



IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Unconstrained Single Variable Optimization: Methods and Applications

(WEEK – 5: LECTURE – 21)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Unconstrained Single Variable Optimization

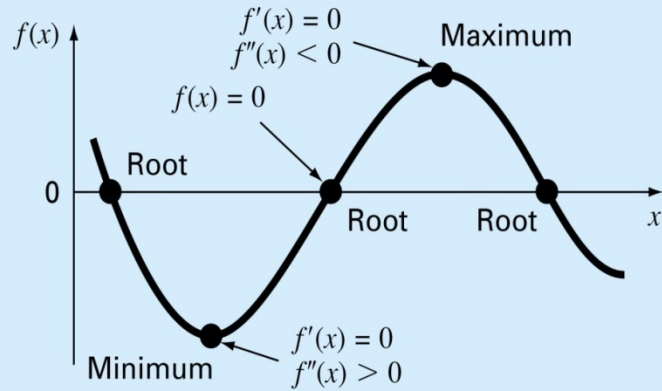
Week 5:

- General Principles of optimization algorithms
- Direct search methods
 - Bracketing method: Exhaustive search
 - Region elimination method
 - Interval halving, Fibonacci, Golden search methods
- Methods requiring derivatives
 - Newton – Raphson Method
 - Bisection method
 - Secant method

Today's Topic:

- ❑ General Principles of optimization algorithms

Unconstrained Single Variable Optimization



Root finding: searching for zeros of a function

Optimization: finding the minimum or maximum of a function

Weierstrass' Theorem

Let $X \subset \mathbb{R}^n$ be a nonempty compact set and $f : X \rightarrow \mathbb{R}$ be a continuous function on X . Then, f attains a maximum and a minimum on X ; that is, there exist $\mathbf{x}_1$ and $\mathbf{x}_2$ in X such that

$$f(\mathbf{x}_1) \geq f(\mathbf{x}) \geq f(\mathbf{x}_2) \quad \forall \mathbf{x} \in X.$$

Unconstrained Single Variable Optimization Problems

Let a function $f(x)$ is defined in the interval $a \leq x \leq b$. If point x^* , where $a < x^* < b$, is a stationary point, then $\left. \frac{df}{dx} \right|_{x=x^*} = 0$

Second order necessary
condition for a local minimum $\frac{d^2 f}{dx^2} \geq 0$

Second order necessary
condition for a local maximum $\frac{d^2 f}{dx^2} \leq 0$

Second order sufficient
condition for a local minimum $\frac{d^2 f}{dx^2} > 0$

Second order sufficient
condition for a local maximum $\frac{d^2 f}{dx^2} < 0$

A stationary point that is neither minimum nor maximum is known as *inflection point* or *saddle point*.

Unconstrained Single Variable Optimization Problems

Analytical methods are easily applied for simple objective functions. The condition $\left. \frac{df}{dx} \right|_{x=x^*} = 0$ may lead to a nonlinear equation that require numerical solution.

Analytical methods are usually difficult to apply for nonlinear objective functions with more than one variable. The necessary condition may result in n nonlinear equations which can be solved by numerical methods only.

Importance:

1. Some unconstrained problems have one variable only.
2. Many multi-variable optimization techniques require repeated use of one dimensional search methods.

$$\frac{\partial f(\mathbf{x})}{\partial x_1} = 0$$

$$\frac{\partial f(\mathbf{x})}{\partial x_2} = 0$$

$$\vdots$$

$$\frac{\partial f(\mathbf{x})}{\partial x_n} = 0$$



may result in n nonlinear equations that are difficult to solve

A General Optimization Algorithm

Consider the following unconstrained optimization problem: $\min_{x \in \mathcal{R}} f(x)$

Any optimization algorithm starts by an initial point x_0 and performs series of iterations to reach the optimal point x . At any k -th iteration, the next point is given by:

$$x_{k+1} = x_k + \alpha_k d_k$$

Here d_k is a search direction and α_k is a positive scalar determining how far to go in that direction. It is called as step length.

Since we want to minimize a function, we need:

$$f(x_{k+1}) \leq f(x_k)$$
$$f(x_k + \alpha_k d_k) \leq f(x_k)$$

d is descent
direction

A general optimization algorithm begins with an initial point, finds a descent search direction, determines the step length and checks the termination criteria.

A General Optimization Algorithm (Cont'd)

When we try to find the step length, we already know that the direction in which we are going is descent. We then want to go far enough in the descent direction so that the function reaches its minimum. Thus, given the previous point and a descent search direction, we try to find a scalar step length α such that the value of the function is minimum in that direction:

$$\min_{\alpha \geq 0} f(x + \alpha d)$$

Since, x and d are known, this problem reduces to a single variable minimization problem.

Optimality condition: $\nabla f(x + \alpha d) = 0$

All we are doing is trying to find zero of a function. This is known as line search.

Numerical Precision

Solving the first-order optimality conditions $f'(x^*) = 0$ is equivalent to finding the roots of the first derivative of the function to be minimized.

When we use computers, it may not be always possible to find the exact zero due to restriction on machine precision.

So we will be satisfied with finding an x^* that belongs to an interval $[a, b]$ such that the function f satisfies

$$f(a)f(b) < 0 \quad \text{and} \quad |a - b| < \delta$$

Scaling

Optimization algorithms use the values of objective function and derivatives of the objective function and the constraints to determine good search directions and step length. Also, function values are used to determine if constraints are satisfied or not.

The scaling of the variables and constraints determines the relative size of the derivatives and function values. For numerical reasons, it is better if all variables have roughly the same magnitude in an optimization problem. Proper scaling of the variables and constraints improves the chances of success and the quality of the solution obtained. Many software perform scaling internally without users intervention.

$$\begin{array}{ccc} 90 < L < 110 & \xrightarrow{\text{scaled}} & 0.90 < L < 1.10 \\ 0.05 < W < 0.15 & & 0.5 < W < 1.5 \end{array}$$

The objective function and constraint functions should also be scaled such that they are close to unity.

Convergence Rate

Optimization algorithms compute a sequence of approximate solutions that we hope converges to the solution. We ask: Does it converge? How fast does it converge?

Suppose you we have a sequence of points x_k ($k = 1, 2, \dots$) converging to a solution x . For a convergent sequence, we have

$$\lim_{k \rightarrow \infty} x_k - x^* = 0$$

The rate of convergence is a measure of how fast an iterative method converges to the numerical solution. An iterative method is said to converge with order r when r is the largest positive number such that

$$0 \leq \lim_{k \rightarrow \infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^r} < \infty$$

Convergence Rate (Cont'd)

$$0 \leq \lim_{k \rightarrow \infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^r} < \infty \rightarrow \lim_{k \rightarrow \infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^r} < p, \quad 0 \leq p \leq 1$$

Note if $p > 1$, the sequence will diverge

If $r = 1$, the method is said to be linearly convergent . Slow convergence. Here norm of error decreases by a constant factor at each iteration.

Also, superlinear convergence (fast): $r = 1, p = 0$. Sublinear convergence: $r = 1, p = 1$.

If $r = 2$, the method is said to be quadratically convergent. Fast convergence. If the initial error is 10^{-1} and $r = 1$, then the sequence of errors will be $10^{-1}, 10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}$, etc.

These definitions apply to single-variable and multivariable optimization problems.

Error and Convergence Criteria

- Error after k iterations:

- absolute error: $|x_k - x^*|$

- relative error: $|x_k - x^*| / |x^*|$ (defined if $x^* \neq 0$)

- Several rules to check for accuracy:

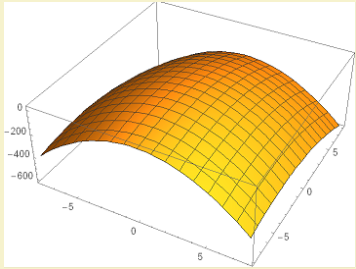
- *X vector criterion:* $|x_{k+1} - x_k| < \text{tolerance}$

- *Function criterion:* $|f(x_{k+1}) - f(x_k)| < \text{tolerance}$

- *Gradient criterion:* $|\nabla f(x_{k+1})| < \text{tolerance}$

Optimization in Chemical Engineering

Thank You





IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Unconstrained Single Variable Optimization: Methods and Applications

(WEEK – 5: LECTURE – 22)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Unconstrained Single Variable Optimization

Week 5:

- ✔ ➤ General Principles of optimization algorithms
- Direct search methods
 - Bracketing method: Exhaustive search
 - Region elimination method
 - Interval halving, Fibonacci, Golden search methods
- Methods requiring derivatives
 - Newton – Raphson Method
 - Bisection method
 - Secant method

Today's Topic:

- Direct search methods
 - Bracketing method:
 - Exhaustive search
 - Bounding phase

Unconstrained Single Variable Optimization Methods: A General Classification

We have learnt how to determine whether or not a given solution is optimal. Now we will learn how to determine the optimal or candidate optimal solutions - numerically

Classification of Single-variable Optimization Methods:

- A. Direct Search Methods: These are zero order methods (use only f)
 - ☐ Bracketing methods
 - ☐ Region Elimination methods
- B. Methods requiring derivatives: Also known as Descent methods
 - ☐ 1st order methods (use f and f')
 - ☐ 2nd order methods (use f , f' and f'')

Unimodality and Bracketing the Optimum

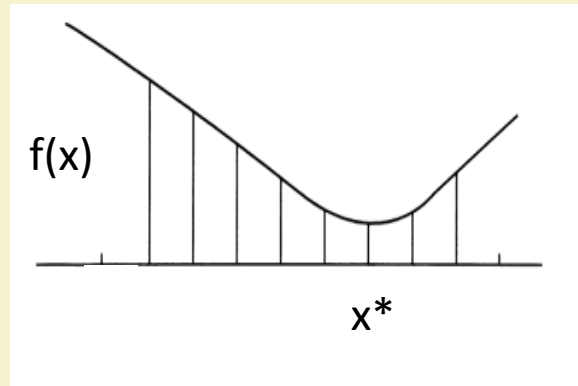
Several optimization methods require that the function to be optimized be unimodal. It means that the function has only one local minimum or maximum in a given interval.

A function of one variable is said to be unimodal if, given that two values of the variable are on the same side of the optimum, the one nearer the optimum gives the better functional value (i.e., the smaller value in the case of a minimization problem).

A function $f(x)$ is unimodal if

$x_1 < x_2 < x^*$ implies that $f(x_2) < f(x_1)$ and

$x_2 > x_1 > x^*$ implies that $f(x_1) < f(x_2)$ where x^* is the minimum point



Scanning and Bracketing the Optimum

Consider: $\min_x f(x) = (x-100)^2$ If x is unbounded ($-\infty < x < \infty$) the minimum is $x^* = 100$

How to bracket the minimum? Several strategies exist.

1. We can discretize the independent variable x by a uniform grid spacing, then look at $f(x)$
2. We can also use an accelerated procedure. $x_{k+1} = x_k + \delta \cdot 2^{k-1}$

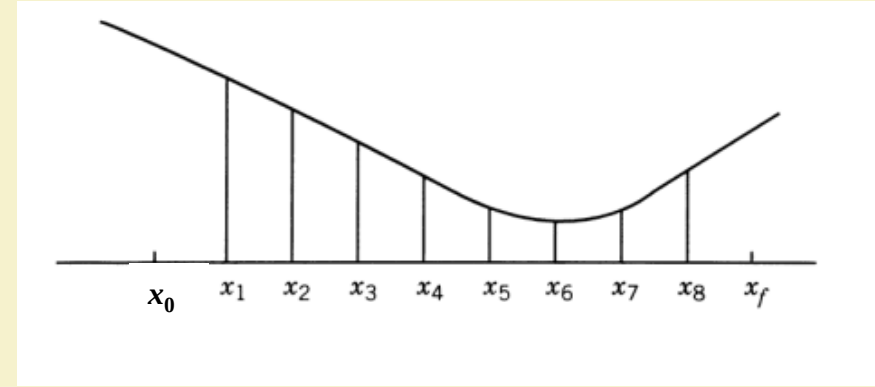
With $\delta = 1$, the minimum of $f(x)$ is bounded between $x=63$ and $x=255$ in 9 function evaluations. $63 < x^* < 255$

x	0	1	3	7	15	31	63	127	255
$f(x)$	10^4	9801	9409	8649	7225	4761	1369	729	2325

Bracketing Method: Exhaustive Search

In this method, the optimum of a function is bracketed by calculating the function values at a number of equally spaced points.

Let the function is defined on the interval (x_0, x_f) , and let it be evaluated at eight equally spaced interior points x_1 to x_8 .



Thus, the minimum must lie, according to the assumption of unimodality, between points x_5 and x_7 . Thus the interval (x_5, x_7) can be considered as the final interval of uncertainty.

This is the simplest of all other methods.

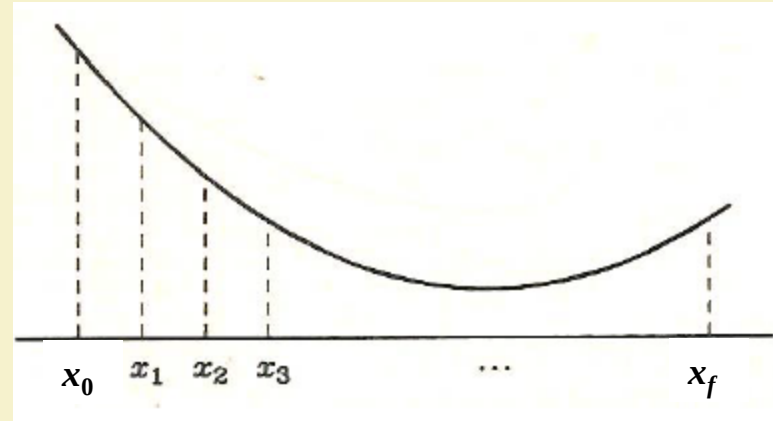
Exhaustive Search Method: Algorithm

Step – 1: Set $x_1 = x_0$, $\Delta x = (x_f - x_0) / (n + 1)$
 $x_2 = x_1 + \Delta x$, $x_3 = x_2 + \Delta x$

n = number of intermediate points

Step – 2: If $f(x_1) \geq f(x_2) \leq f(x_3)$
the minimum point lies
between (x_1, x_3) . Hence, terminate.

Step – 3: If $x_3 \leq x_f$ Go to Step – 2.
Else no minimum exists in (x_0, x_f) or a
boundary point (x_0 or x_f) is the
minimum point.



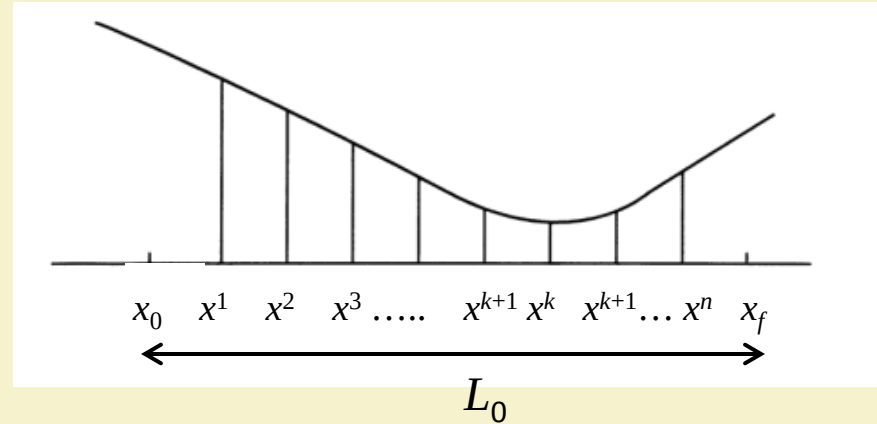
Exhaustive Search Method: Analysis

In the interval (x_0, x_f) , the objective function has been evaluated at n equally spaced points:

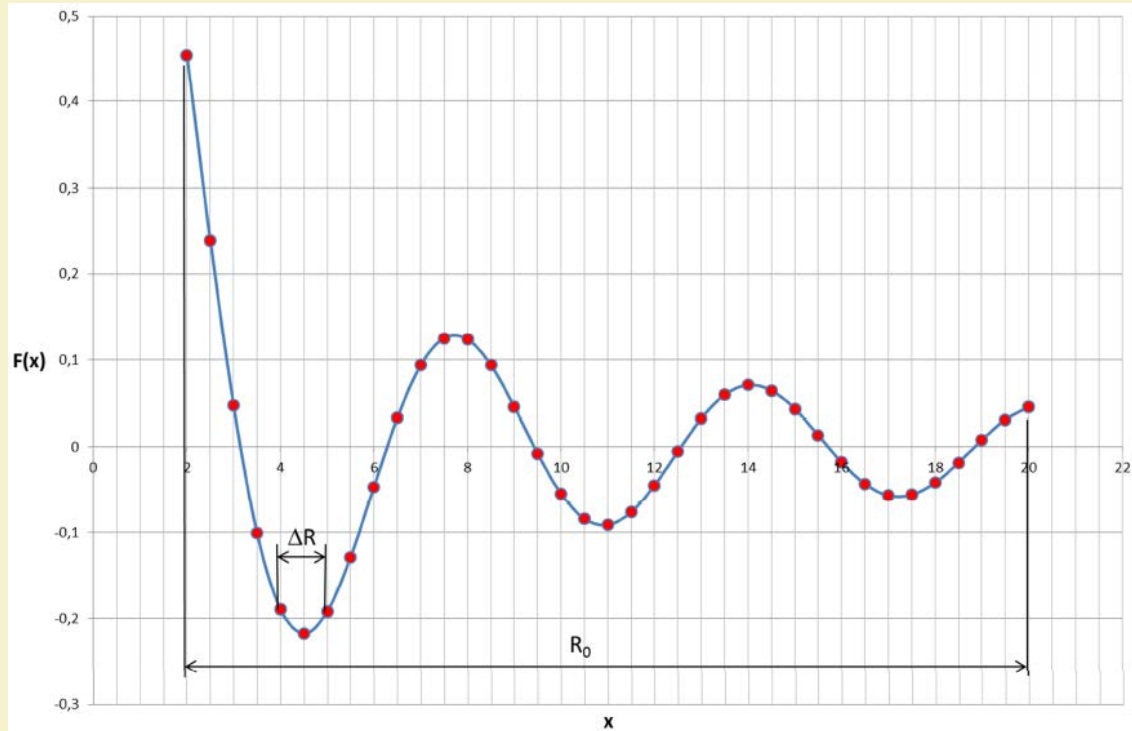
$$x_0 < x^1 < x^2 \dots < x^n < x_f$$

If the minimum value among the n function values is x^k , then the final interval of uncertainty is $[x^{k-1}, x^{k+1}]$ with length of

$$L_n = x^{k+1} - x^{k-1} = \frac{2}{n+1} L_0, \quad \text{where } L_0 = x_f - x_0$$



Exhaustive Search Method

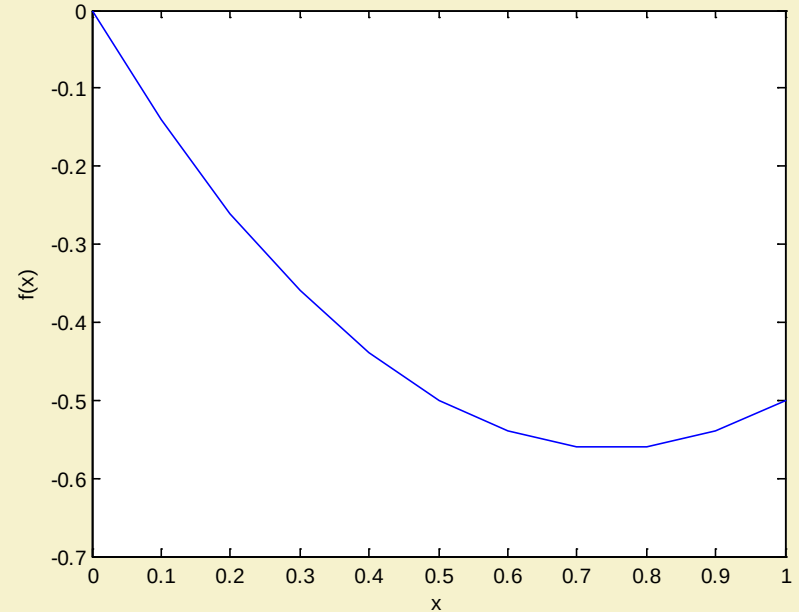


Range of
uncertainty = ΔR

Exhaustive Search Method: Example-1

Find the minimum of $f(x) = x(x - 1.5)$ in the interval $[0, 1]$ to within 10 % of the exact value.

Plot x Vs $f(x)$ for $x = 0$ to $x = 1$



Exhaustive Search Method: Example-1 (Cont'd)

Find the minimum of $f = x(x-1.5)$ in the interval $[1, 2]$ to within 10 % of the exact value.

Solution:

If the middle point of the final interval of uncertainty is taken as the approximate optimal point, the maximum deviation could be $1/(n+1)$ times the initial interval of uncertainty. Thus, to find the optimum within 10% of the exact value, we should have $\frac{1}{n+1} \leq \frac{1}{10}$ or $n \geq 9$

i	1	2	3	4	5	6	7	8	9
x_i	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$f(x_i)$	-0.14	-0.26	-0.36	-0.44	-0.50	-0.54	-0.56	-0.56	-0.54



Exhaustive Search Method: Homework

Let heat loss from a closed chamber is expressed as: $Q = \frac{1}{x} + 10 \frac{\text{kJ}}{\text{h}}$ where x is the insulation thickness in cm.

It will cost Rs. 50 to generate 1kJ of heat by furnace and insulation will cost Rs. 100/year for each centimetre of thickness over the course of its lifetime. What is the optimal insulation thickness that minimizes the total cost of lost heat and insulation?

Cost of heat loss:

$$C_{T,heat} = \left(\left(\frac{1}{x} + 10 \right) \frac{\text{kJ}}{\text{h}} \right) \left(24 \frac{\text{h}}{\text{day}} \right) \left(365 \frac{\text{day}}{\text{yr}} \right) \left(50 \frac{\text{Rs}}{\text{kJ}} \right) = \frac{438000}{x} + 4380000 \frac{\text{Rs}}{\text{yr}}$$

Exhaustive Search Method: Homework (Cont'd)

Cost of heat loss:

$$C_{T,heat} = \left(\left(\frac{1}{x} + 10 \right) \frac{\text{kJ}}{\text{h}} \right) \left(24 \frac{\text{h}}{\text{day}} \right) \left(365 \frac{\text{day}}{\text{yr}} \right) \left(50 \frac{\text{Rs}}{\text{kJ}} \right) = \left(\frac{438000}{x} + 4380000 \right) \frac{\text{Rs}}{\text{yr}}$$

Cost of insulation: $C_{T,ins} = 100x \frac{\text{Rs}}{\text{yr}}$

Total cost: $C_{T,total} = \left(\frac{438000}{x} + 4380000 + 100x \right) \frac{\text{Rs}}{\text{yr}}$

Use necessary condition: $\frac{d}{dx} C_{T,total} = -\frac{438000}{x^2} + 100 = 0$
 $\Rightarrow x^2 = 4380 \Rightarrow x = 66.18$

Check sufficient condition:

$$\begin{aligned} \frac{d^2}{dx^2} C_{T,total} &= (2) \frac{438000}{x^3} \\ &= \frac{876000}{x^3} > 0 \text{ at } x = 66.18 \end{aligned}$$

Bracketing Method: Bounding Phase Method

Bounding phase method guarantees to bracket the minimum of a unimodal function.

1. Starting with an initial guess, find a search direction based on two or more function evaluations in the neighborhood of the initial guess.
2. Then an exponential search strategy is used to reach the optimum (Swann's method).

Select initial guess $x^{(0)}$ and an increment Δ

If $f(x^{(0)} - |\Delta|) \geq f(x^{(0)}) \geq f(x^{(0)} + |\Delta|)$, then the minimum lies to the RHS of $x^{(0)}$

If $f(x^{(0)} - |\Delta|) \geq f(x^{(0)}) \leq f(x^{(0)} + |\Delta|)$, then the minimum lies between $(x^{(0)} - |\Delta|)$ and $(x^{(0)} + |\Delta|)$

Note: $f(x^{(0)} - |\Delta|) \leq f(x^{(0)}) \geq f(x^{(0)} + |\Delta|)$, is ruled out by unimodality assumption

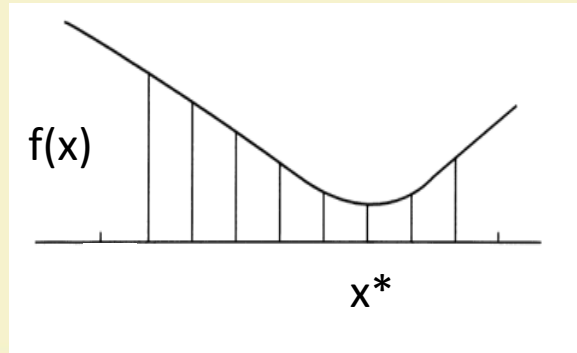
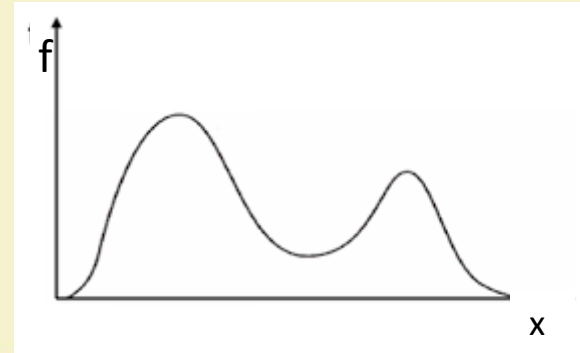
Bracketing Method: Bounding Phase Method

Select initial guess $x^{(0)}$ and an increment Δ

If $f(x^{(0)} - |\Delta|) \geq f(x^{(0)}) \geq f(x^{(0)} + |\Delta|)$, then the minimum lies to the RHS of $x^{(0)}$

If $f(x^{(0)} - |\Delta|) \geq f(x^{(0)}) \leq f(x^{(0)} + |\Delta|)$, then the minimum lies between $(x^{(0)} - |\Delta|)$ and $(x^{(0)} + |\Delta|)$

Note: $f(x^{(0)} - |\Delta|) \leq f(x^{(0)}) \geq f(x^{(0)} + |\Delta|)$, is ruled out by unimodality assumption



Bounding Phase Method: Algorithm

Step – 1: Set iteration counter $k = 0$.

Select initial guess $x^{(0)}$ and an increment Δ

Step – 2: If $f(x^{(0)} - |\Delta|) \geq f(x^{(0)}) \geq f(x^{(0)} + |\Delta|)$, then $\Delta > 0$

else if $f(x^{(0)} - |\Delta|) \leq f(x^{(0)}) \leq f(x^{(0)} + |\Delta|)$, then $\Delta < 0$

else go to *Step – 1*

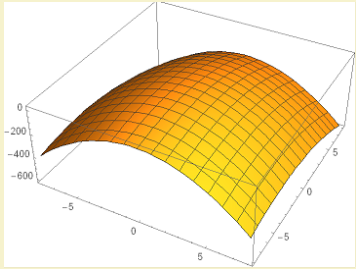
Step – 3: Set $x^{(k+1)} = x^{(k)} + 2^k \Delta$

Step – 4: If $f(x^{(k+1)}) < f(x^{(k)})$, set $k = k + 1$ and go to *Step – 3*

else the minimum lies in the interval $(x^{(k-1)}, x^{(k+1)})$. Stop.

Optimization in Chemical Engineering

Thank You





IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Unconstrained Single Variable Optimization: Methods and Applications

(WEEK – 5: LECTURE – 23)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Unconstrained Single Variable Optimization

Week 5:

- ✓ ➤ General Principles of optimization algorithms
- Direct search methods
 - ✓ ➤ Bracketing method: Exhaustive search
 - Region elimination method
 - Interval halving, Fibonacci, Golden search methods
- Methods requiring derivatives
 - Newton – Raphson Method
 - Bisection method
 - Secant method

Today's Topic:

- Direct search methods
 - Region elimination method
 - Dichotomous search
 - Interval halving

Unconstrained Single Variable Optimization Methods: A General Classification

We have learnt how to determine whether or not a given solution is optimal. Now we will learn how to determine the optimal or candidate optimal solutions - numerically

Classification of Single-variable Optimization Methods:

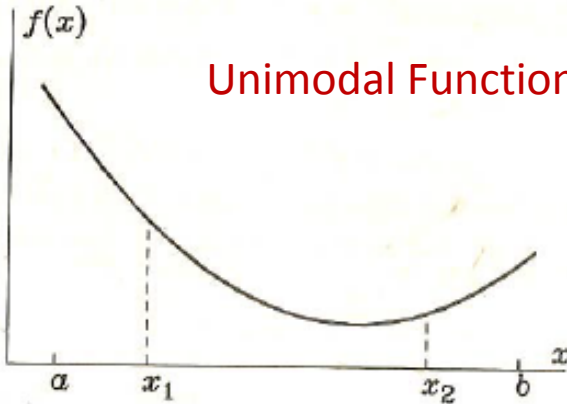
- A. Direct Search Methods: These are zero order methods (use only f)
 - ☐ Bracketing methods
 - ☐ Region Elimination methods
- B. Methods requiring derivatives: Also known as Descent methods
 - ☐ 1st order methods (use f and f')
 - ☐ 2nd order methods (use f , f' and f'')

Region Elimination Method

Direct Search methods that locate optimal point of a single-variable function by successively eliminating subintervals so as to reduce the remaining interval of search are called Region Elimination methods.

After we have bracketed the optimum (minimum) point, Region Elimination method can be used to improve the accuracy of the solution.

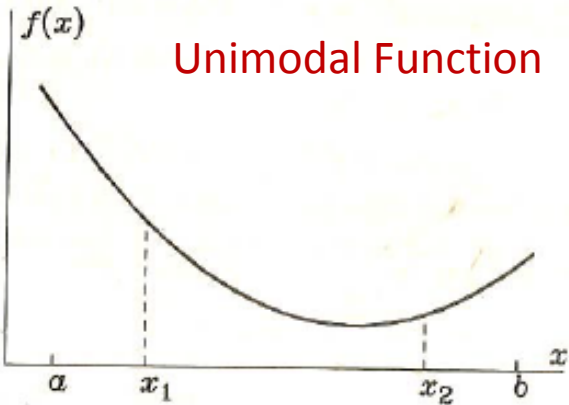
Unimodal Function



Fundamental Rule for Region Elimination

If	Then minimum does not lie in
$f(x_1) > f(x_2)$	(a, x_1)
$f(x_1) < f(x_2)$	(x_2, b)
$f(x_1) = f(x_2)$	(a, x_1) and (x_2, b)

Region Elimination Method: How to Place Trial Points?



Fundamental Rule for Region Elimination

If	Then minimum does not lie in
$f(x_1) > f(x_2)$	(a, x_1)
$f(x_1) < f(x_2)$	(x_2, b)
$f(x_1) = f(x_2)$	(a, x_1) and (x_2, b)

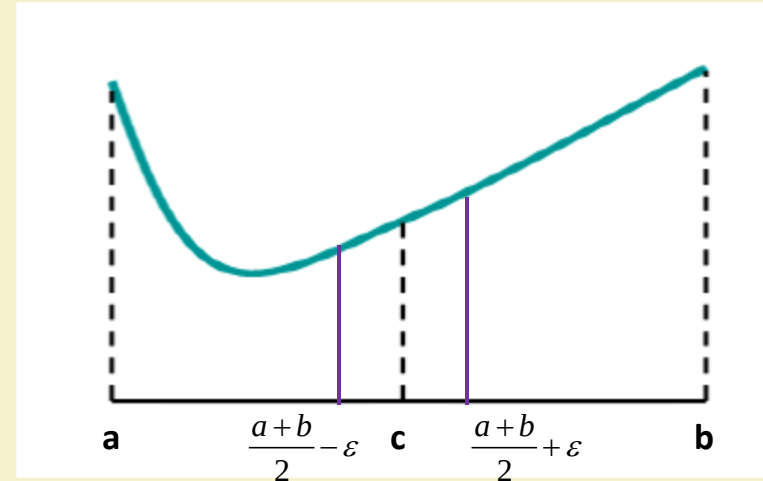
Note that depending on function values, we will delete $[a, x_1]$, $[x_2, b]$ or both. In order to reduce the interval of uncertainty, we would like to maximize the length of $[a, x_1]$ or $[x_2, b]$. To maximize both, we should place x_1 and x_2 symmetrically in the interval $[a, b]$.

Region Elimination Method: Dichotomous Search

Let the optimum lie between $[a, b]$. The dichotomous method first computes the mid-point as $(a+b)/2$ and then move slightly to either side of the mid-point to compute two test-points: $\frac{a+b}{2} \pm \varepsilon$

Based on the function values and unimodality assumption, the interval is updated by eliminating one part and the procedure continues until the optimal solution is contained in a small interval.

This method is also known as method of bisection.



Dichotomous Method: Algorithm

Consider: $\min_x f(x)$

Given: Initial interval of uncertainty, $[a, b]$

Set iteration counter $k = 0$, $a^k = a$, $b^k = b$, $\varepsilon > 0$,

L = final length of uncertainty

The final interval of uncertainty
after n experiments (n is even):

$$L_n = \frac{b-a}{2^{n/2}} + \varepsilon \left(1 - \frac{1}{2^{n/2}}\right)$$

While $(b^k - a^k) > L$

$$\alpha^k = \frac{a^k + b^k}{2} - \varepsilon, \quad \beta^k = \frac{a^k + b^k}{2} + \varepsilon$$

if $f(\alpha^k) \geq f(\beta^k)$

$$a^{k+1} = \alpha^k, b^{k+1} = b^k$$

else

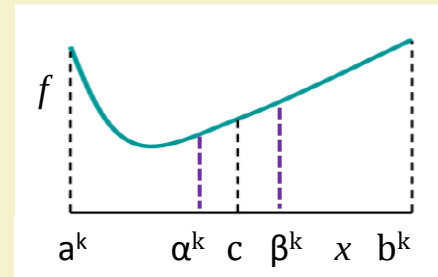
$$b^{k+1} = \beta^k, a^{k+1} = a^k$$

end if

$$k = k + 1$$

end while

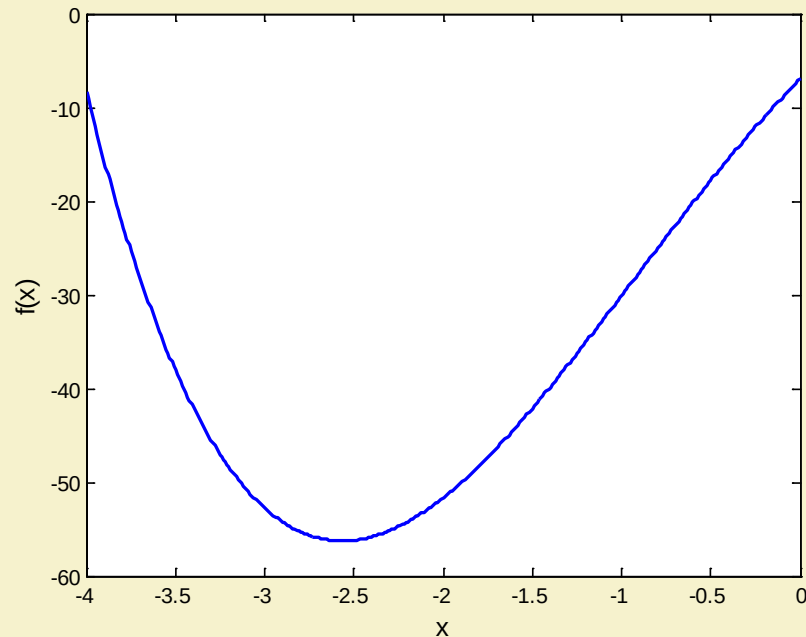
$$\text{output: } x^* = \frac{a^k + b^k}{2}$$



Dichotomous Method: Example

Consider: $\min_x f(x) = \frac{1}{4}x^4 - \frac{5}{3}x^3 - 6x^2 + 19x - 7$

Use $\varepsilon = 0.01$



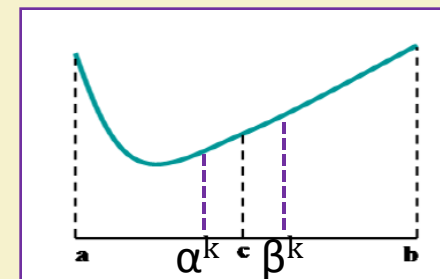
Dichotomous Method: Example

Consider: $\min_x f(x) = \frac{1}{4}x^4 - \frac{5}{3}x^3 - 6x^2 + 19x - 7$

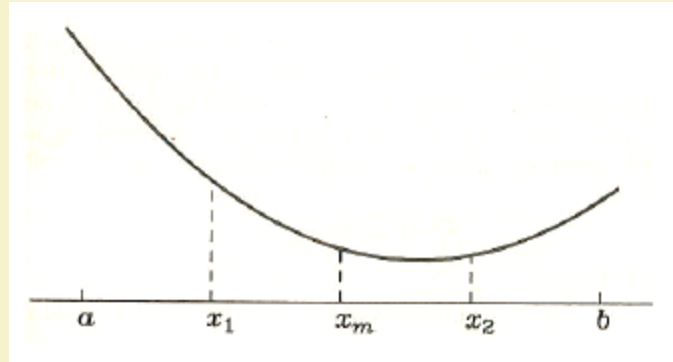
Solution: $x^* = -2.56$, $f(x^*) = -56.26$

k	a^k	b^k	$b^k - a^k$	$f(a^k)$	$f(b^k)$
0	-4	0	4	-8.33	-7
1	-4	-1.99	2.01	-8.33	-51.66
2	-3.00	-1.99	1.01	-52.74	-51.66
3	-3.00	-2.49	0.51	-52.74	-56.19
..	..	..	..	..	..
9	-2.5704	-2.5624	0.0080	-56.2622	-56.2625
10	-2.5665	-2.5624	0.0003	-56.2626	-56.2625

Use $\epsilon = 0.01$



Region Elimination: Interval Halving Method



Once the optimum has been bracketed, Region Elimination method gives us a more refined estimate of the optimum by eliminating a certain amount of subinterval at each step.

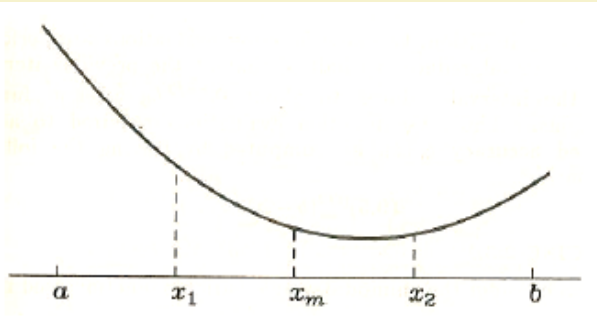
Interval Halving method eliminates exactly one-half of the interval at each stage by considering three equally spaced trial points. These 3 points divide the interval $[a, b]$ into 4 equal regions.

If $f(x_1) < f(x_m)$, the minimum can not lie beyond x_m . Eliminate $[x_m \text{ to } b]$, this is 50%.

If $f(x_1) > f(x_m)$, the minimum can not lie in $[a, x_1]$. Eliminate this $[a, x_1]$, which is 25%.

Compare function value at x_m and x_2 to eliminate further 25% of the search space.

Region Elimination: Interval Halving Method: Algorithm



Step – 1: Given : $x^* \in [a, b]$, $L_0 = L = (b - a)$, $\varepsilon > 0$

Let $x_m = (a + b) / 2$, Evaluate $f(x_m)$

Step – 2: Set $x_1 = a + L / 4$, $x_2 = b - L / 4$. Evaluate $f(x_1)$, $f(x_2)$

Step – 3: If $f(x_1) < f(x_m)$, set $b = x_m$; $x_m = x_1$; go to *Step – 5*;

Else go to *Step – 4*

Step – 4: If $f(x_2) < f(x_m)$, set $a = x_m$; $x_m = x_2$; go to *Step – 5*;

Else set $a = x_1$; $b = x_2$; go to *Step – 5*

Step – 5: Evaluate $L = (b - a)$. If $|L| < \varepsilon$, Stop;

Else go to *Step – 2*

Interval Halving Method: Analysis

At each stage of the algorithm, exactly half the length of the search interval is removed.

The mid-point of subsequent intervals is always equal to one of the previous trial points – x_1 , x_2 , or x_m . Thus at most two function evaluations are necessary at each subsequent step.

The interval of uncertainty remaining at the end of n function evaluations ($n \geq 3$ and odd) is given by

$$L_n = \left(\frac{1}{2}\right)^{(n-1)/2} L_0$$

Interval Halving Method: Example

Find the minimum of $f(x) = x(x-1.5)$ in the interval $[0, 1]$ to within 10% of the exact value.

Solution:

If the middle point of the final interval of uncertainty is taken as the optimum point, the specified accuracy can be achieved if:

$$\frac{1}{2}L_n \leq \frac{L_0}{10} \quad \text{or} \quad \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \leq \frac{L_0}{5}$$

Since $L_0=1$, we can write

$$\frac{1}{2^{(n-1)/2}} \leq \frac{1}{5} \quad \text{or} \quad 2^{(n-1)/2} \geq 5 \quad \Rightarrow n = 7 \text{ (} n \text{ is odd)}$$

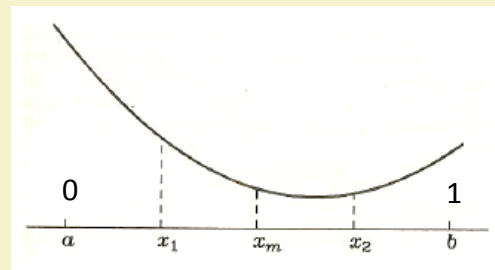
Interval Halving Method: Example (Cont'd)

Stage: 1

$$x_1 = 0.25, \quad f_1 = 0.25(-1.25) = -0.3125$$

$$x_m = 0.50, \quad f_m = 0.50(-1.0) = -0.5000$$

$$x_2 = 0.75, \quad f_2 = 0.75(-0.75) = -0.5625$$



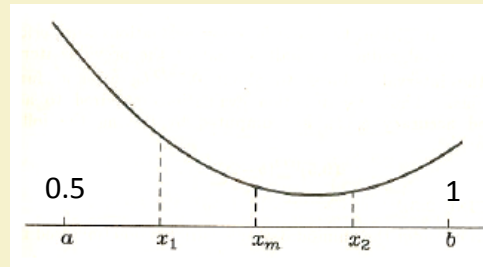
Since $f_1 > f_m > f_2$, delete the interval $[a, x_m] = [0.0, 0.5]$. Now set x_2 and x_m as the new x_m and a , respectively. Thus now $a=0.5$, $x_m=0.75$, and $b=1.0$. Divide the new interval of uncertainty $[0.5, 1.0]$ into four equal parts and go to Stage-2.

Stage: 2

$$x_1 = 0.625, \quad f_1 = 0.625(-0.875) = -0.546875$$

$$x_m = 0.750, \quad f_m = 0.750(-0.750) = -0.562500$$

$$x_2 = 0.875, \quad f_2 = 0.875(-0.625) = -0.546875$$



Interval Halving Method: Example (Cont'd)

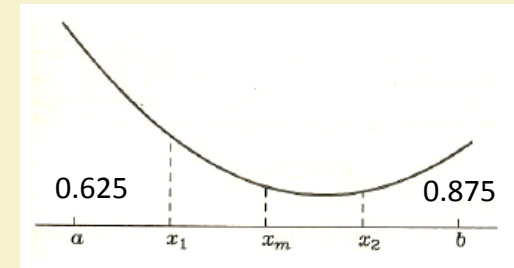
Since $f_1 > f_m$ and $f_2 > f_m$, delete both the intervals $[a, x_1]$ and $[x_2, b]$. Set x_1 , x_m and x_2 as the new a , x_m , and b , respectively. The new interval of uncertainty will be $[0.625, 0.875]$. Divide this interval into four equal parts and go to Stage-3.

Stage: 3

$$x_1 = 0.6875, \quad f_1 = 0.6875(-0.8125) = -0.558594$$

$$x_m = 0.75, \quad f_m = 0.75(-0.75) = -0.5625$$

$$x_2 = 0.8125, \quad f_2 = 0.8125(-0.6875) = -0.558594$$

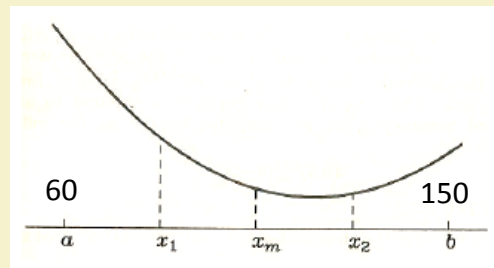


Continue like this and obtain $x_{\text{opt}} \simeq 0.75$

Interval Halving Method: Homework

Consider: $\min_x f(x) = (100 - x)^2$

Find x_{opt} by Interval Halving method. Take $x = [60, 150]$

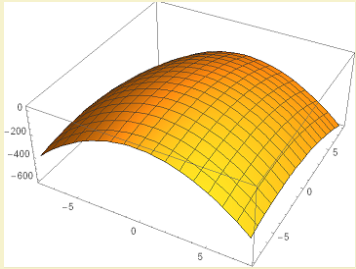


Note: $x_{\text{opt}} = 100$.

Perform 3 iterations and see that the mid-point of the interval after 3 iterations is already 99.375.

Optimization in Chemical Engineering

Thank You





IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Unconstrained Single Variable Optimization: Methods and Applications

(WEEK – 5: LECTURE – 24)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Unconstrained Single Variable Optimization

Week 5:

- ✓ ➤ General Principles of optimization algorithms
- Direct search methods
 - ✓ ➤ Bracketing method: Exhaustive search
 - ⚠ ➤ Region elimination method
 - Interval halving, Fibonacci, Golden search methods
- Methods requiring derivatives
 - Newton – Raphson Method
 - Bisection method
 - Secant method

Today's Topic:

- Direct search methods
 - Region elimination method
 - Golden section search
 - Fibonacci search

Region Elimination Methods

Consider that we have an interval of uncertainty and the function has been evaluated at the boundaries. In order to reduce the interval of uncertainty, we have to evaluate two new points inside the interval at every iteration.

In case of Dichotomous search or Interval Halving method, although the function value at an interior point is available at the beginning of every new iteration, it is not used.

Fibonacci Search method and the Golden Section Search method use the available function value at an interior point and thus they require only one function evaluation for every iteration – except for the first iteration where they require two function evaluations.

Region Elimination: Fibonacci Search Method



Fibonacci

Fibonacci search method uses the sequence of Fibonacci numbers, $\{F_n\}$, to reduce the interval of uncertainty. These numbers are defined as:

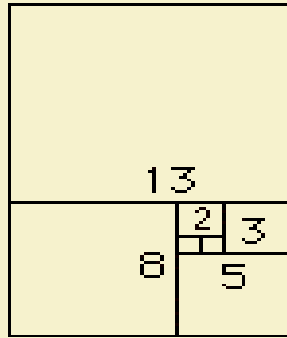
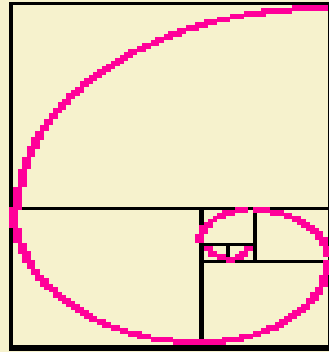
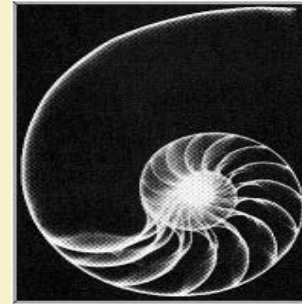
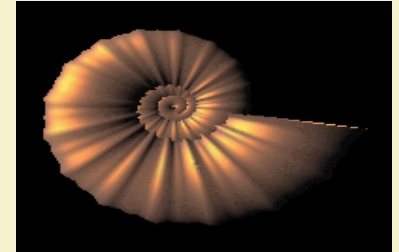
$$F_0 = F_1 = 1$$

$$F_n = F_{n-1} + F_{n-2}, \quad n = 2, 3, 4, \dots$$

Each number after the first two represents the sum of the preceding two.

First few Fibonacci numbers are: 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89,...

The Fibonacci Numbers in Nature



Fibonacci spiral found in both snail and sea shells

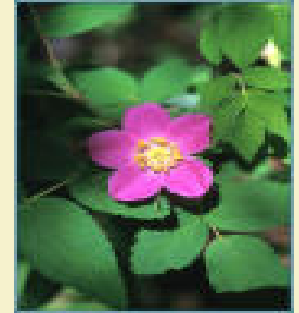
The Fibonacci Numbers in Nature



3 petals



5 petals



13 petals



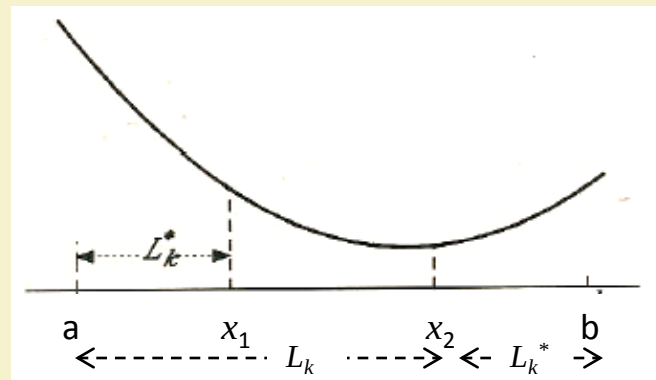
21 petals

Fibonacci Search Method: How Does it Work?

In this search, at each iteration the length of the interval is chosen according to the Fibonacci numbers.

$$F_0 = F_1 = 1$$

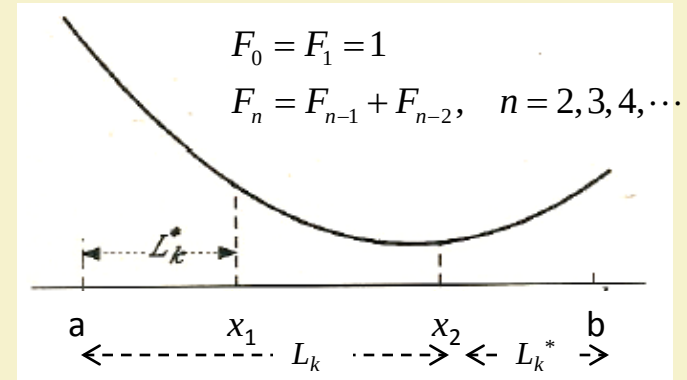
$$F_n = F_{n-1} + F_{n-2}, \quad n = 2, 3, 4, \dots$$



We require two points for region elimination. In Fibonacci search, out of these two points, one is always the previous point and the other point is new. Therefore, only one function evaluation is required at each iteration for Fibonacci search method.

Fibonacci Search Method: How Does it Work?

Let the initial interval is $L = (b - a)$. At iteration k , two intermediate points are chosen so that each is L_k^* distance away from either end. Now a part of region is eliminated based on function values. After region elimination, the remaining interval is L_k .



If we define: $L_k^* = \left(\frac{F_{n-k+1}}{F_{n+1}} \right) L$ and $L_k = \left(\frac{F_{n-k+2}}{F_{n+1}} \right) L$, then $L_k - L_k^* = L_{k+1}^*$

Thus any of the two points used in iteration k remains as a point in $(k+1)$ iteration.

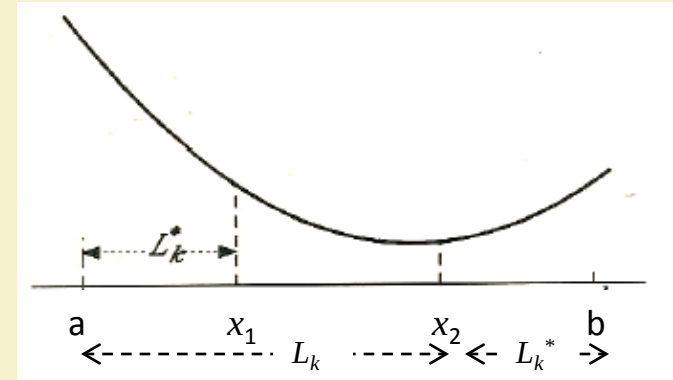
Fibonacci Search Method: Algorithm

Step – 1: Given : $x^* \in [a, b]$, $L = (b - a)$,
 n = number of function evaluations,
Set iteration counter $k = 2$

Step – 2: Set $L_k^* = \left(\frac{F_{n-k+1}}{F_{n+1}} \right) L$; $x_1 = a + L_k^*$; $x_2 = b - L_k^*$

Step – 3: Evaluate $f(x_1)$ or $f(x_2)$ – one will be known from previous step.
Use unimodality of function to eliminate a part of the interval.
Set new a and b .

Step – 4: If $k = n$, Stop;
Else set $k = k + 1$ and go to Step – 2



Fibonacci Search Method: Analysis

Fibonacci numbers have to be calculated and stored at the start of algorithm. At every iteration the proportion of the eliminated region is not the same. Number of iterations required need to be specified in advance.

Fibonacci algorithm is optimum in the sense that it gives the largest ratio of initial to final interval for a fixed number of function evaluations.

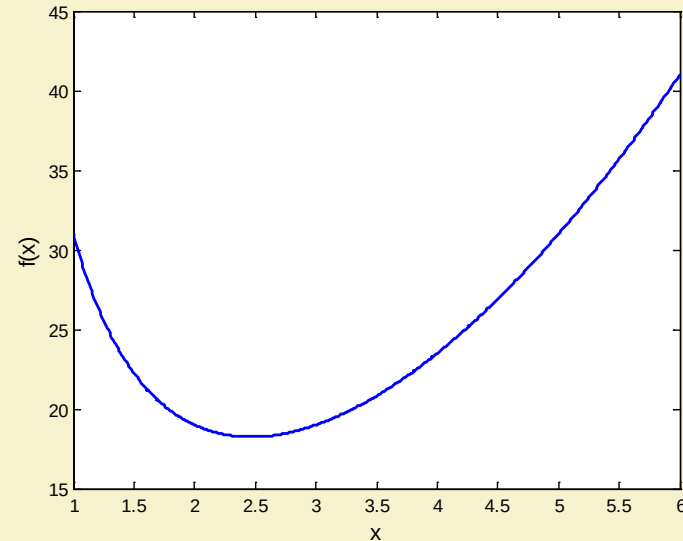
After n function evaluations, the interval of uncertainty reduces to: $\frac{2}{F_{n+1}}(b-a)$

Thus for a desired accuracy δ , the number of function evaluations required can be computed from: $\frac{2}{F_{n+1}}(b-a) = \delta$

Fibonacci Search Method: Example

Using Fibonacci search method, minimize the following function in the interval $x = [1, 6]$.
Perform 3 iterations ($n = 3$).

$$\min_x f(x) = x^2 + \frac{30}{x}$$



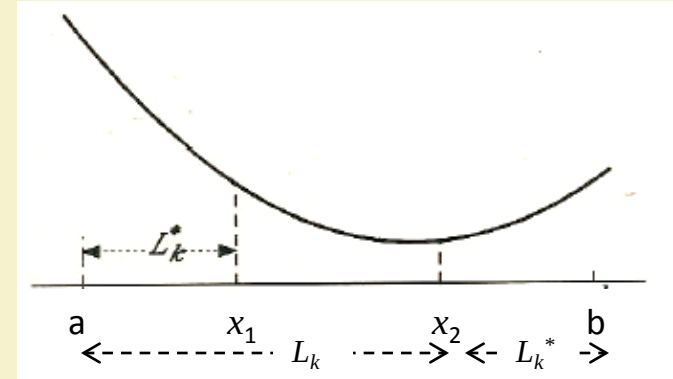
Fibonacci Search Method: Example (Cont'd)

$$\min_x f(x) = x^2 + \frac{30}{x} \quad x = [1, 6].$$

Iteration-1, Step-1:

$a = 1$; $b = 6$; Initial interval, $L = (b-a) = (6-1) = 5$.

$n = 3$. Set iteration counter $k = 2$.



Iteration-1, Step-2:

$$L_2^* = \left(\frac{F_{n-k+1}}{F_{n+1}} \right) L = \left(\frac{F_{3-2+1}}{F_{3+1}} \right) L = \left(\frac{F_2}{F_4} \right) L = \left(\frac{2}{5} \right) 5 = 2$$

Thus, $x_1 = (a + L_2^*) = (1 + 2) = 3$; $x_2 = (b - L_2^*) = (6 - 2) = 4$

Fibonacci numbers are: 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89,...

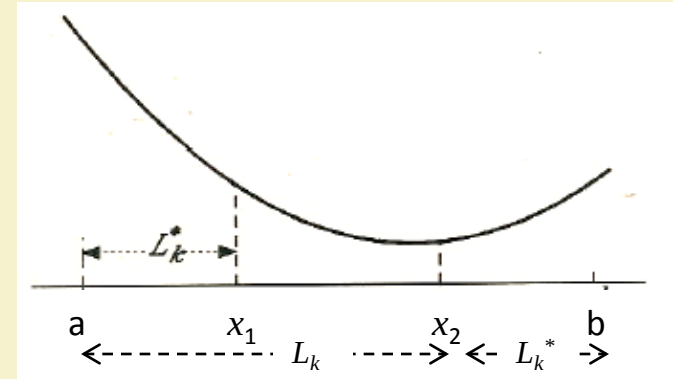
Fibonacci Search Method: Example (Cont'd)

Iteration-1, Step-3:

Compute: $f(x_1) = f(3) = 19$; $f(x_2) = f(4) = 23.5$

Since $f(x_1) < f(x_2)$, we eliminate $[x_2, b] = [4, 6]$

Set $a = 1$; $b = 4$



First iteration complete.

Fibonacci Search Method: Example (Cont'd)

Iteration-2, Step-2:

$$L_3^* = \left(\frac{F_{3-3+1}}{F_{3+1}} \right) L = \left(\frac{F_1}{F_4} \right) L = \left(\frac{1}{5} \right) 5 = 1$$

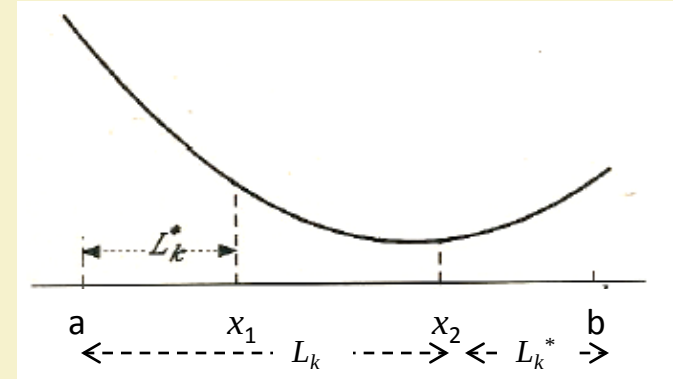
Thus, $x_1 = 1 + 1 = 2$; $x_2 = 4 - 1 = 3$

Iteration-2, Step-3:

Compute: $f(x_1) = f(2) = 19$; $f(x_2) = f(3) = 19$

Since $f(x_1) = f(x_2)$, we eliminate $[a, x_1] = [1, 2]$
and $[x_2, b] = [3, 4]$

Set $a = 2$; $b = 3$ **Second iteration complete.**



Minimum is bracketed between $[2, 3]$. In actual practice, we should consider higher value of n and proceed as shown.

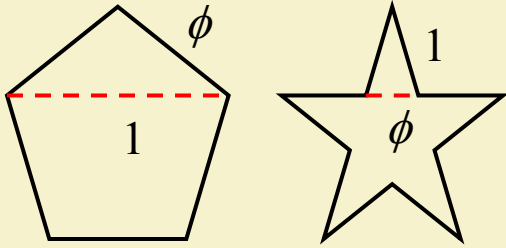
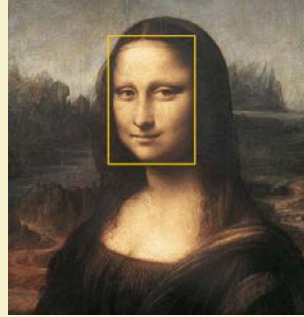
Region Elimination: Golden Section Search Method

Two numbers, p and q, are in a golden ratio if $\frac{p}{p+q} = \frac{q}{p}$

We can write this as: $\frac{q}{p} = \tau \quad \Rightarrow \quad 1 + \tau = \frac{1}{\tau} \quad \Rightarrow \quad \tau^2 + \tau - 1 = 0$

By solving: $\tau = \frac{-1 + \sqrt{1 - 4(-1)}}{2} = \frac{\sqrt{5} - 1}{2} = 0.61803\dots$ Golden ratio

Golden Section Search Method: Golden Ratio



The Parthenon in Athens, Greece

Golden Ratio and Fibonacci Numbers

Fibonacci sequence:

$$F_0 = F_1 = 1$$

$$F_n = F_{n-1} + F_{n-2}, \quad n = 2, 3, 4, \dots$$

First few Fibonacci numbers are:

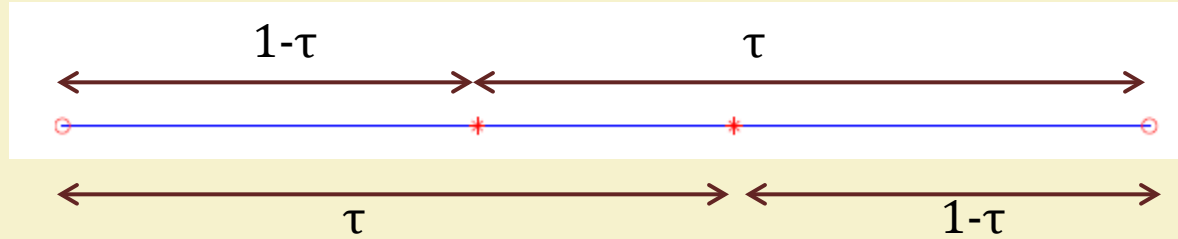
1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ...

Consider the ratio of consecutive numbers in Fibonacci sequence:

$0/1 = 0$, $1/1 = 1$, $1/2 = 0.5$, $2/3 = 0.667$, $3/5 = 0.6$, $5/8 = 0.625$, $8/13 = 0.615$, $13/21 = 0.619$,
 $34/21 = 0.617$, and so on.

As one proceeds, the ratio of consecutive numbers approaches the golden ratio.

Golden Section Search Method: Algorithm



1. Start with a unit interval for convenience. Thus the given interval may be scaled to $[0, 1]$.
2. Place two trial points a fraction τ from either end.
3. Suppose RHS subinterval is eliminated. The remaining subinterval has length τ and it has one old trial point located interior to it at a distance $(1-\tau)$ from the left endpoint.
4. Each subsequent iteration will eliminate $(1-\tau)$ of the remaining interval. Thus after n function evaluation, the interval remaining will be τ^{n-1}

Golden Section Search Method: Algorithm

Note:

We require two points for region elimination. Out of these two points, one is always the previous point and the other point is new. Therefore, only one function evaluation is required at each iteration. Also equal portion is eliminated always.

Step – 1: Given : $x^* \in [a, b]$, $L = (b - a)$, $\varepsilon > 0$

Normalize the variable x by: $w = (x - a) / (b - a)$

Thus $a_w = 0, b_w = 1, L_w = 1$. Set iteration counter $k = 1$

Step – 2: Set $w_1 = a_w + 0.618L_w$; $w_2 = b_w - 0.618L_w$

Step – 3: Evaluate $f(w_1)$ or $f(w_2)$ – one will be known from previous step.

Use unimodality of function to eliminate a part of the interval.

Set new a_w and b_w .

Step – 4: If $|L_w| < \varepsilon$, Stop;

Else set $k = k + 1$ and go to *Step – 2*

Golden Section Search Method: Example

$$\min_x f(x) = (100 - x)^2, \quad 60 \leq x \leq 150$$

Solution:

Let us first rescale the given interval $[60, 150]$ to $[0, 1]$ and reformulate the problem:

$$w = \frac{x - 60}{150 - 60} = \frac{x - 60}{90}$$

$$\min_x f(w) = (40 - 90w)^2, \quad 0 \leq w \leq 1$$

Golden Section Search Method: Example

$$\min_x f(w) = (40 - 90w)^2, \quad 0 \leq w \leq 1$$

Iteration-1:

$$a_w = 0; b_w = 1;$$

$$\text{Initial interval, } L_w = (b_w - a_w) = (1 - 0) = 1.$$

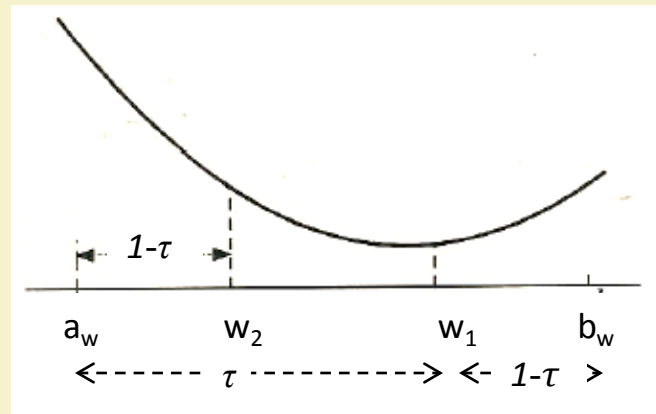
$$w_1 = a_w + \tau L_w = 0 + (0.618)1 = 0.618;$$

$$w_2 = b_w - \tau L_w = 1 - (0.618)1 = 0.382$$

$$f(w_1) = 244; f(w_2) = 31.6$$

Since $f(w_2) < f(w_1)$ and $w_2 < w_1$, the interval $w \geq w_1$ is eliminated

$$\text{Set } a_w = 0; b_w = 0.618; L_w = 0.618 - 0 = 0.618$$



Golden Section Search Method: Example

Iteration-2:

$$a_w = 0; b_w = 0.618;$$

$$\text{Interval, } L_w = (b_w - a_w) = (0.618 - 0) = 0.618$$

$$w_1 = a_w + \tau L_w = 0 + (0.618)(0.618) = 0.382;$$

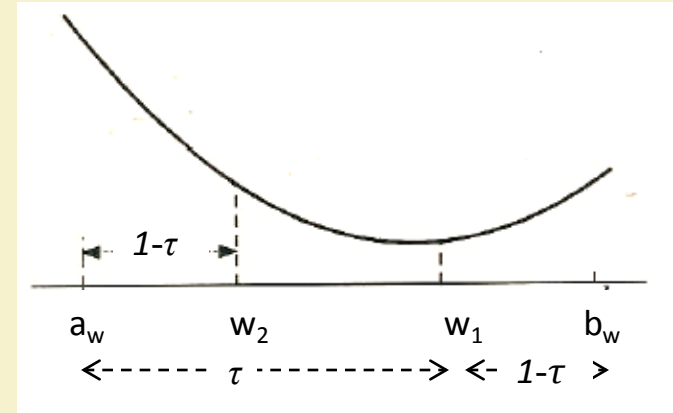
$$w_2 = b_w - \tau L_w = 0.618 - (0.618)(0.618) = 0.236;$$

Note : w_1 was computed in previous iteration.

$$f(w_1) = 31.6; f(w_2) = 352$$

Since $f(w_2) > f(w_1)$ and $w_2 < w_1$, the interval $w \leq w_2$ is eliminated

$$\text{Set } a_w = 0.236; b_w = 0.618; L_w = 0.618 - 0.236 = 0.382$$



Golden Section Search Method: Example

Iteration-3:

$$a_w = 0.236; b_w = 0.618;$$

$$\text{Interval, } L_w = (b_w - a_w) = (0.618 - 0.236) = 0.382$$

$$w_1 = a_w + \tau L_w = 0.236 + (0.618)(0.382) = 0.472;$$

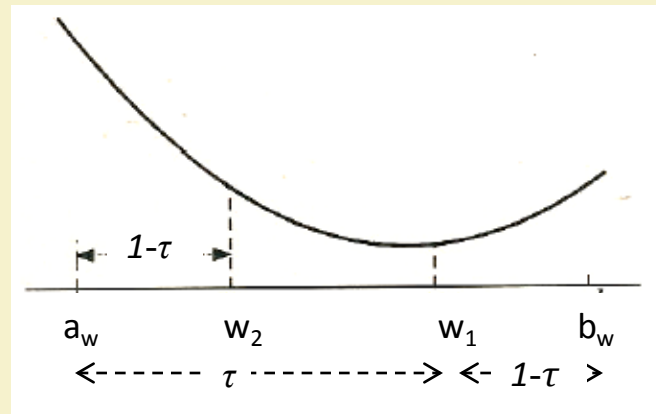
$$w_2 = b_w - \tau L_w = 0.618 - (0.618)(0.382) = 0.382;$$

Note : w_2 was computed in previous iteration.

$$f(w_1) = 6.15; f(w_2) = 31.6$$

Since $f(w_1) < f(w_2)$ and $w_1 > w_2$, the interval $w \leq w_2$ is eliminated

$$\text{Set } a_w = 0.382; b_w = 0.618; L_w = 0.618 - 0.382 = 0.236$$



We now have

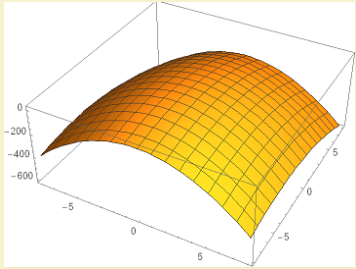
$$0.382 \leq w \leq 0.618$$

$$\Rightarrow 94.4 \leq x \leq 115.6$$

Continue to get x close to 100

Optimization in Chemical Engineering

Thank You





IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Unconstrained Single Variable Optimization: Methods and Applications

(WEEK – 5: LECTURE – 25)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Unconstrained Single Variable Optimization

Week 5:

- General Principles of optimization algorithms
- Direct search methods
 - Bracketing method: Exhaustive search
 - Region elimination method
 - Interval halving, Fibonacci, Golden search methods
- Methods requiring derivatives
 - Newton – Raphson Method
 - Bisection method
 - Secant method

➤ Today's Topic:

- Methods requiring derivatives
 - Newton – Raphson Method
 - Bisection method
 - Secant method

Gradient Based Methods

Gradient-based methods are more effective and popular. However, it is not always easy to obtain derivative information for real-life problems.

But when the derivative information is available, these methods are very fast compared to direct search methods.

Termination criteria:

Gradient is zero at local or global minimum.

In practice, algorithm stops when the gradient is less than a predetermined small value.

Newton – Raphson Method

The Newton-Raphson method requires that the function $f(x)$ be twice differentiable.

We start with an initial estimate of the stationary point x_1 – that is the initial estimate of the root of $f'(x)=0$.

A linear approximation of the function $f'(x)$ at the point x_1 is obtained, and the point at which the linear approximation is zero is taken as the next improved approximation of the root of $f'(x)=0$.

Isaac Newton



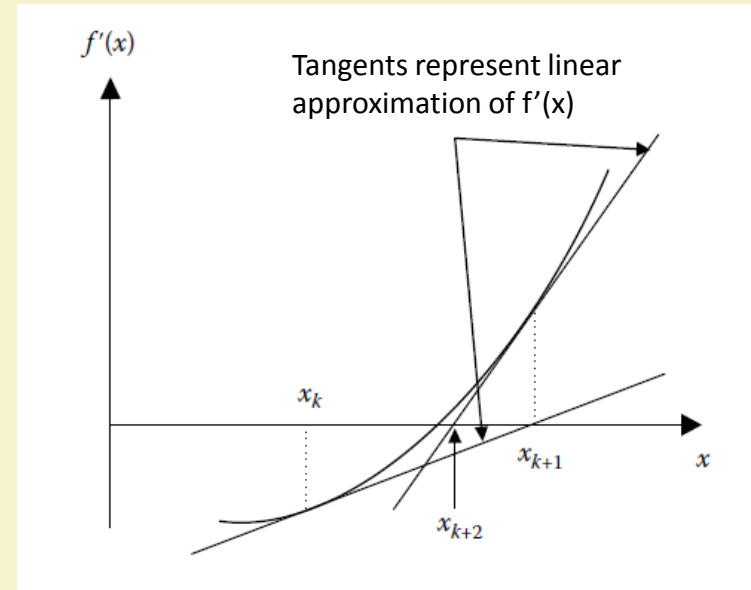
Newton – Raphson Method

Given a current estimate of stationary point x_k , the linear approximation of the function $f'(x)$ at x_k can be set to zero to get next estimate:

$$\tilde{f}'(x; x_k) = f'(x_k) + f''(x_k)(x - x_k) = 0$$

$$\Rightarrow x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

Depending on the starting point and the nature of the function, it may be possible to diverge instead of converging to true stationary point.



Newton – Raphson Method: Algorithm

Step – 1: Set initial guess = x_1 ; tolerance $\varepsilon > 0$;
iteration counter $k = 1$; Compute $f'(x_k)$

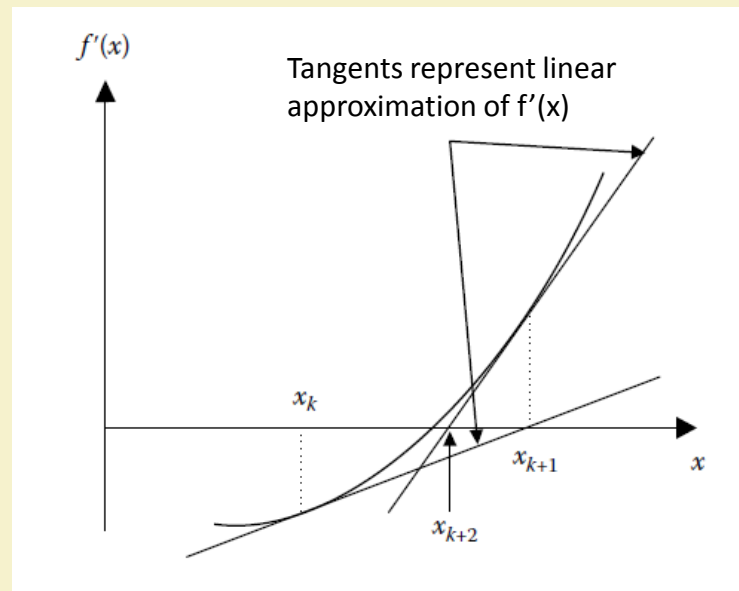
Step – 2: Compute $f''(x_k)$

Step – 3: Compute $x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$;

Compute $f'(x_{k+1})$

Step - 4: If $|f'(x_{k+1})| < \varepsilon$, Stop

Else set $k = k + 1$ and go to *Step – 2*



Newton – Raphson Method: Numerical Derivatives

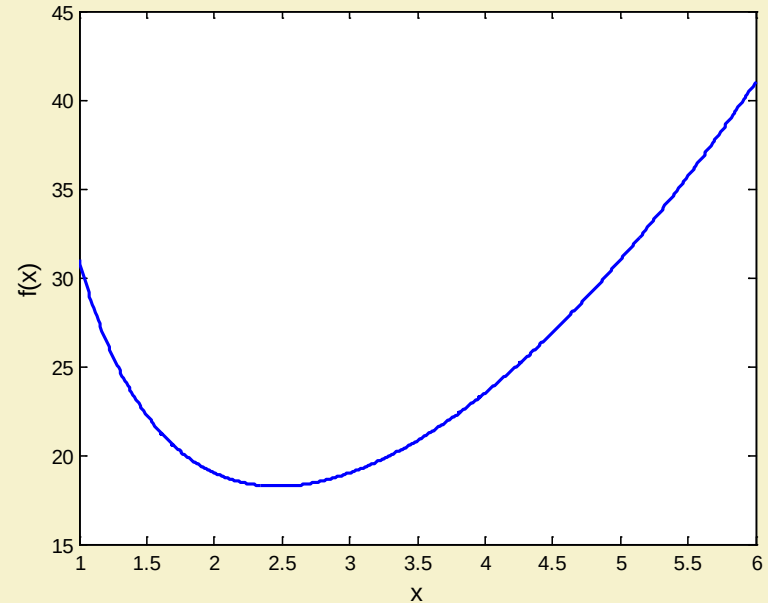
Many expressions are available. The following expressions use central difference method.

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Newton – Raphson Method: Example

$$\min_x f(x) = x^2 + \frac{30}{x}$$



Newton – Raphson Method: Example

$$\min_x f(x) = x^2 + \frac{30}{x}$$

Initial guess: $x_1 = 2$

Solution:

$$f'(x) = 2x - \frac{30}{x^2}; \quad f''(x) = 2 + \frac{60}{x^3}$$

Step – 1: $x_1 = 2$; $f'(x_1) = -3.5$; $f''(x_1) = 9.5$

$$x_2 = x_1 - \frac{f'(x_1)}{f''(x_1)} = 2 - \frac{-3.5}{9.5} = 2.3684$$

Step – 2: $x_2 = 2.3684$; $f'(x_2) = -0.6114$; $f''(x_2) = 6.5163$

$$x_3 = x_2 - \frac{f'(x_2)}{f''(x_2)} = 2 - \frac{-0.6114}{6.5163} = 2.4622$$

Step – 2: $x_3 = 2.4622$; $f'(x_3) = -0.0241$; $f''(x_3) = 6.0196$

$$x_4 = x_3 - \frac{f'(x_3)}{f''(x_3)} = 2 - \frac{-0.0241}{6.0196} = 2.4662$$

Bisection Method

Bisection method uses function value and sign of first derivative at two points to eliminate a part of search space. It does not use second derivative. Unimodality of function is assumed.

At the maximum or minimum of a function, $f'(x) = 0$. Since the function is assumed to be unimodal, the gradient of the function changes sign near the optimum point. If $f'(x_1)$ and $f'(x_2)$ are the derivatives of a function computed at points x_1 and x_2 , then the minimum of the function is bracketed between x_1 and x_2 if the sign of $f'(x_1)$ and $f'(x_2)$ are different – one is positive and the other is negative:

$$f'(x_1) f'(x_2) < 0$$

Bisection Method: Algorithm

Step – 1: Choose two points $[a, b]$ such that $f'(a) < 0$ and $f'(b) > 0$.

Set $x_1 = a$; $x_2 = b$; tolerance $\varepsilon > 0$;

Step – 2: Compute $z = \frac{x_1 + x_2}{2}$ and evaluate $f'(z)$

Step – 3: If $|f'(z)| < \varepsilon$, Stop

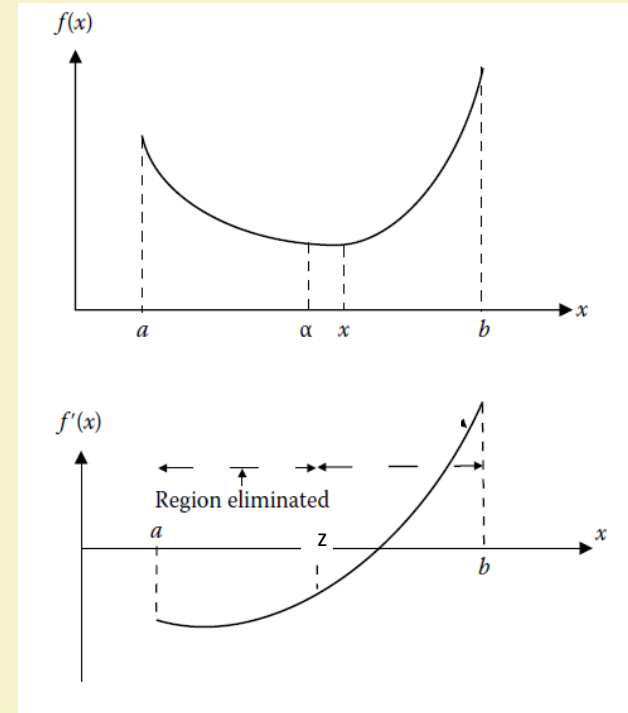
Else if $f'(z) < 0$ set $x_1 = z$ and go to Step – 2

Else if $f'(z) > 0$ set $x_2 = z$ and go to Step – 2

Consider sign of first derivative at mid-point.

If derivative is negative, eliminate left-half.

If derivative is positive, eliminate right-half.



Secant Method

In the bisection method, we used only the sign of the derivative to locate the zero of $f'(x)$. In the secant method, both the magnitude and the sign of the derivative are used to locate the zero of $f'(x)$.

We start with two point x_1 and x_2 such that $f'(x_1)$ and $f'(x_2)$ have opposite sign: $f'(x_1)f'(x_2) < 0$

Next we assume that $f'(x)$ varies linearly between points x_1 and x_2 . A secant line is drawn between the two points x_1 and x_2 . The point z where the secant line crosses the x -axis is taken as the improved guess for the zero of $f'(x)$ in the next iteration.

One of the points (x_1 or x_2) is then replaced by z using sign of $f'(z)$ and either $[x_1, z]$ or $[z, x_2]$ is eliminated. More (or smaller) than half the search space may be eliminated.

Secant Method: Algorithm

Algorithm is same as bisection method. Note the change in computation of point z .

Step – 1: Choose two points $[a, b]$ such that $f'(a) < 0$ and $f'(b) > 0$.

Set $x_1 = a$; $x_2 = b$; tolerance $\varepsilon > 0$;

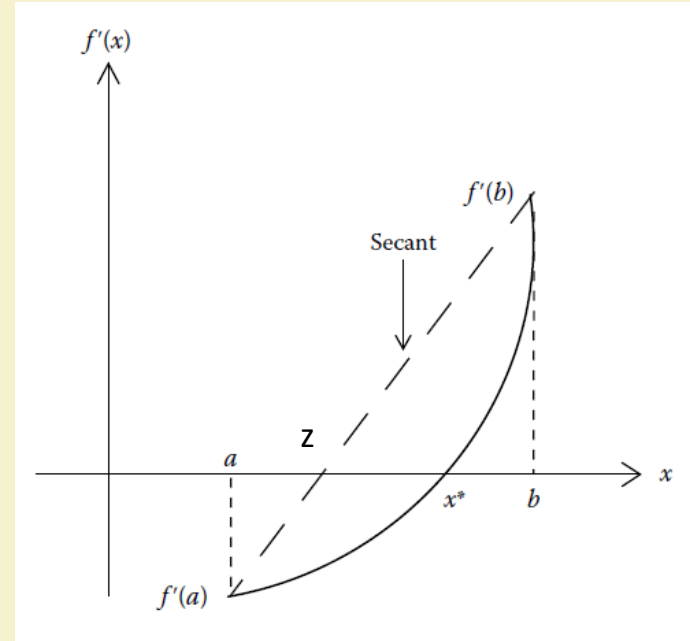
Step – 2: Compute $z = x_2 - \frac{f'(x_2)}{[f'(x_2) - f'(x_1)] / (x_2 - x_1)}$;

Evaluate $f'(z)$

Step – 3: If $|f'(z)| < \varepsilon$, *Stop*

Else if $f'(z) < 0$ set $x_1 = z$ and go to *Step – 2*

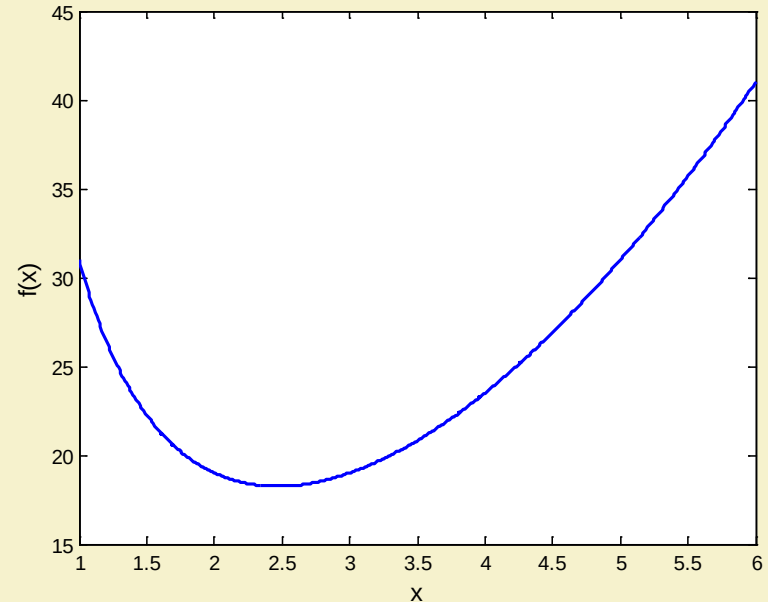
Else if $f'(z) > 0$ set $x_2 = z$ and go to *Step – 2*



Exercise

$$\min_x f(x) = x^2 + \frac{30}{x}$$

Solve using Bisection method and Secant method. Compare your results with the results obtained using Newton-Raphson method.



Optimization in Chemical Engineering

Thank You

