Chapter 2

Functions of a Single Variable

Single-variable optimization problem is of central importance to optimization theory and practice:

- not only because it is a type of problem that the engineer commonly encounters in practice,
- but also because single-variable optimization often arises as a subproblem within the iterative procedures for solving multivariable optimization problems.

2.1 Properties of Single-Variable Functions

Problem 2.1 *Minimize*

$$f(x) = x^3 + 2x^2 - x + 3$$

subject to

$$x \in \mathbf{S}$$

- If $\mathbf{S} = \mathbf{R}$, Problem 2.1 is an unconstrained problem.
- If $\mathbf{S} = \{x| - 5 \leq x \leq 5\}$ Problem 2.1 is a constrained problem.

In engineering optimization,

- f: objective function
- $\mathbf{S}$: *feasible region*, *constraint set*, or *domain* of interest of x

Classification of functions (Figure 2.1)

- Continuous function
- Discontinuous function
- Discrete function

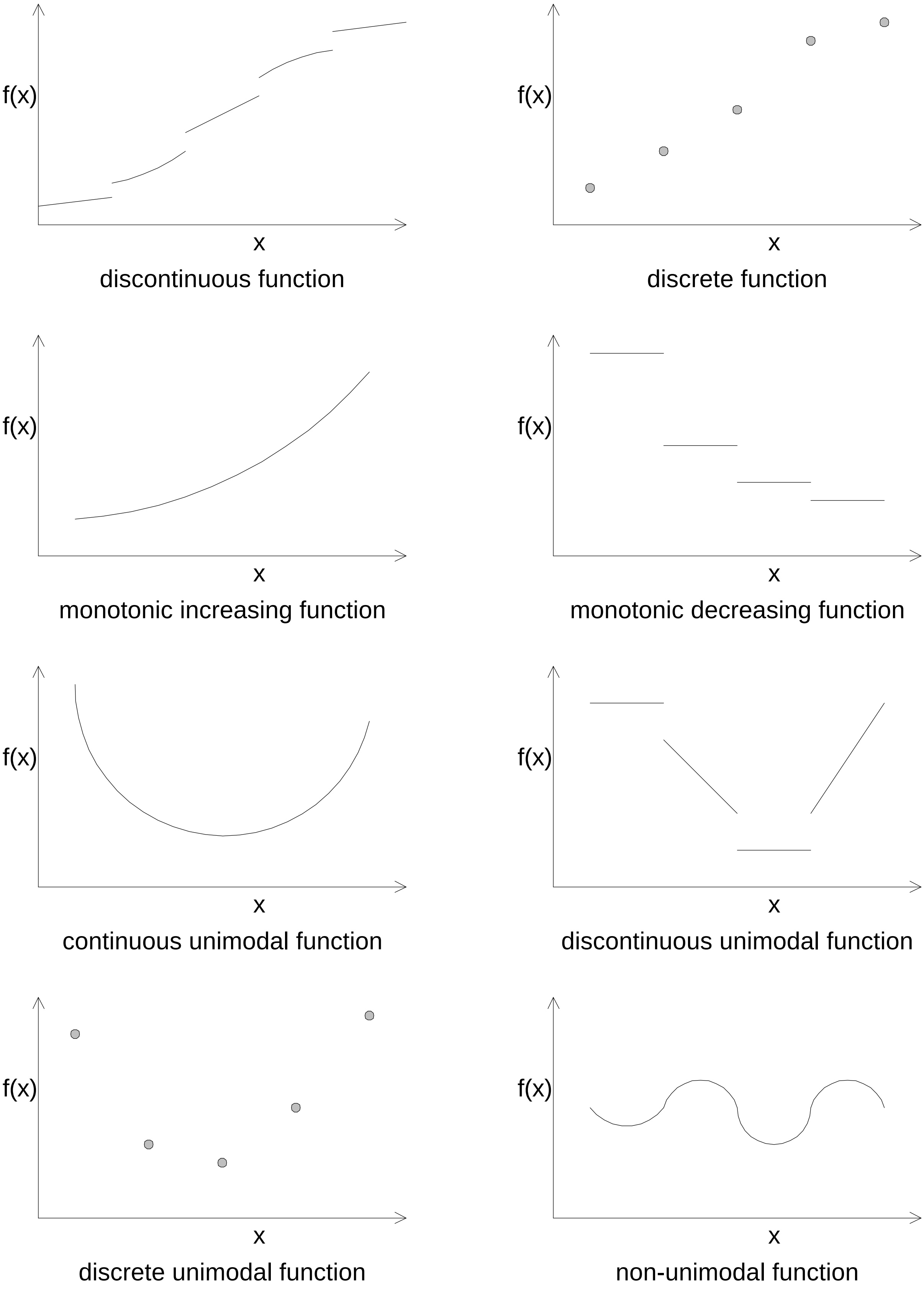

Figure 2.1: Various single variable functions

- Monotonic function
- Unimodal function

Definition 2.1 (Monotonic Function) *A function $f(x)$ is* monotonic *(either increasing or decreasing) if for any two points x_1 and x_2 with $x_1 \leq x_2$, it follows that*

$$f(x_1) \leq f(x_2) \qquad \textit{monotonically increasing}$$

$$f(x_1) \geq f(x_2) \qquad \textit{monotonically decreasing}$$

Definition 2.2 (Unimodal Function) *A function $f(x)$ is* unimodal *on the interval $a \leq x \leq b$ if and only if it is monotonic on either side of the single optimal point x^* in the interval. In other words, if x^* is the single minimum point of $f(x)$ in the range $a \leq x \leq b$, then $f(x)$ is unimodal on the interval if and only if for any two points x_1 and x_2,*

$$x^* \leq x_1 \leq x_2 \qquad \textit{implies that} \qquad f(x^*) \leq f(x_1) \leq f(x_2)$$

and

$$x^* \geq x_1 \geq x_2 \qquad \textit{implies that} \qquad f(x^*) \leq f(x_1) \leq f(x_2)$$

2.2 Optimality Criteria

In considering optimization problems, two questions generally must be addressed

1. *The static question*: How can one determine whether a given point x^* is the optimal solution? (Figure 2.2)
2. *The dynamic question*: If x^* is not the optimal point, then how does one go about finding a solution that is optimal?

Definition 2.3 (Global Minimum) *A function $f(x)$ defined on a set $\mathbf{S}$ attains its* global minimum *at a point $x^{**} \in \mathbf{S}$ if and only if*

$$f(x^{**}) \leq f(x) \qquad \forall x \in \mathbf{S}$$

Definition 2.4 (Local minimum) *A function $f(x)$ defined on $\mathbf{S}$ has a* local minimum *(*relative minimum*) at a point $x^* \in \mathbf{S}$ if and only if there exist an $\varepsilon > 0$ such that*

$$f(x^*) \leq f(x)$$

for all $x \in \mathbf{S}$ satisfying $| x - x^*| < \varepsilon$.

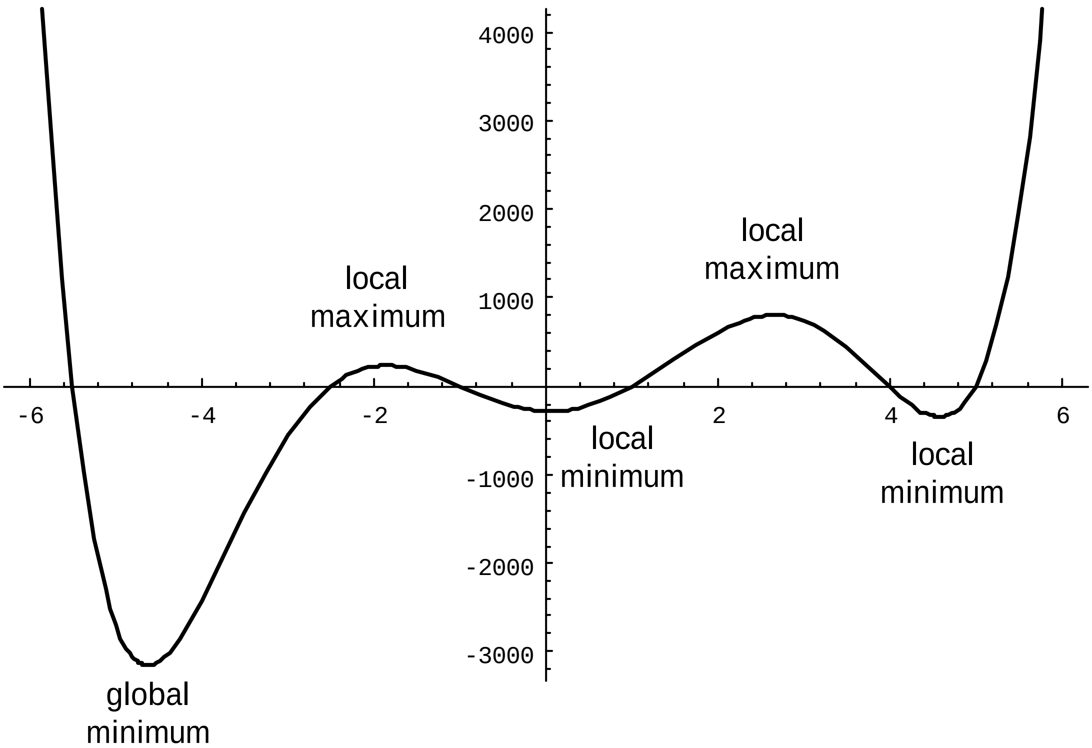

Figure 2.2: Local and global optima

Remarks

1. By reversing the directions of inequality, we can get the equivalent definitions of *global maximum* and *local maximum.*

2. Under the assumption of unimodality, the local minimum automatically becomes the global minimum.

3. When the function is not unimodal, multiple local optima are possible and the global minimum can be found only by locating all local optima and selecting the best one.

Identification of Single-Variable Optima For $x \in (a, b)$, let $x = x^* + \varepsilon$ then

$$f(x^* + \varepsilon) - f(x^*) = \varepsilon \left.\frac{df}{dx}\right|_{x=x^*} + \frac{\varepsilon^2}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=x^*} + \cdots + \frac{\varepsilon^n}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=x^*} + O(\varepsilon^{n+1}) \tag{2.1}$$

If x^* is a local minimum of f on (a, b), then there must be an ε-neighborhood of x^* such that for all x within a distance ε,

$$f(x) \geq f(x^*) \tag{2.2}$$

which implies that

$$\varepsilon \left.\frac{df}{dx}\right|_{x=x^*} + \frac{\varepsilon^2}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=x^*} + \cdots + \frac{\varepsilon^n}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=x^*} + O(\varepsilon^{n+1}) \geq 0 \tag{2.3}$$

Theorem 2.1 (Necessary Condition) *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. $\left.\dfrac{df}{dx}\right|_{x=x^*} = 0$

2. $\left.\dfrac{d^2 f}{dx^2}\right|_{x=x^*} \geq 0 \ (\leq 0)$

Definition 2.5 (Stationary Point) *A* stationary point *is a point x^* at which*

$$\left.\frac{df}{dx}\right|_{x=x^*} = 0$$

Definition 2.6 (Inflection Point) *An* inflection point *or* saddle point[1] *is a stationary point that does not correspond to a local optimum (minimum or maximum).*

[1] The term *inflection point* is preferred for single-variable functions, while *saddle point* is preferred for multivariable functions

Theorem 2.2 (Sufficient Condition) *Suppose at a point x^* the first derivative is zero and the first nonzero higher order derivative is denoted by n.*

(i) If n is odd, then x^* is a point of inflection.

(ii) 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.

2.3 Region Elimination Methods

Theorem 2.3 (Elimination Property) *Suppose f is strictly unimodal on the interval $[a, b]$ with a minimum at x^*. Let x_1 and x_2 be two points in the interval such that $a < x_1 < x_2 < b$. Comparing the functional values at x_1 and x_2, we can conclude:*

(i) 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, $x^* \in (x_1, b]$

(ii) 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, $x^* \in [a, x_2)$ (Figure 2.3)

(iii) When $f(x_1) = f(x_2)$, we could eliminate both ends, $[a, x_1)$ and $(x_2, b]$, and the minimum must occur in the interval $[x_1, x_2]$

The region elimination methods can be broken down into two phases

- *Bounding Phase*: An initial coarse search that will bound or bracket the optimum
- *Interval Refinement Phase*: A finite sequence of interval reductions or refinements to reduce the initial search interval to desired accuracy

2.3.1 Bounding Phase

Assuming unimodality, the $(k + 1)$st test point is generated using the recursion

$$x_{k+1} = x_k + 2^k \Delta$$

for $k = 0, 1, 2, \ldots$ where x_0 is an arbitrarily selected starting point and Δ is a step-size parameter of suitably chosen magnitude.

- If $f(x_0 - |\Delta|) \geq f(x_0) \geq f(x_0 + |\Delta|)$ then $\Delta = |\Delta|$
- If $f(x_0 - |\Delta|) \leq f(x_0) \leq f(x_0 + |\Delta|)$ then $\Delta = -|\Delta|$
- If $f(x_0 - |\Delta|) \geq f(x_0)$ and $f(x_0) \leq f(x_0 + |\Delta|)$ then the minimum is bracketed between $x_0 - |\Delta|$ and $x_0 + |\Delta|$.

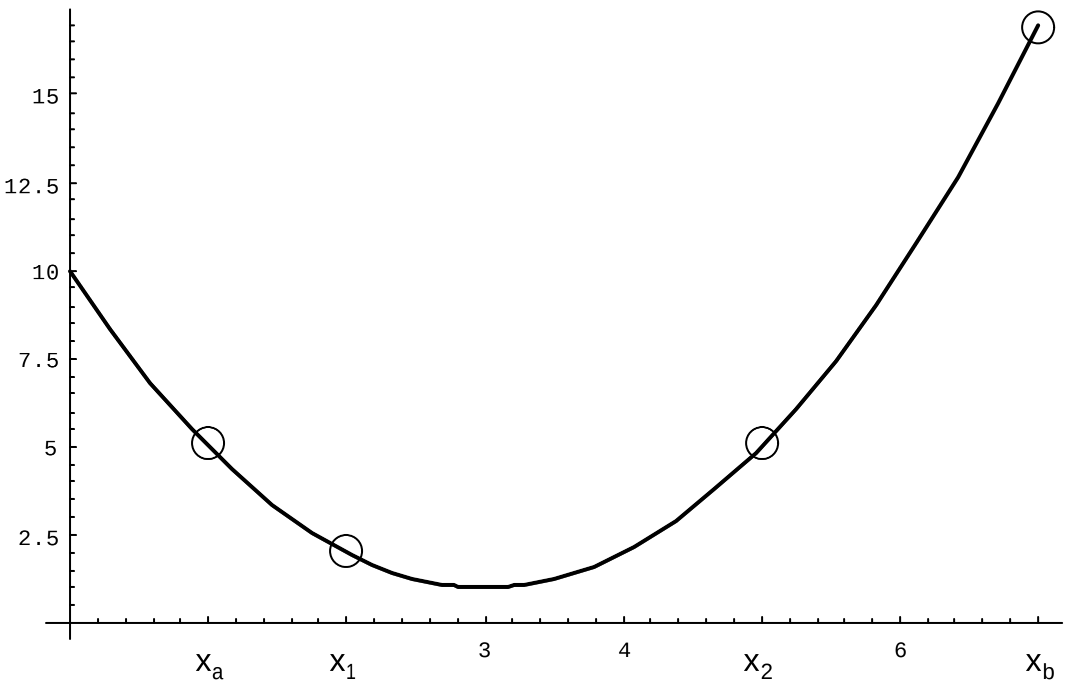

Figure 2.3: Case (ii) of Theorem 2.3

- The remaining case, $f(x_0 - |\Delta|) \leq f(x_0)$ and $f(x_0) \geq f(x_0 + |\Delta|)$, is ruled out by the unimodality assumption.

Example 2.1 *Starting with* $x_0 = 30$ *and* $|\Delta| = 5$, *minimize*

$$f(x) = (100 - x)^2$$

Bounding phase

$$\begin{aligned} f(x_0) &= f(30) &= 4900 \\ f(x_0 + |\Delta|) &= f(35) &= 4225 \\ f(x_0 - |\Delta|) &= f(25) &= 5625 \end{aligned}$$

$\Delta = |\Delta| = +5$ $65 \leq x^* \leq 185$

Table 2.1: Bounding procedure

k	x_k	$f(x_k)$
0	30	4900
1	35	4225
2	45	3025
3	65	1225
4	105	25
5	185	7225

2.3.2 Interval Refinement Phase

Interval Halving (Three-Point Equal-Interval Search) This Method deletes *exactly* one-half the interval at each stage.

Let a, x_1, x_m, x_2, and b are equally-spaced:

Table 2.2: Interval halving

Cases	a	x_m	b
$f(x_1) < f(x_m) \leq f(x_2)$	a	x_1	x_m
$f(x_1) \geq f(x_m) > f(x_2)$	x_m	x_2	b
$f(x_1) \geq f(x_m)$ and $f(x_m) \leq f(x_2)$	x_1	x_m	x_2

Golden Section Search Figure 2.4

1. If only two trials are available, then it is best to locate them equi-distant from the center of the interval.
2. In general, the minimax strategy suggests that trials be placed symmetrically in the interval so that the subinterval eliminated will be of the same length regardless of the outcome of the trials.
3. The search scheme should require the evaluation of *only one* new point at each step.

$$1 - \tau = \tau^2$$
$$\tau = \frac{\sqrt{5} - 1}{2} = 0.61803\cdots$$

2.3.3 Comparison of Region-Elimination Methods

Fractional reduction $\mathrm{FR}(N) = L_N/L_1$ where L_i is the interval of uncertainty after i functional evaluations (Figure 2.5).

- interval halving
$$\mathrm{FR}(N) = \left(\frac{1}{2}\right)^{N/2} = (0.707\cdots)^N$$
- golden section search
$$\mathrm{FR}(N) = \left(\frac{\sqrt{5} - 1}{2}\right)^N = (0.618\cdots)^N$$
- exhaustive search
$$\mathrm{FR}(N) = \frac{2}{N+1}$$

Common characteristics of interval halving & golden section searches

- requires unimodality, but not differentiability
- applicable to both continuous and discontinuous functions as well as to discrete variables
- does not utilize the magnitude of the difference between the function values

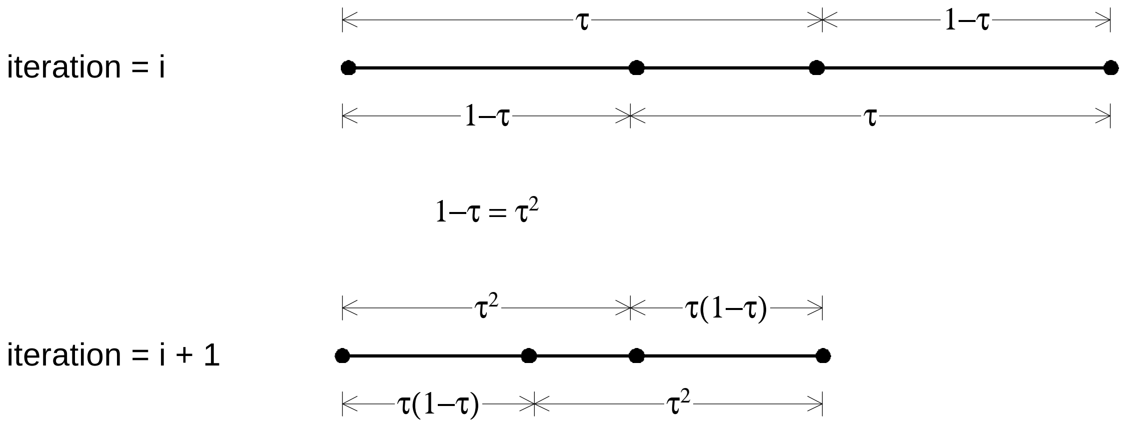

Figure 2.4: Golden section search

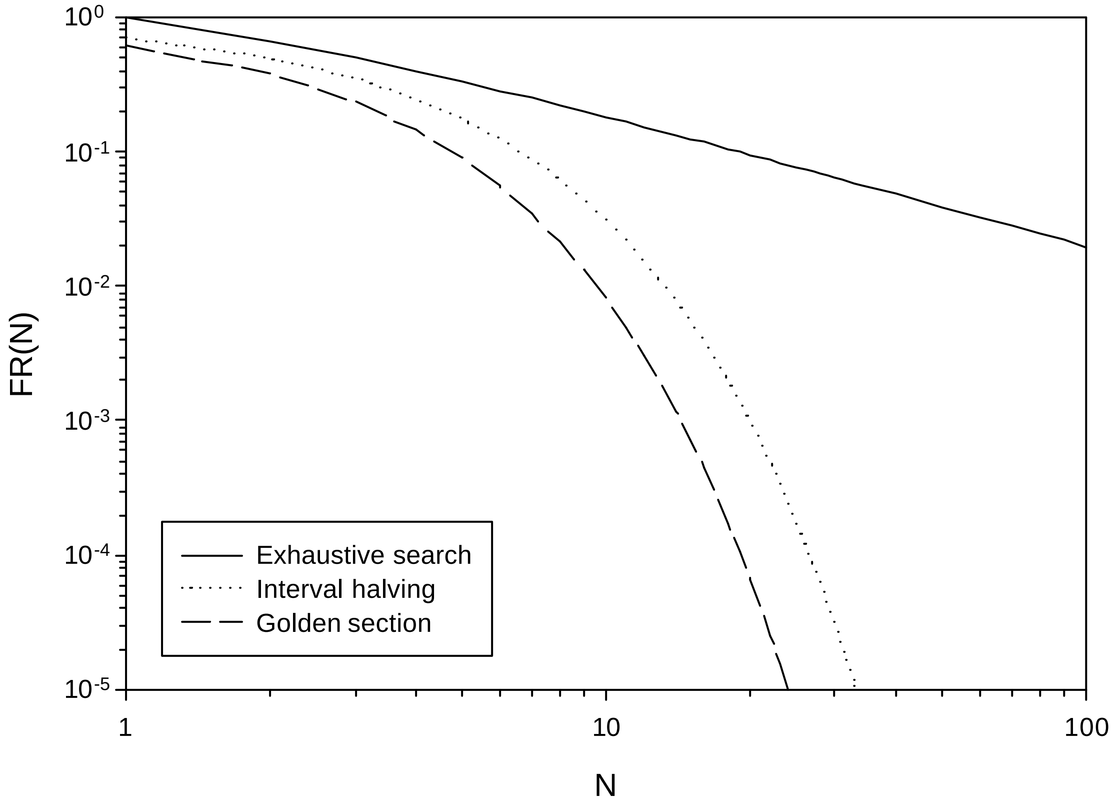

Figure 2.5: Fractional reduction achieved

2.4 Polynomial Approximation or Point Estimation Methods

Quadratic Estimation Methods For

$$q(x) = a_0 + a_1(x - x_1) + a_2(x - x1)(x - x_2)$$

let $f_1 = q(x_1)$, $f_2 = q(x_2)$, and $f_3 = q(x_3)$ then

$$a_0 = f_1 \qquad a_1 = \frac{f_2 - f_1}{x_2 - x_1} \qquad a_2 = \frac{1}{x_3 - x_2}\left(\frac{f_3 - f_1}{x_3 - x_1} - a_1\right)$$

and

$$\bar{x} = \frac{x_2 + x_1}{2} - \frac{a_1}{2a_2}$$

Powell's Successive Quadratic Estimation Method Using $\bar{x}$ and the two points bracketing $\bar{x}$, repeat quadratic estimation.

2.5 Methods Requiring Derivatives

Most single-variable optimization methods requireing derivatives are to find the solution of the first-order necessary condition for optimality:

$$f'(x^*) = \left.\frac{df}{dx}\right|_{x=x^*} = 0$$

2.5.1 Newton-Raphson Method

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

2.5.2 Bisection Method

$$x_{k+1} = \frac{b + a}{2}$$

2.5.3 Secant Method

$$x_{k+1} = b - \frac{f'(b)}{[f'(b) - f'(a)]/(b - a)}$$

2.5.4 Cubic Search Method

Given cubic approximation

$$\bar{f}(x) = a_0 + a_1(x - x_1) + a_2(x - x_1)(x - x_2) + a_3(x - x_1)^2(x - x_2)$$

where

$$a_0 = f_1 \qquad a_1 = \frac{f_2 - f_1}{x_2 - x_1} \qquad a_2 = \frac{a_1 - f_1'}{x_2 - x_1} \qquad a_3 = \frac{f_1' + f_2' - 2a_1}{(x_2 - x_1)^2}$$

If $f'(x_1)f'(x_2) < 0$, find $\bar{x}$ such that $\bar{f}'(\bar{x}) = 0$

2.6 Comparison of Methods

- point estimation methods is intrinsically superior from a theoretical point of view
  - without derivatives: Powell's quadratic search exhibits superlinear convergence
  - requiring first derivative: cubic search
- region-elimination methods: golden section search exhibits linear convergence

2.7 Assignments

2.7.1 Reading Materials

- Reklaitis, *et. al.*'s Chapter 2 [19]
- Edgar & Himmelblau's Chapters 4 & 5 [5]
- Rao's §2.1 – 2.2 & Chapter 5 [17]
- Chong & Żak's Chapters 6 & 7 [4]

Bibliography

[1] Beveridge, G. S. & R. S. Schechter, 1970, *Optimization: Theory and Practice*, McGraw-Hill.

[2] Biegler, L. T., E. I. Grossmann & A. W. Westerberg, 1997, *Systematic Methods of Chemical Process Design*, Prentice-Hall.

[3] Bryson, Jr., A. E. & Y.-C. Ho, 1975, *Applied Optimal Control: Optimization, Estimation, and Control*, Revised Printing, Hemisphere.

[4] Chong, E. K. P. & S. H. Żak, 1996, *An Introduction to Optimization*, Wiley.

[5] Edgar, T. F. & D. M. Himmelblau, 1989, *Optimization of Chemical Processes*, McGraw-Hill.

[6] Edgeworth, F. Y., 1987, *Mathematical Psychics*, University Microfilms International (Out-of Print Books on Demand, the original edition in 1881).

[7] Floudas, C. A. & P. M. Pardalos (eds.), 2001, *Encyclipedia of Optimization*, Kluwer.

[8] Floudas, C. A., 2000, *Deterministic Global Optimization: Theory, Methods and Applications*, Kluwer.

[9] Floudas, C. A. & P. M. Pardalos (eds.), 2000, *Optimization in Computational Chemistry and Molecular Biology*, Kluwer.

[10] Gelfand, I. M. & S. V. Fomin, 1963, *Calculus of Variation*, Revised English editon translated and edited by R. A. Silverman, Prentice-Hall.

[11] Horst, R. & P. M. Pardolos (eds.), 1995, *Handbook of Global Optimization*, Kluwer.

[12] Horst, R. & H. Tuy, 1996, *Global Optimization: Deterministic Approach*, 3rd ed., Springer.

[13] McCormick, G. P., 1967, "Second order conditions for constrained minima," *SIAM J. Appl. Math.*, **15**(3), 641 – 652.

[14] Miettinen. K. M., 1999, *Nonlinear Multiobjective Optimization*, Kluwer.

[15] Pareto, V., 1964, *Cours d'Economie Politique*, Libraire Droz, Genève (the first edition in 1896).

[16] Pareto, V., 1971, *Manual of Political Economy*, MacMillan Press (the original edition in French in 1927).

[17] Rao, S. S., 1996, *Engineering Optimization: Theory and Practice*, 3rd ed., Wiley.

[18] Ray, W. H., 1981, *Advanced Process Control*, McGraw-Hill.

[19] Reklaitis, G. V., A. Ravindran & K. M. Ragsdell, 1983, *Engineering Optimization: Methods and Applications*, Wiley.

Optimization Journals

- AIAA Journal
- ASCE Journal of Structural Engineering
- ASME Journal of Mechanical Design
- Computers and Chemical Engineering
- Computers and Operations Research
- Computers and Structures
- Engineering Optimization
- International Journal for Numerical Methods in Engineering
- Journal of Optimization Theory and Applications
- Management Sceience
- Operations Research
- SIAM Journal of Optimization
- Structural Optimization