LECTURE NOTE I

Chapter 1

Introduction to Optimization

"Of the evils, always choose the lesser."

Optimization: Selecting the best among the entire set by efficient quantitative methods.

1.1 Requirements for the application of optimization method

- **Defining system boundaries**

  Too small: easy to handle, but misleading

  Too large: real, but hard to handle

- **Performance criteria**

  Defining "what the best is"

  (In terms of economic measure, operation measure, errors, and etc.)

- **Independent Variables**

  What you can manipulate. (Optimization variables, system parameters)

- **System Model**

  Relation between performance criteria and independent variables

  Equality and inequality constraints

1.2 Application of optimization in engineering

- Design of components or entire system
- Planning and analysis of existing operation
- Engineering analysis and data reduction
- Control of dynamic systems
-

Example 1.1 Design of Oxygen supply system

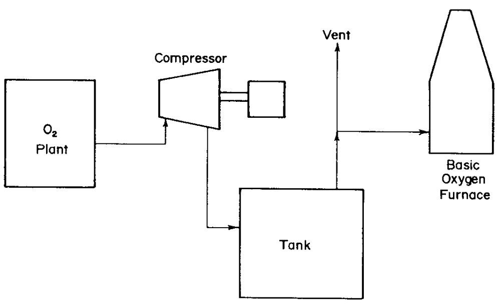


Figure 1.3. Design of oxygen production system, Example 1.1.

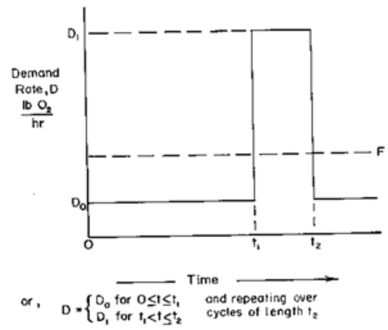


Figure 1.2. Oxygen demand cycle, Example 1.1.

Oxygen plant: production rate F (lb O_2/hr)

Compressor capacity: H (hp)

Holder tank volume: V (ft^3)

Tank pressure constraint: $P_0 \le P \le P_{max}$

P_0 is the delivery pressure to BOF.

If tank pressure is over the limit, then the extra oxygen will be vent in the air.

Cyclic operation: low O_2 demand period until t_1 and then high demand period up to t_2

Operation objectives: Supply O_2 to BOF as needed (demand) while maintaining holder tank pressure limits. If possible, minimize the energy consumption.

→ The holder tank should be large enough to handle the situation where the demand is larger while the supply is normal for the period between t_1 and t_2..

Feasibility: $Ft_2 \ge D_0 t_1 + D_1(t_2 - t_1)$ (if not, expand the O_2 plant production capacity)

Objective function (J): Total cost

J=(annual cost of O_2 plant)+(capital cost of tank)+(annual cost of compressor)

Constraints: Plant model (tank pressure)

$$P(t) = \begin{cases} (F - D_0)t\phi + P(0) & \text{for } 0 \le t \le t_1 \\ \quad \text{if } P(t) > P_{max}, & P(t) = P_{max} \\ P(t_1) - (D_1 - F)(t - t_1)\phi & \text{for } t_1 < t \le t_2 \end{cases}$$

where $\phi = \dfrac{RT}{MV} z$

$$P^{max}(t) = \min((F - D_0)t_1\phi + P(0), P_{max}) \quad \text{(automatically satisfied)}$$

$$P^{min}(t) = \min(P(t_1), P_{max}) - (D_1 - F)(t_2 - t_1)\phi \ge P_0 \quad \text{(inequality constraint)}$$

$$Ft_2 \ge D_0 t_1 + D_1(t_2 - t_1) \quad \text{(inequality constraint)}$$

Optimization variable: V, H, F

System parameters: physical properties, plant design characteristics, etc.

→ Depending on the nature of project, i.e., designing plant or finding a better operating conditions, optimization variables will be chosen differently.

Example 1.4 Data fitting

$$P = \frac{RT}{v-b} - \frac{a}{T^{0.5}v(v+b)}$$

Objectives: From the series of PvT measurements, find the parameters for semiempirical Redlich-Kwong equation

Then solve $\min_{a,b} \sum_{i=1}^{n} \left(P_i - \frac{RT_i}{v_i - b} - \frac{a}{T_i^{0.5} v_i (v_i + b)} \right)^2$

1.3 Structure of optimization problems

- General form: constrained minimization

$$\min_x f(x)$$

$$\text{subject to } h_k(x) = 0 \quad (k = 1, \cdots, K)$$

$$g_j(x) \geq 0 \quad (j = 1, \cdots, J)$$

$$x_i^U \geq x_i \geq x_i^L \quad (i = 1, \cdots, N)$$

- If J=K=0 and $x_i^U = -x_i^L = \infty$ for i=1 to N, then the problem is unconstrained.

1.4 Class of Optimization

- One dimensional vs. multi-dimensional optimization
- Unconstrained vs. constrained optimization
- Based on the type of objective function and constraints

LP (Linear Programming): linear objective function and linear constraints

QP (Quadratic Programming): quadratic objective function and linear constraints

NLP (NonLinear Programming): nonlinear objective function and nonlinear constraints

IP (Integer Programming): LP with integer variables only

MILP (Mixed Integer LP): LP with integer variables and continuous variables

MINLP (Mixed Integer NLP): NLP with integer variables and continuous variables

Chapter 2

Functions of a Single Variable

Single variable: The variable is a scalar. (not a vector)

2.1 Properties of single-variable functions

- $y = f(x)$: y is a function of x.

  y: dependent variable x: independent variable

  $y \in R$ $x \in S \subset R$

  If S=R, then f is an *unconstrained function*.

- In optimization

  f: objective function (scalar)

  S: feasible region (constraint set, domain of interest of x)

  x: independent variable or optimization variable

- *Continuous*: $\forall x_0 \in S, \quad \lim_{x \to x_0^+} f(x) = \lim_{x \to x_0^-} f(x)$

  1. A sums or products of a continuous function is continuous.
  2. The ratio of two continuous functions is continuous at all points where the denominator does not vanish.

- *Smooth*: differentiable indefinitely

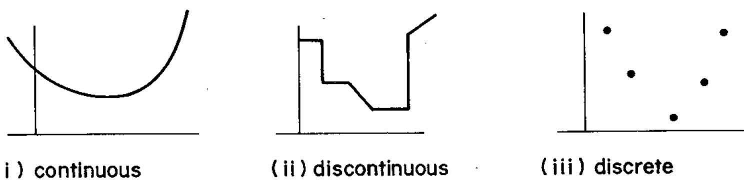


Figure 2.6. Unimodal functions.

- A *continuous* function on a closed interval (compact set) has the minimum (absolute minimum) and the maximum (absolute maximum).
- *Piecewise continuous*

  Discontinuous only at a finite number of points

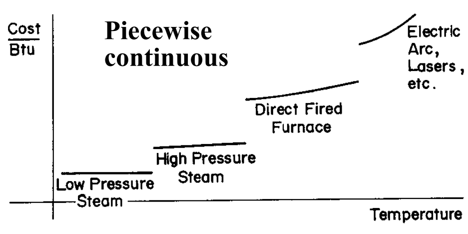
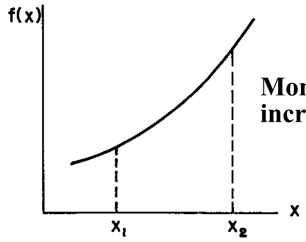


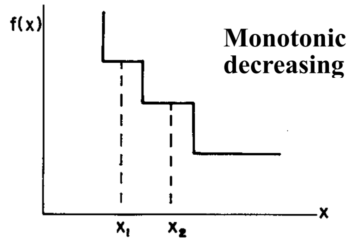
Figure 2.1. A discontinuous function.

- Monotonic function

$\forall x_1, x_2 \in S,$ if $x_1 \le x_2$ and $f(x_1) \le f(x_2),$ then f is a monotomic increasing function,

$\forall x_1, x_2 \in S,$ if $x_1 \le x_2$ and $f(x_1) \ge f(x_2),$ then f is a monotomic decreasing function,





- Unimodality

A function *f*(*x*) is *unimodal* on the interval $a \le x \le b$ if and only if it is monotonic on either side of a single optimal point x* in the interval.

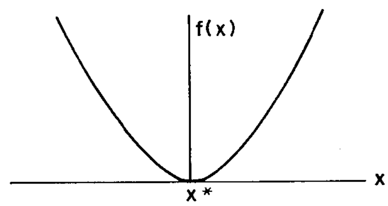


Figure 2.5. Unimodal function.

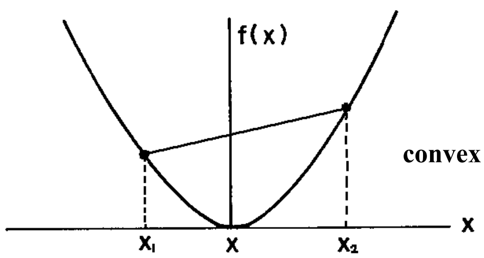
$$\rightarrow \begin{array}{l} x^* \ge x_1 \ge x_2 \rightarrow f(x^*) \le f(x_1) \le f(x_2) \\ x^* \le x_1 \le x_2 \rightarrow f(x^*) \le f(x_1) \le f(x_2) \end{array}$$

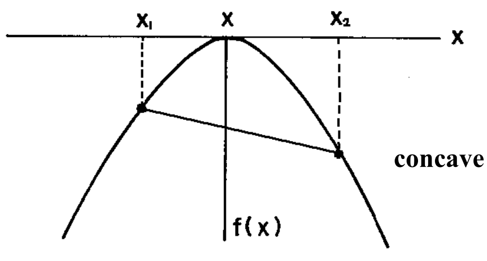
cf) bimodal, multimodal

- Convex and concave functions

For $x_1 \le x \le x_2,$ if $f(x)$ is smaller than the value of line segment from $(x_1, f(x_1))$ to $(x_2, f(x_2))$ then the function is *convex*.

For $x_1 \le x \le x_2,$ if $f(x)$ is larger than the value of line segment from $(x_1, f(x_1))$ to $(x_2, f(x_2))$ then the function is *concave*.





$\forall x_1, x_2 \in S,$ and $0 \le \alpha \le 1$

The $f(x)$ is *convex* if $f(\alpha x_1 + (1-\alpha)x_2) \le \alpha f(x_1) + (1-\alpha) f(x_2)$

The $f(x)$ is *concave* if $f(\alpha x_1 + (1-\alpha)x_2) \ge \alpha f(x_1) + (1-\alpha) f(x_2)$

- All positive linear combination of convex function is convex.
- If $f(x)$ is convex on S, then a subset $\Gamma_C = \{f(x) \le C,\ \forall x \in S\}$ is also convex.
- $\forall x, y \in S,$ $f(x)$ is convex iff $f(y) \ge f(x) + \nabla f(x)(y-x)$

(For $x<y$, $f(y)$ is not smaller than the increased value from x with slope at x.)

2.2 Optimality criteria

- *Global* and *Local optima*

$x^{**} \in S$ is the *global minimum* iff $f(x^{**}) \le f(x)\ \forall x \in S$.

$x^{*} \in S$ is a *local minimum* iff $f(x^{*}) \le f(x)\ \forall x \in [x^{*}-\varepsilon, x^{*}+\varepsilon]$.

1. By reversing the direction of the inequality, the equivalent definitions of *global* and *local maxima* can be obtained.
2. Under the assumption of unimodality, the local optimum automatically becomes the *global optimum*.
3. When the function is not unimodal, multiple local optima are possible and the global optimum can be found only by locating all local optima and selecting the best one.

- Identification of single-variable optima

$$f(x^{*}+\varepsilon) - f(x^{*}) = \left.\frac{df}{dx}\right|_{x=x^{*}} \varepsilon + \left.\frac{d^2 f}{dx^2}\right|_{x=x^{*}} \frac{\varepsilon^2}{2!} + O_3(\varepsilon)$$

For minimum, with arbitrarily small ε

$$f(x^{*}) \le f(x)$$

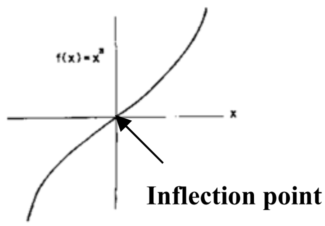
$$f'(x^{*})\varepsilon + f''(x^{*})\frac{\varepsilon^2}{2!} + O_3(\varepsilon) \ge 0 \Rightarrow f'(x^{*}) = 0 \text{ and } f''(x^{*}) \ge 0$$

- **Theorem 2.1**

Necessary conditions for x^* to be a local minimum (maximum) of f on the open interval (a, b), providing that f is twice differentiable, are that

1. $\left.\frac{df}{dx}\right|_{x=x^{*}} = 0$ (*Stationary point* condition)

2. $\left.\frac{d^2 f}{dx^2}\right|_{x=x^{*}} \ge 0 \quad (\le 0)$



- *Inflection* (*saddle*) point: a stationary point that does not correspond to a local optimum.

- **Theorem 2.2**

Suppose at a point x^* the first derivative is zero and the first nonzero higher order derivative is denoted by n.

1. If n is odd, then x^* is a point of inflection
2. If n is even then x^* is a local optimum. Moreover,
   A. If that derivative is positive, then the point x^* is a local minimum.
   B. If that derivative is negative, then the point x^* is a local maximum.

cf) For vector-matrix cases, the positive (negative) should be positive (negative) definite.

- Global optimum for single-variable functions in bounded interval of x, $[a, b]$.

Possible optima will reside at

1. stationary points where $f'(x)=0$
2. end points, $f(a)$ and $f(b)$
3. the points where $f(x)$ is discontinuous
4. the points where $f'(x)$ is discontinuous

Thus, the global optimum is located at one of the above candidates which has smallest (largest) function value.

2.3 Regional Elimination Methods

- **Theorem 2.3**

Suppose f is *strictly unimodal* on the interval $a \le x \le b$ with a minimum at x^*. Let x_1 and x_2 be two points in the interval such that $a < x_1 < x_2 < b$,

1. If $f(x_1) > f(x_2)$, then the minimum of $f(x)$ does not lie in the interval (a, x_1). In other words, $x^* \in (x_1, b)$
2. If $f(x_1) < f(x_2)$, then the minimum of $f(x)$ does not lie in the interval (x_2, b). In other words, $x^* \in (a, x_2)$

cf) *strictly unimodal*:
$$x^* > x_1 > x_2 \rightarrow f(x^*) < f(x_1) < f(x_2)$$
$$x^* < x_1 < x_2 \rightarrow f(x^*) < f(x_1) < f(x_2)$$

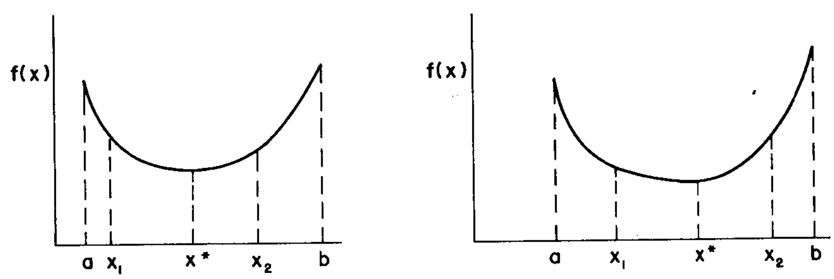


Figure 2.10. Case (i) and case (ii) of Theorem 2.3.

- **Bounding Phase**: An *initial* coarse search that will bound or bracket the optimum.
  - <u>*Swann's method*</u> (minimization for strictly unimodal case)

    For a given initial guess x_0 and a step size parameter Δ, start with k=1.

    i) Decision of direction

    If $f(x_0-|\Delta|)\ge f(x_0)\ge f(x_0+|\Delta|)$, choose positive Δ.
    If $f(x_0-|\Delta|)\le f(x_0)\le f(x_0+|\Delta|)$, choose negative Δ,
    and let $x_{-1}=x_0-\Delta$ and $x_1=x_0+\Delta$.
    If $f(x_0-|\Delta|)\le f(x_0)\ge f(x_0+|\Delta|)$, conclude f is not unimodal and stop.
    If $f(x_0-|\Delta|)\ge f(x_0)\le f(x_0+|\Delta|)$, then $x_0-|\Delta|\le x^*\le x_0+|\Delta|$ and stop.

    ii) Test point generation:

    k=k+1
    $x_k=x_{k-1}+2^{k-1}\Delta$
    If $f(x_k)<f(x_{k-1})$, repeat step ii)

    iii) Termination of bracketting

    If $f(x_k)\ge f(x_{k-1})$, conclude that x^* lies in between x_k and x_{k-2} and stop.

    cf) If Δ is too small, it could take quite long to get the initial bracket and if Δ is too large, the initial bracket could be too wide.

- **Interval Refinement Phase**: With the initial bracket (a, b) from bounding phase, locate the minimum in the reasonably small range.
  - <u>*Interval Halving method*</u> (three-point equal-interval search)

    i) Let x_m=(a+b)/2 and L=b-a. Compute $f(x_m)$.
    ii) Set x_1=a+L/4 and x_2=b-L/4. Compute $f(x_1)$ and $f(x_2)$.
    iii) If $f(x_1)<f(x_m)$, drop (x_m, b) and let b= x_m and x_m = x_1. Then go to vi).
    iv) If $f(x_2)<f(x_m)$, drop (a, x_m) and let a= x_m and x_m = x_2.
    v) If $f(x_2)\ge f(x_m)$, drop (a, x_1) and (x_2, b) let a= x_1 and b = x_2.
    vi) Recompute L=b-a.
    vii) If L is small enough, conclude x^* lies in (a, b) and stop. Else go to ii).

    Remark 1: At each subsequent step, two function evaluations are needed.
    Remark 2: After n function evaluations, $L^{new}=L^{initial}(0.5)^{n/2}$.
    Remark 3: Among equal interval searches (2-, 3-, 4-point search), the 3-point search is the most efficient method.

  - <u>*Golden Section method*</u>

    Golden section number:
    $\tau=(-1+\sqrt{5})/2\approx 0.618$
    (positive solution of $\tau^2=1-\tau$)

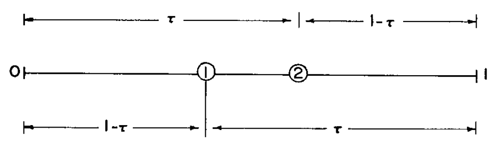


Figure 2.11. Golden section search.

Start from k=1 and prespecified termination criterion ε ..

i) Let $x_k^1 = b - \tau(b-a)$ and $x_k^2 = a + \tau(b-a)$.

ii) Compute $f(x_k^1)$ and/or $f(x_k^2)$.

iii) If $f(x_k^1) \le f(x_k^2)$, set $b = x_k^2$, $x_{k+1}^2 = x_k^1$, and $x_{k+1}^1 = b - \tau(b-a)$.

iv) If $f(x_k^1) > f(x_k^2)$, set $a = x_k^1$, $x_{k+1}^1 = x_k^2$, and $x_{k+1}^2 = a + \tau(b-a)$.

v) If $b - a > \varepsilon$, k=k+1 and go to ii).

vi) Conclude that

If $f(x_{k+1}^1) < f(x_{k+1}^2)$, $x^* = [a \; x_{k+1}^2]$.
If $f(x_{k+1}^1) > f(x_{k+1}^2)$, $x^* = [\, x_{k+1}^1 \; b]$.
If $f(x_{k+1}^1) = f(x_{k+1}^2)$, $x^* = [\, x_{k+1}^1 \; x_{k+1}^2]$.

Remark 1: At each subsequent step, only one function evaluation is needed.

Remark 2: After n function evaluations, $L^{new} = L^{initial}(\tau)^{n-1}$.

- <u>*Fibonacci method*</u>

Fibonacci numbers: $F_0 = F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$ $(n \ge 2)$ (1, 1, 2, 3, 5, 8, 13, …)

Start from k=1 and predetermined N.

i) Let $x_k^1 = a + (b-a)F_{N-k} / F_{N+2-k}$ and $x_k^2 = a + (b-a)F_{N+1-k} / F_{N+2-k}$.

ii) Compute $f(x_k^1)$ and/or $f(x_k^2)$.

iii) If $f(x_k^1) \le f(x_k^2)$, set $b = x_k^2$, $x_{k+1}^2 = x_k^1$, and $x_{k+1}^1 = a + (b-a)F_{N-1-k} / F_{N+1-k}$.

iv) If $f(x_k^1) > f(x_k^2)$, set $a = x_k^1$, $x_{k+1}^1 = x_k^2$, and $x_{k+1}^2 = a + (b-a)F_{N-k} / F_{N+1-k}$.

v) If k<N, k=k+1 and go to ii).

vi) Conclude that

If $f(x_{k+1}^1) < f(x_{k+1}^2)$, $x^* = [a \; x_{k+1}^2]$.
If $f(x_{k+1}^1) > f(x_{k+1}^2)$, $x^* = [\, x_{k+1}^1 \; b]$.
If $f(x_{k+1}^1) = f(x_{k+1}^2)$, $x^* = [\, x_{k+1}^1 \; x_{k+1}^2]$.

Remark 1: (N+1) Fibonacci numbers have to be generated initially.

Remark 2: At each subsequent step, only one function evaluation is needed.

Remark 3: After N function evaluations, $L^{new} = L^{initial} / F_{N+1}$. For 1% accuracy N=11 (F_{12}=144) and for 0.1% N=17 (F_{11}=1577).

- Comparison of the regional elimination methods

Table 2.1 Fractional Reduction Achieved

	Number of Functional Evaluations				
Search Method	$N = 2$	$N = 5$	$N = 10$	$N = 15$	$N = 20$
Interval halving	0.5	0.177	0.031	.006	.0009
Golden section	0.618	0.146	0.013	.001	.0001
Exhaustive	0.667	0.333	0.182	.125	.095

2.4 Polynomial Approximation or Point-estimation methods

- Quadratic equation

$$y = az^2 + bz + c$$

Given data: $y_1 = y(z_1)$, $y_2 = y(z_2)$, $y_3 = y(z_3)$ ($z_1 < z_2 < z_3$ WLOG)

By Cramer's rule,

For $\begin{pmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$ (Let the matrix be A.)

$$a = \frac{1}{\det(A)}\begin{vmatrix} y_1 & x_1 & 1 \\ y_2 & x_2 & 1 \\ y_3 & x_3 & 1 \end{vmatrix},\quad b = \frac{1}{\det(A)}\begin{vmatrix} x_1^2 & y_1 & 1 \\ x_2^2 & y_2 & 1 \\ x_3^2 & y_3 & 1 \end{vmatrix},\quad c = \frac{1}{\det(A)}\begin{vmatrix} x_1^2 & x_1 & y_1 \\ x_2^2 & x_2 & y_2 \\ x_3^2 & x_3 & y_3 \end{vmatrix}$$

$$\begin{aligned}\det(A) &= (x_2^2x_3 - x_3^2x_2) - (x_1^2x_3 - x_3^2x_1) + (x_1^2x_2 - x_2^2x_1) \\ &= -(x_1 - x_2)(x_2 - x_3)(x_3 - x_1)\end{aligned}$$

$$\therefore \quad \begin{aligned} a &= \frac{(z_2 - z_3)y_1 + (z_3 - z_1)y_2 + (z_1 - z_2)y_3}{-(z_1 - z_2)(z_2 - z_3)(z_3 - z_1)} \\ b &= \frac{(z_2^2 - z_3^2)y_1 + (z_3^2 - z_1^2)y_2 + (z_1^2 - z_2^2)y_3}{(z_1 - z_2)(z_2 - z_3)(z_3 - z_1)} \end{aligned}$$

Check that if a>0. If not, the minimum does not exist.

The minimum point of the quadratic equation: $\frac{dy}{dz} = 2az + b = 0 \Rightarrow z^* = -\frac{b}{2a}$

- *Powell's method*

Start from x_1 and step size Δ and termination criteria ε_x and ε_f.

i) Find three points using *bracketing method* in bounding phase of regional elimination. (The middle point has the lowest value and let $x_1 < x_2 < x_3$.)

ii) Find the minimum using the formula:

$$x^* = \frac{1}{2}\frac{(z_2^2 - z_3^2)y_1 + (z_3^2 - z_1^2)y_2 + (z_1^2 - z_2^2)y_3}{(z_2 - z_3)y_1 + (z_3 - z_1)y_2 + (z_1 - z_2)y_3}$$

iii) If $|x_2 - x^*| < \varepsilon_x$ and $|f(x_2) - f(x^*)| < \varepsilon_f$, then stop and the minimum is x^*.

iv) Else, let $x_2 = \arg\min\{f(x_1), f(x_2), f(x_3), f(x^*)\}$ and x_1 and x_3 are the left and right points of x_2 and go to ii).

- *Equally-spaced quadratic approximation method*

$$y = a(z - z_2)^2 + b(z - z_2) + c$$

Given data: $y_1 = y(z_1)$, $y_2 = y(z_2)$, $y_3 = y(z_3)$ $(z_1 + h = z_2 = z_3 - h)$

$$y_1 = a(z_1 - z_2)^2 + b(z_1 - z_2) + y_2 = ah^2 - bh + y_2$$
$$y_3 = a(z_3 - z_2)^2 + b(z_3 - z_2) + y_2 = ah^2 + bh + y_2$$

$$a = (y_1 + y_3 - 2y_2)/(2h^2) \text{ and } b = (y_3 - y_1)/(2h)$$
$$\therefore z^* = -\frac{b}{2a} = z_2 + \frac{h(y_1 - y_3)}{2(y_1 + y_3 - 2y_2)}$$

Start from x_1 and step size Δ and termination criteria ε_x and ε_f.

i) Find three points using *bracketing method* in bounding phase of regional elimination.

ii) From the last point, back out by a half of the last step size. (4 equally-spaced points)

iii) Let the minimum point be x_2 and choose x_1 and x_3 as the left and right points of x_2

iv) Find the minimum using the formula:

$$x^* = x_2 + \frac{h(y_1 - y_3)}{2(y_1 + y_3 - 2y_2)}$$

v) If $|x_2 - x^*| < \varepsilon_x$ and $|f(x_2) - f(x^*)| < \varepsilon_f$, then stop and the minimum is x^*.

vi) Starting from the best point, repeat the procedure.

2.5 Methods requiring derivatives

These methods are for continuous. The differentiability helps the efficiency of the algorithms. The derivative can be obtained either analytically or numerically.

• <u>*Newton-Raphson method*</u> (assume twice differentiable)

- It can be used to find the root or the minimum of a function.

$$f(x^*) = f(x_k) + f'(x_k)(x^* - x_k) \Rightarrow x^* = x_k - f(x_k)/f'(x_k)$$
$$f'(x^*) = f'(x_k) + f''(x_k)(x^* - x_k) \Rightarrow x^* = x_k - f'(x_k)/f''(x_k)$$

Start from x_0 (k=0) and the termination criteria ε_x and ε_f.

i) $x_{k+1} = x_k - f'(x_k)/f''(x_k)$

ii) If $|x_{k+1} - x_k| < \varepsilon_x$ and $|f(x_{k+1}) - f(x_k)| < \varepsilon_f$, then stop and the minimum is x_{k+1}.

iii) k=k+1 and go to step i).

Remark 1: If the initial guess is bad, the algorithm may diverge.

→ Robustness problem to initial guess (Sensitive to initial guess)

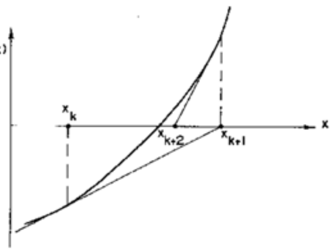


Figure 2.14. Newton-Raphson method (convergence).

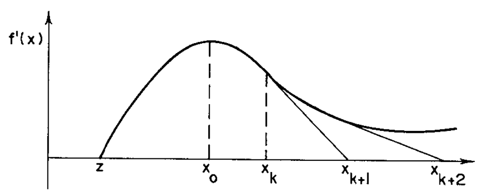


Figure 2.15. Newton-Raphson method (divergence).

- *Bisection method* (Bolzano search)

  Start from x_0 (k=1) and the termination criterion ε.

  i) Find the (a, b) for minimum using bracketting so that $f'(a) < 0$ and $f'(b) > 0$.

  ii) Let $x_k = (a+b)/2$ and evaluate $f'(x_k)$.

  iii) If $|f'(x_k)| \le \varepsilon$, then step and x_k is the optimum point.

  iv) If $f'(x_k) < 0$, a=x_k and if $f'(x_k) > 0$, b=x_k and go to ii).

- *Secant method*

  Start from x_0 (k=1) and the termination criterion ε.

  v) Find the (a, b) for minimum using bracketting so that $f'(a) < 0$ and $f'(b) > 0$.

  vi) Let $x_k = b - (b-a)f'(b)/(f'(b) - f'(a))$ and evaluate $f'(x_k)$.

  vii) If $|f'(x_k)| \le \varepsilon$, then step and x_k is the optimum point.

  viii) If $f'(x_k) < 0$, a=x_k and if $f'(x_k) > 0$, b=x_k and go to ii).

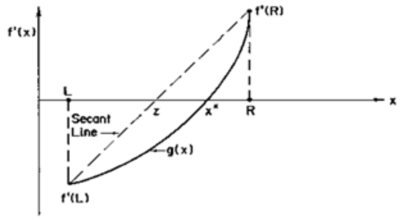


Figure 2.16. Secant method.

- *Cubic search method*

  - Cubic equation

$$y = a(z-z_1)^3 + b(z-z_1)^2 + c(z-z_1) + d \quad (a>0)$$

Given data: $y_1 = y(z_1)$, $y_2 = y(z_2)$, $y_1' = y'(z_1)$, $y_2' = y'(z_2)$ (z_1<z_2)

$$d = y(z_1) \qquad c = y'(z_1)$$

$$y_2 = a(z_2-z_1)^3 + b(z_2-z_1)^2 + y_1'(z_2-z_1) + y_1$$

$$y_2' = 3a(z_2-z_1)^2 + 2b(z_2-z_1) + y_1'$$

$$\begin{bmatrix} (z_2-z_1)^3 & (z_2-z_1)^2 \\ 3(z_2-z_1)^2 & 2(z_2-z_1) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_2 - y_1 - y_1'(z_2-z_1) \\ y_2' - y_1' \end{bmatrix}$$

$$a = \frac{2(y_1-y_2)+(z_2-z_1)(y'_1+y'_2)}{(z_2-z_1)^3} \quad b = -\frac{3(y_1-y_2)+(z_2-z_1)(2y'_1+y'_2)}{(z_2-z_1)^2}$$

$$z^* = z_1 + \frac{-b+\sqrt{b^2-3ac}}{3a} = z_2 - (z_2-z_1)\frac{u_2-u_1+y'_2}{2u_2-y'_1+y'_2}$$

where $u_1 = y_1' + y_2' + 3(y_1-y_2)/(z_2-z_1)$

$u_2 = (u_1^2 - y'_1 y'_2)^{0.5}$

Remark 1: This equation does not apply if $y_1 = y_2$ and $y_1' = -y_2'$.

Remark 2: If $b^2 - 3ac < 0$, the minimum does not exist.

Start from x_0 (k=1) and the termination criterion ε.

i) Find the (a, b) for minimum using bracketting so that $f'(a) < 0$ and $f'(b) > 0$.

ii) Let x_k from the above cubic approximation and evaluate $f'(x_k)$.

iii) If $|f'(x_k)| \le \varepsilon$, then step and x_k is the optimum point.

iv) If $f'(x_k) < 0$, a=x_k and if $f'(x_k) > 0$, b=x_k and go to ii).

2.6 Comparison of the methods

- For very high accuracy, polynomial approximation methods are superior.
- For strongly skewed or possibly multimodal functions, Powell's search has been known to converge at a much slower rate than regional-elimination methods.
- For reliability, choose golden-section method is an ideal choice.
- Cubic search usually shows faster convergence at the cost of computation.
- It is recommended that the Powell-type search method generally be used along with a golden-section search to which the program can default if it encounters difficulties in the course of iterations.