Optimization

1-D optimization

Chapter 13:

Optimization

- Often in engineering we first learn how to design units or systems that simply meet a set of specifications

- In practical application, the design must also be optimized to:
  - Reduce: cost, raw material, waste, downtime, environmental impact, inventory
  - Increase: profits, yields, safety, reliability

Optimization

- So the trick is to formulate a function to be optimized
- For a given operation, costs can be minimized
- For a given supply, product can be maximized
- For an existing process, recycle ratios, purge rates, temperatures, etc can be manipulated to increase yeild

Optimization

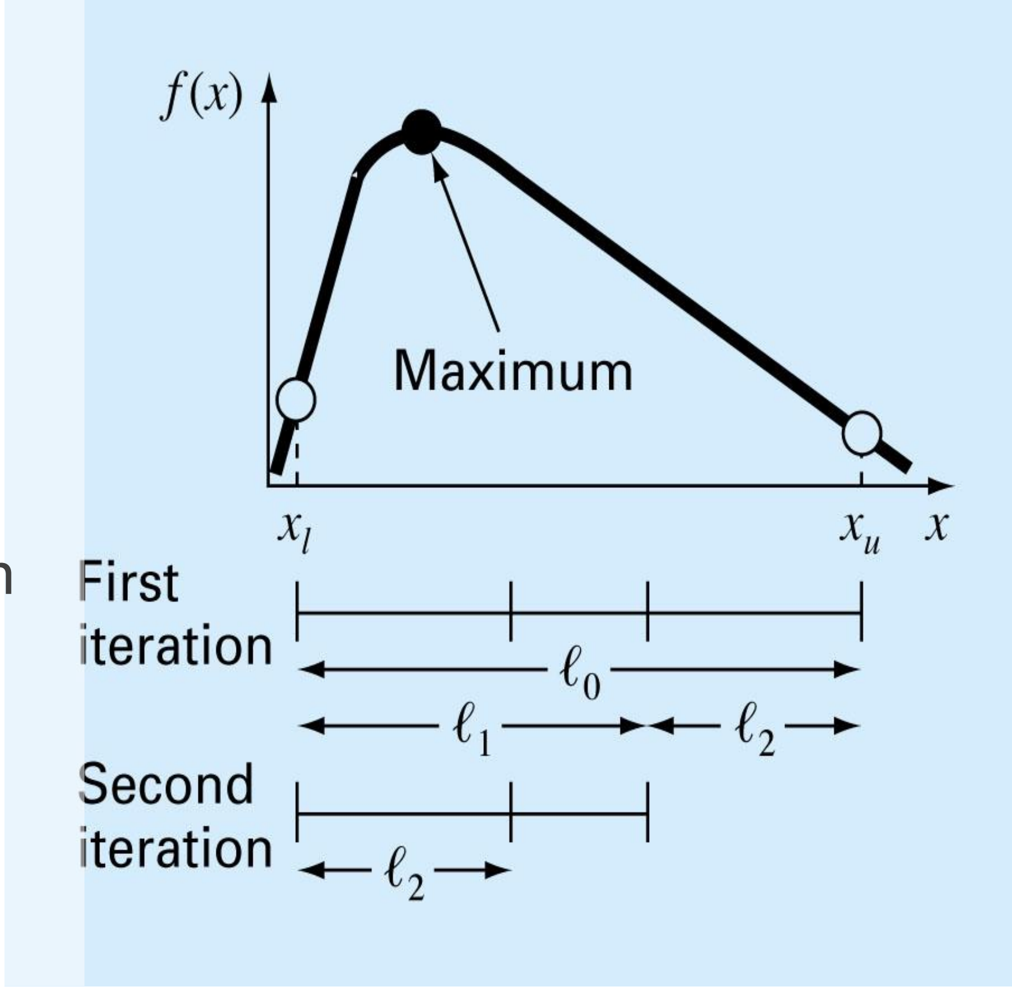
- Objective function
  - goal of the optimization
- Design variables
  - Which independent variables can be manipulated to achieve the goal
- Constraints
  - External limitations of the system
  - Often in terms of inequalities
  - Limitation of the range of the desired solution (e.g. no negative temperatures)

One Dimensional Optimization

- Minimizing or maximizing a function of a single independent variable is quite common in engineering design, especially in unit ops
- Common methods include:
  - Newton’s method, if the function is differentiable
  - Quadratic interpolation, which is analogous to Müller’s Method and the Secant method
  - Golden-section search, which is analogous to the bracketed bisection method

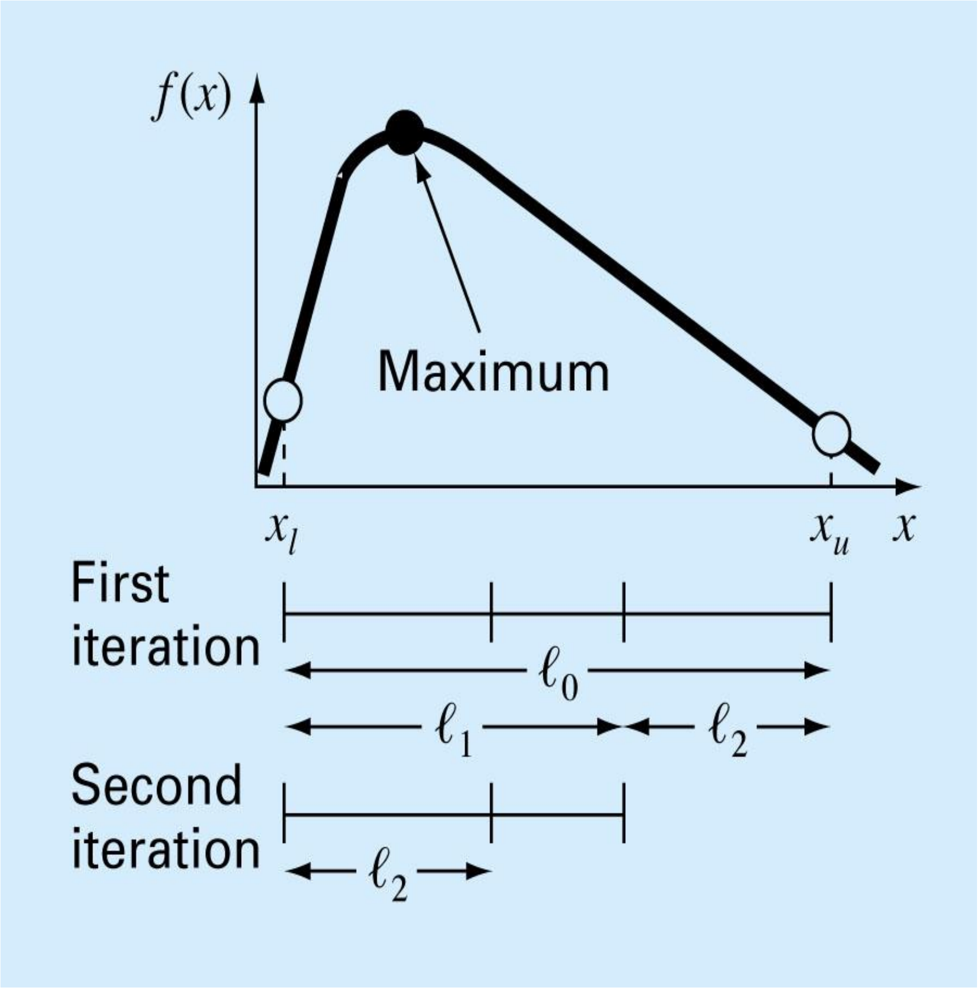
Golden Section Search

- This method starts at to initialization points, x_l and x_u
- Then these and two interior points, x_1 and x_2, are all evaluated
- Since we are looking for the maximum, the lowest of the values $f(x_1)$, $f(x_2)$ determines which side of the interval to continue with
- Assuming you have the optimum bracketed, this method will always find it
- It is similar to the bisection method in that it converges predictably although slightly slower



Golden Section Search

- The two interior points are chosen carefully, so that the ratio of the intervals are equal
- This allows us to 'recycle' the function values and reduce computations
- Only one new x value per iteration



Golden Section Search

- Example 13.1

Use the golden-section search to find the maximum of the function f(x) within the interval $X_L = 0$ and $X_u = 4$.

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

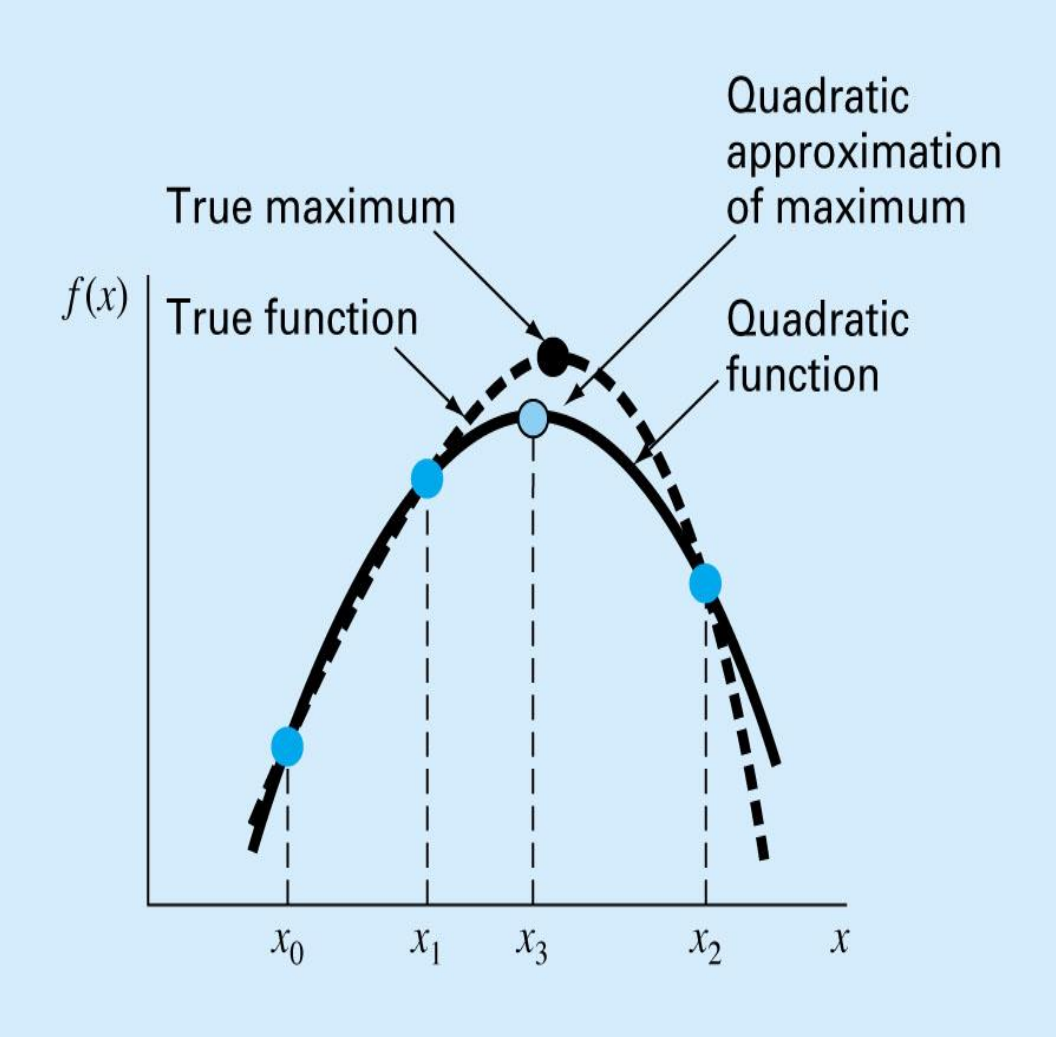
- Start at x=0, 4 and calculate d=GR*(4-0)
- Calculate x1,x2 and f(x1),f(x2)
- Throw away xl or xu
- Replace x1 or x2

Golden Section Search

	A	B	C	D	E	F	G	H	I	J	K	L
1	Example 13.1			Ratio	0.618034		Solver Solution					
2							x_max	1.427551	f(x)	1.775726		
3	i	xl	f(xl)	x1	f(x1)	x2	f(x2)	xu	f(xu)	d	Throw away	max
4	1	0.00000	0.0[illegible]00	1.52786	1.76472	2.47214	0.62997	4.00000	-3.11360	2.4721	upper	1.76472
5	2	0.00000	0.00000	0.94427	1.53098	1.52786	1.76472	2.47214	0.62997	1.5279	lower	1.76472
6	3	0.94427	1.53098	1.52786	1.76472	1.88854	1.54322	2.47214	0.62997	0.9443	upper	1.76472
7	4	0.94427	1.53098	1.30495	1.75945	1.52786	1.76472	1.88854	1.54322	0.5836	lower	1.76472
8	5	1.30495	1.75945	1.52786	1.76472	1.66563	1.71358	1.88854	1.54322	0.3607	upper	1.76472
9	6	1.30495	1.75945	1.44272	1.77547	1.52786	1.76472	1.66563	1.71358	0.2229	upper	1.77547
10	7	1.30495	1.75945	1.39010	1.77420	1.44272	1.77547	1.52786	1.76472	0.1378	lower	1.77547
11	8	1.39010	1.77420	1.44272	1.77547	1.47524	1.77324	1.52786	1.76472	0.0851	upper	1.77547
12	9	1.39010	1.77420	1.42262	1.77570	1.44272	1.77547	1.47524	1.77324	0.0526	upper	1.77570
13	10	1.39010	1.77420	1.41020	1.77540	1.42262	1.77570	1.44272	1.77547	0.0325	lower	1.77570
14	11	1.41020	1.77540	1.42262	1.77570	1.43030	1.77572	1.44272	1.77547	0.0201	lower	1.77572
15	12	1.42262	1.77570	1.43030	1.77572	1.43504	1.77566	1.44272	1.77547	0.0124	upper	1.77572
16	13	1.42262	1.77570	1.42736	1.77573	1.43030	1.77572	1.43504	1.77566	0.0077	upper	1.77573
17	14	1.42262	1.77570	1.42555	1.77572	1.42736	1.77573	1.43030	1.77572	0.0047	lower	1.77573
18	15	1.42555	1.77572	1.42736	1.77573	1.42848	1.77572	1.43030	1.77572	0.0029	upper	1.77573
19	16	1.42555	1.77572	1.42667	1.77572	1.42736	1.77573	1.42848	1.77572	0.0018	lower	1.77573
20	17	1.42667	1.77572	1.42736	1.77573	1.42779	1.77573	1.42848	1.77572	0.0011	upper	1.77573
21	18	1.42667	1.77572	1.42710	1.77573	1.42736	1.77573	1.42779	1.77573	0.0007	lower	1.77573
22	19	1.42710	1.77573	1.42736	1.77573	1.42753	1.77573	1.42779	1.77573	0.0004	lower	1.77573
23	20	1.42736	1.77573	1.42753	1.77573	1.42763	1.77573	1.42779	1.77573	0.0003	upper	1.77573
24	21	1.42736	1.77573	1.42747	1.77573	1.42753	1.77573	1.42763	1.77573	0.0002	lower	1.77573
25	22	1.42747	1.77573	1.42753	1.77573	1.42757	1.77573	1.42763	1.77573	0.0001	lower	1.77573
26	23	1.42753	1.77573	1.42757	1.77573	1.42759	1.77573	1.42763	1.77573	0.0001	upper	1.77573
27	24	1.42753	1.77573	1.42755	1.77573	1.42757	1.77573	1.42759	1.77573	0.0000	upper	1.77573
28												
29			Twenty interations to get error less than four decimal places									

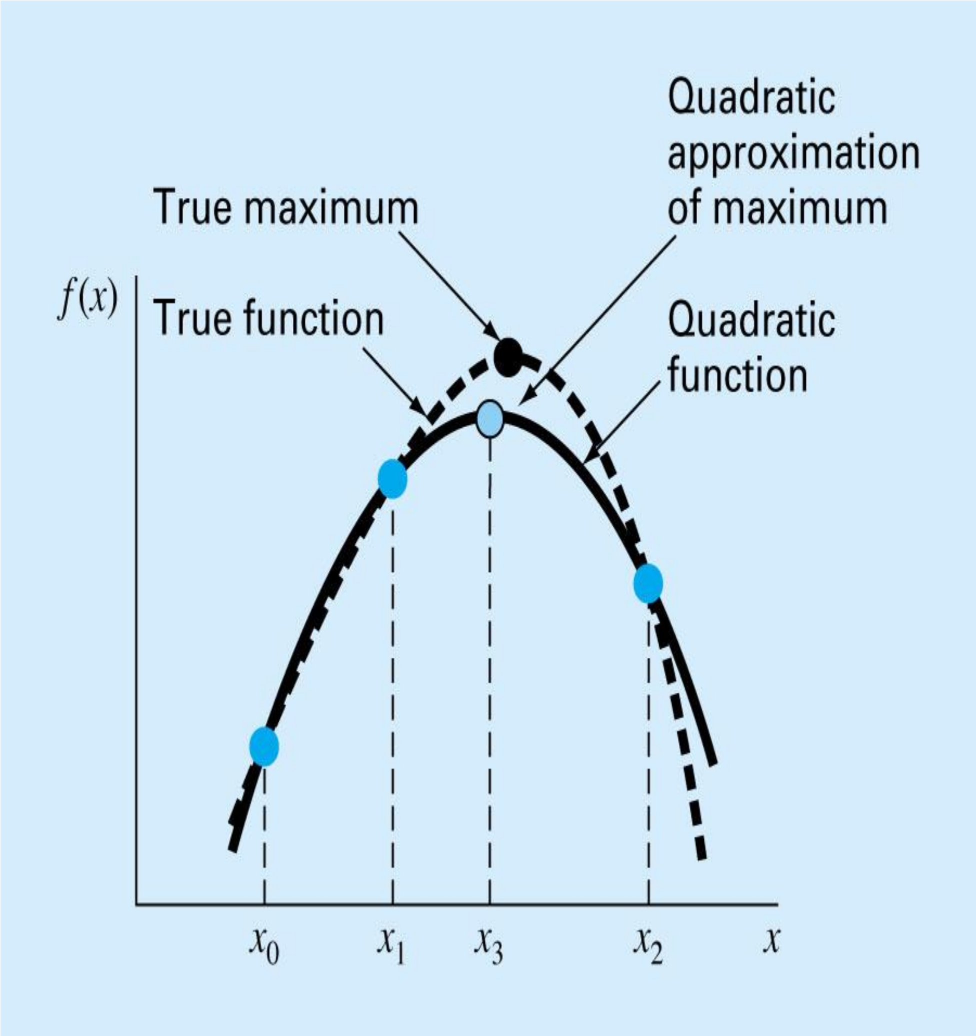
Quadratic Interpolation

- For three points there is one parabola that can be fitted to the points (like Müller’s method)
- We can analytically determine the location of the maximum of this parabola
- Then evaluate the function at this location and determine a new range to consider



Quadratic Interpolation

- The selection criteria for which endpoint to discard, is similar to Golden Search
- But still only one new function evaluation is required per iteration
- Although this can be a bracketing method, it will work as an open method as well
- Questions?



Newton's Method

- Basically finding the root of the derivative
- When the derivative equals zero a minimum or maximum has been found
- Find the roots of $g(x)=f'(x)$ using methods discussed in part 3
- Then plug x into $f(x)$ to find the value at the maximum
- Questions?

Summary

- The methods discussed today have the same weaknesses and strengths of their analogous methods for roots
- Golden Section
  - Must know the range containing a single optimum point
  - Slow
- Quadratic Interpolation
  - Like false-position, this method can get hung up on one side of the range and slowly converge
- Newton’s
  - Need first and second derivative
  - Must be ‘close’ with intial guesses
  - Fast convergence