ME 310

Numerical Methods

Optimization

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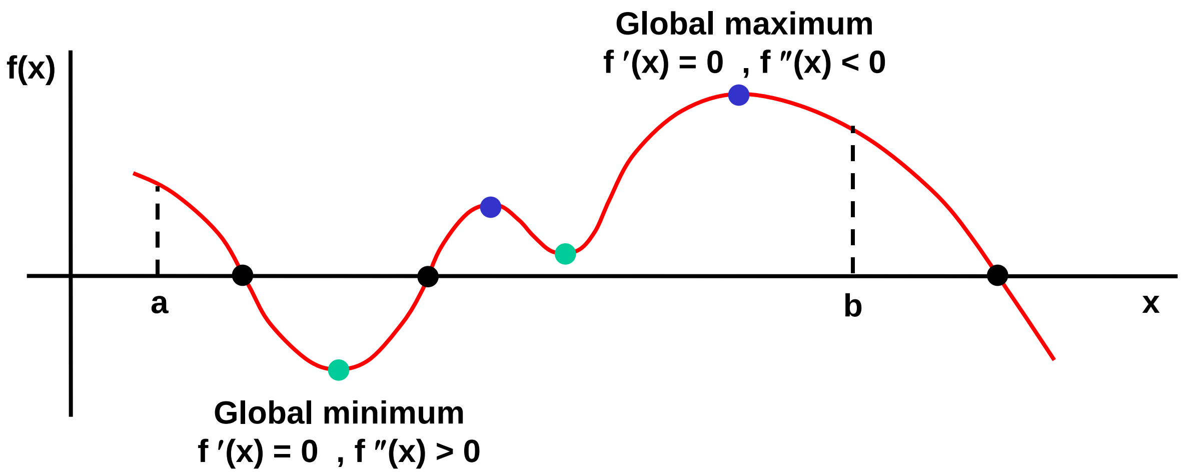
Optimization

• Optimization is similar to root finding. Both involve guessing and searching for a point on a function.



• Optimum is the point where f ′(x) = 0. f ″(x) indicates whether it is a minimum or a maximum.

• In this range there can be only one global minimum and one global maximum. These can be at the end points of the interval.

• There can be several local minimums and local maximums.

• Practical optimization problems are complicated and include several constraints.

  • Minimization of cost of a manufactured part (time, quality, quantity, etc.).

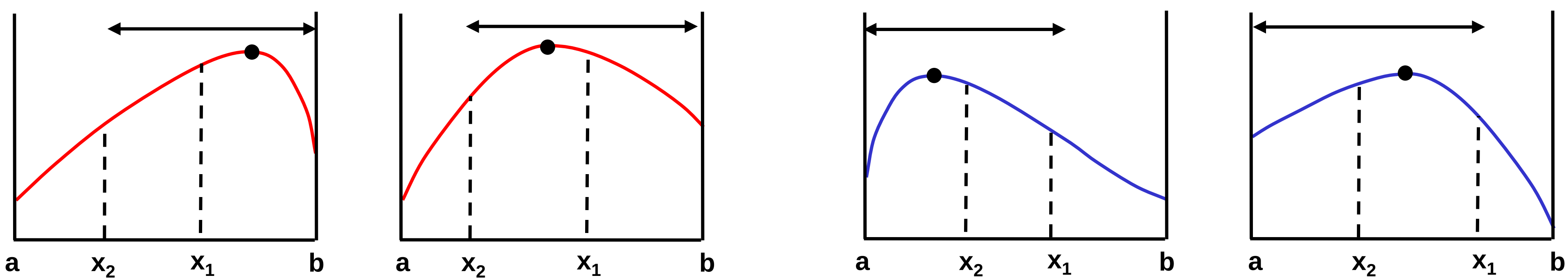
  • Maximization of efficiency of a cooling unit (size, material, safety, ergonomics, cost, etc.).

  • Transportation problem (manage the shipping between several sources and several warehouses).

- We will study 1D ($f=f(x)$), unconstrained optimization using the following methods.
  - Bracketing methods (Golden Section Search, Quadratic Interpolation)
  - Open Methods (Newton's Method)

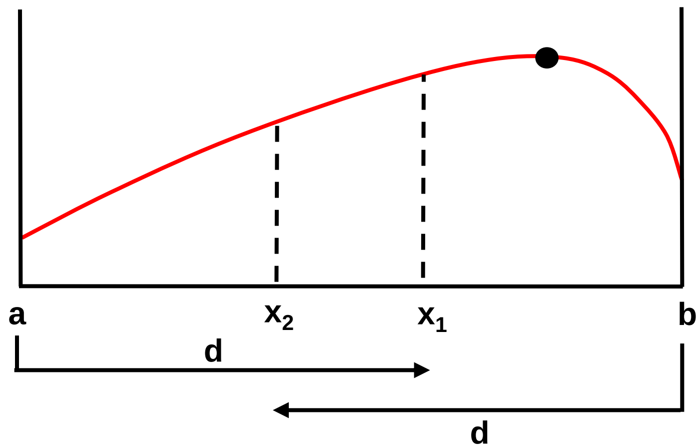
Bracketing Methods

- Consider finding the maximum of a function $f(x)$ in the interval [a,b].
- Consider a function that has only one maximum (or minimum) in [a,b].
- Similar to the bracketing methods used for root finding, we will iteratively narrow the interval [a,b] to locate the minimum.
- Remember that in root finding (for example in the Bisection method), only one intermediate point was enough to narrow the interval.
- In finding a maximum we need two intermediate points (x_1 and x_2).
- If $f(x_1) > f(x_2)$ than the maximum is between $[x_2,b]$. Otherwise it is between $[a,x_1]$



Golden Section Search

- There are several different ways in selecting the two intermediate points x_1 and x_2.
- In Golden Section Search these two points are selected as



$x_1 = a + d$

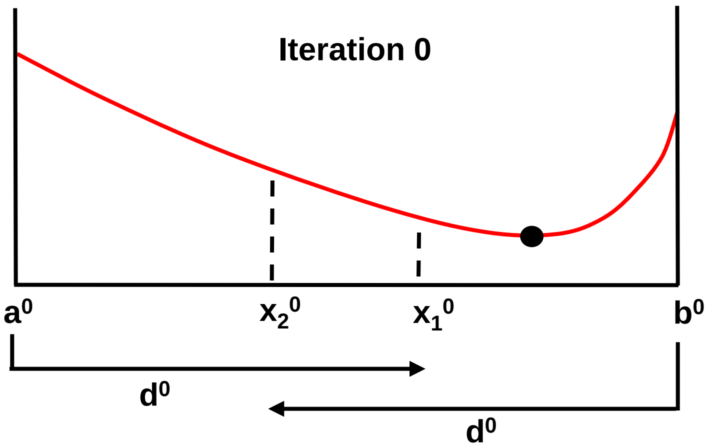
$x_2 = b - d$

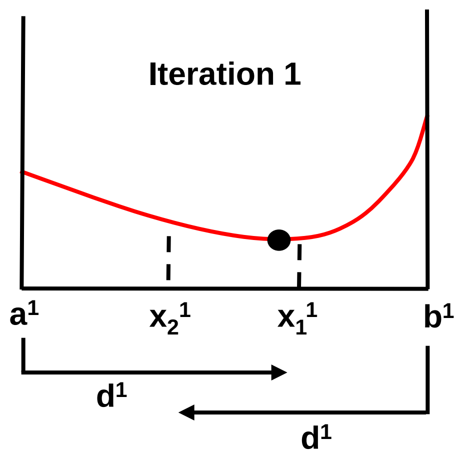
where $d = R\,(b\text{-}a)$.

- $\mathbf{R} = \dfrac{\sqrt{5}-1}{2} = \mathbf{0.618034\ ...}$ is called the golden-ratio. It is the positive root of $r^2 + r - 1 = 0$.
- If $f(x_1) > f(x_2)$ than continue with the interval $[x_2,b]$. Otherwise continue with $[a,x_1]$. This works to locate a maximum. To locate a minimum do the opposite.
- Calculate two new intermediate points in the narrowed interval and iterate like this.
- At each iteration, the interval drops by a factor of R ($d^{i+1} = R\,d^{i}$).
- Stop when $(x_1\text{-}x_2)$ drops below the specified tolerance. See page 347 for an alternative stopping criteria.

Golden Ratio

- What is the importance of the golden ratio, R = 0.618034 ?
- Consider the following case. Superscripts show the iteration number.





- At iteration 0,

$$x_1^0 = a^0 + \frac{\sqrt{5}-1}{2}(b^0 - a^0) \quad , \quad x_2^0 = b^0 - \frac{\sqrt{5}-1}{2}(b^0 - a^0)$$

- $f(x_1^0) < f(x_2^0)$, therefore continue with $[x_2^0, b^0]$.

- At iteration 1, $a^1 = x_2^0$, $b^1 = b^0$

$$x_1^1 = a^1 + \frac{\sqrt{5}-1}{2}(b^1 - a^1)$$

$$x_2^1 = b^1 - \frac{\sqrt{5}-1}{2}(b^1 - a^1) \quad = \quad x_1^0$$

- Therefore there is no need to calculate x_2^1 and $f(x_2^1)$.

  This saves computations.

Exercise: Show that $x_2^1 = x_1^0$

Pseudocode for the Golden Section Search

```
R = 0.618033988
READ  a,  b,  maxIter,  tolerance
CALCULATE   fa,  fb

LOOP  k  from  1  to  maxIter
    x1 = a + R(b-a)    ;   f1 = func(x1)
    x2 = b - R(b-a)    ;   f2 = func(x2)

    IF ( f1 > f2) THEN
        a = x2    ;   x2 = x1   ;   f2 = f1
        x1 = a + R(b-a)    ;   f1 = func(x1)
    ELSE
        b = x1    :   x1 = x2   ;   f1 = f2
        x2 = b - R(b-a)    ;   f2 = func(x2)
    ENDIF

    WRITE   k, x1, x2
    IF ( (x1 – x2) < tolerance)  STOP

ENDLOOP
```

Exercise 21: This pseudocode is written to find a maximum. Modify it so that it can find a minimum too.

Exercise 22: Change the stopping criteria with the one given in the book.

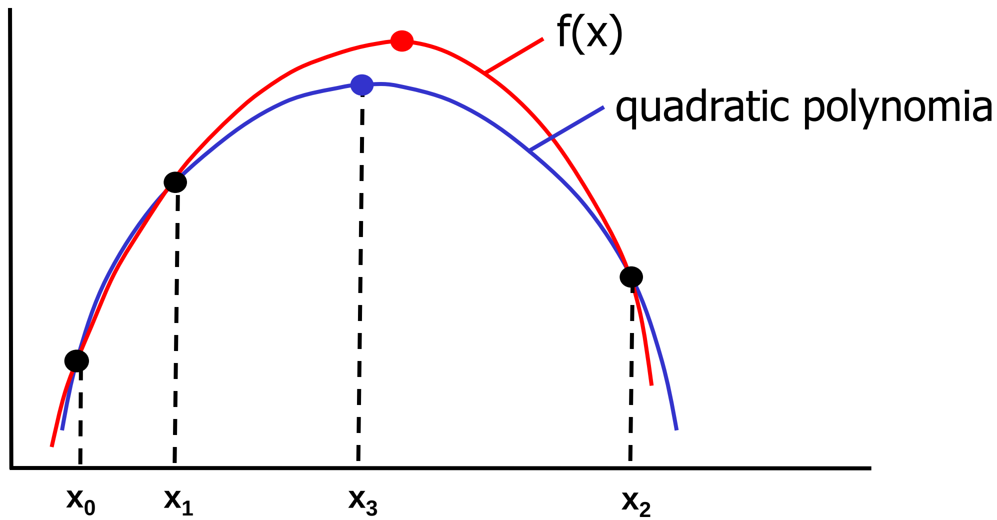
Exercise 23: What happens if

(i) the initial interval [a,b] contains more than one min or max?

(ii) a is the maximum and b is the minimum, or vice versa?

Quadratic Interpolation

- Based on the fact that a quadratic (2nd order) polynomial often provides a good approximation of a function near an optimum point.



- Select 3 points (x_0, x_1 and x_2) that contains only 1 optimum point of a function.
- Only one quadratic will pass through these points. Find the equation of this quadratic.
- Equate its first derivative to zero and find its optimum point, x_3.

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

- Similar to the Golden Section Search, narrow the interval by discarding one of the points.
- Continue with the remaining 3 points and calculate a new optimum (x_3).
- Iterate like this and stop when the approximate relative error drops below the tolerance value.

Newton's Method

• Recall that Newton-Raphson method is used to find the root of f(x) =0 as $\mathbf{x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}}$

• Similarly the optimum points of f(x) can be found by applying N-R to f ′(x) = 0. $\mathbf{x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}}$

• This open method requires only one starting point.

• It also requires the 1st and 2nd derivative of f(x).

• It converges fast, but convergence is not guaranteed.

• At the end one can check the sign of f ″(x) to determine whether the optimum point is a minimum or a maximum.

• If the derivatives are not known than their approximations can be used. This is similar to the Secant method that we learned in root finding.

• To avoid divergence, it is a good idea to use this method when we are close enough to the optimum point. So we can use a hybrid technique, where we start with a bracketing method and safely narrow the interval and than continue with the Newton's method.

Example 23:

Find the maximum of $f(x) = 2x - 1.75x^2 + 1.1x^3 - 0.25x^4$ using

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

(b) Quadratic interpolation ($x_0 = -1.75$, $x_1 = 2$, $x_2 = 2.25$, perform 5 iterations)

(c) Newton's method ($x_0 = 2.5$, $\varepsilon_s = 1\%$)

(a) Golden Section Search

iter 1: $a = -2$, $b = 4$, $x_1 = a + R(b-a) = 1.708$, $x_2 = b - R(b-a) = 0.292$

$f(x_1) = 1.664$, $f(x_2) = 0.460$ $f(x_1) > f(x_2)$ than continue with $[x_2 , b]$.

$f(x_1) > f(x_2)$ than $x_{opt} = x_1 = 1.708$, $\varepsilon_a = (1-R) * (b-a) / |x_{opt}| * 100 = 134\ \%$

iter 2: $a = 0.292$, $b = 4$, $x_1 = a + R(b-a) = 2.584$, $x_2 = 1.708$

$f(x_1) = 1.316$, $f(x_2) = 1.664$ $f(x_1) < f(x_2)$ than continue with $[a , x_1]$.

$f(x_1) < f(x_2)$ than $x_{opt} = x_2 = 1.708$, $\varepsilon_a = (1-R) * (b-a) / |x_{opt}| * 100 = 83\ \%$

iter 3: $a = 0.292$, $b = 2.584$, $x_1 = 1.708$, $x_2 = b - R(b-a) = 1.167$

$f(x_1) = 1.664$, $f(x_2) = 1.235$ $f(x_1) > f(x_2)$ than continue with $[x_2 , b]$.

$f(x_1) > f(x_2)$ than $x_{opt} = x_1 = 1.708$, $\varepsilon_a = (1-R) * (b-a) / |x_{opt}| * 100 = 51\ \%$

. . . .

iter 11: $x_{opt} = 2.073$, $\varepsilon_a = 0.9\ \%$

Example 23 (cont'd)

(b) Quadratic Interpolation

iter 1: $x_0 = -1.75$, $x_1 = 2.0$, $x_2 = 2.25$

Calculate $x_3 = 2.0617$

iter 2: $x_0 = 2.0$, $x_1 = 2.0617$, $x_2 = 2.25$

Calculate $x_3 = 2.0741$

iter 3: $x_0 = 2.0617$, $x_1 = 2.0741$, $x_2 = 2.25$

Calculate $x_3 = 2.0779$

iter 4: $x_0 = 2.0741$, $x_1 = 2.0779$, $x_2 = 2.25$

Calculate $x_3 = 2.0791$

iter 5: $x_0 = 2.0779$, $x_1 = 2.0791$, $x_2 = 2.25$

Calculate $x_3 = 2.0786$

$\varepsilon_a = | (x_3^{present} - x_3^{previous}) / x_3^{present} | * 100 = 0.02\ \%$

Example 23 (cont'd)

(c) Newton's Method

$f'(x) = 2 - 3.5\,x + 3.3\,x^2 - x^3$, $f''(x) = -3.5 + 6.6\,x - 3\,x^2$

$x_0 = 2.25$

iter 1: $x_1 = x_0 - f'(x_0) / f''(x_0) = 2.19565$

$\varepsilon_a = |\,(x_1 - x_0) / x_1\,| * 100 = 13.9\ \%$

iter 2: $x_2 = x_1 - f'(x_1) / f''(x_1) = 2.0917$

$\varepsilon_a = |\,(x_2 - x_1) / x_2\,| * 100 = 5.0\ \%$

iter 3: $x_3 = x_2 - f'(x_2) / f''(x_2) = 2.07951$

$\varepsilon_a = |\,(x_3 - x_2) / x_3\,| * 100 = 0.6\ \%$