 < f2 THEN
     xℓ = x2
     x2 = x1
     x1 = xℓ+d
     f2 = f1
     f1 = f(x1)
  ELSE
     xu = x1
     x1 = x2
     x2 = xu-d
     f1 = f2
     f2 = f(x2)
  END IF
  iter = iter+1
  IF f1 > f2 THEN                                  IF f1 < f2 THEN
     xopt = x1
     fx = f1
  ELSE
     xopt = x2
     fx = f2
  END IF
  IF xopt ≠ 0. THEN
     ea = (1.-R) *ABS((xu - xℓ)/xopt) * 100.
  END IF
  IF ea ≤ es OR iter ≥ maxit EXIT
END DO
Gold = xopt
END Gold
```

(*a*) **Maximization** (*b*) **Minimization**

Finding maximum through Quadratic Interpolation



If we have 3 points that jointly bracket a maximum (or minimum), then:

1. Fit a parabola to 3 points (using Lagrange approach) and find *f(x)*
2. Then solve $df/dx = 0$ to find the optimum point.

Example (from the textbook):

Use the Golden-section search to find the maximum of

$f(x) = 2 \, \mathbf{sin} \, x - x^2/10$ within the interval $x_l=0$ and $x_u=4$

Newton's Method

- A similar approach to Newton- Raphson method can be used to find an optimum of *f(x)* by finding the root of *f'(x)* (i.e. solving *f'(x)*=0):

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

- <u>Disadvantage</u>: it may be divergent

- If it is difficult to find *f'(x)* and *f''(x)* analytically, then a secant-like version of Newton's technique can be developed by using finite-difference approximations for the derivatives.

Example 13.3:

Use Newton's method to find the maximum of

$f(x) = 2 \sin x - x^2/10$ with an initial guess of $x_0 = 2.5$

Solution:

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

$$x_1 = 2.5 - \frac{2\cos 2.5 - 2.5/5}{-2\sin 2.5 - 1/5} = 0.995 \quad \text{and} \quad f(0.995) = 1.578$$

i	*x*	*f(x)*	*f'(x)*	*f''(x)*
0	2.5	0.572	-2.102	-1.3969
1	0.995	1.578	0.8898	-1.8776
2	1.469	1.774	-0.0905	-2.1896
3	1.4276	1.77573	-0.0002	-2.17954
4	1.4275	1.77573	0.0000	-2.17952