Θεωρία Βελτιστοποίησης

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Μη γραμμικός προγραμματισμός: μέθοδοι μονοδιάστατης ελαχιστοποίησης

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Τι παρουσιάστηκε έως σήμερα

- Αναλυτικές μέθοδοι επίλυσης προβλημάτων βελτιστοποίησης.
- Μέθοδοι γραμμικού προγραμματισμού για την επίλυση προβλημάτων με γραμμική αντικειμενική συνάρτηση και γραμμικούς περιορισμούς ισότητας ή ανισότητας.

Τι θα παρουσιαστεί

- Μέθοδοι επίλυσης μη γραμμικών προβλημάτων.
- Η συγκεκριμένη διάλεξη θα εστιάσει σε μονοδιάστατα προβλήματα, δηλαδή σε προβλήματα με μία μεταβλητή.
- Θα παρουσιαστούν προσεγγίσεις, οι οποίες ανήκουν σε κάποια από τις εξής κατηγορίες:
- Μέθοδοι απαλοιφής.
- Μέθοδοι παρεμβολής.

Αριθμητικές μέθοδοι

- Αρκετές αριθμητικές μέθοδοι παράγουν μια σειρά διαδοχικών εκτιμήσεων της αντικειμενικής συνάρτησης, επιδιώκοντας να προσεγγίσουν το βέλτιστο. Αυτές ονομάζονται *επαναληπτικές* και ένας τυπικός τρόπος λειτουργίας είναι ως εξής:
- 1. Εκκίνηση από ένα δοκιμαστικό σημείο $\mathbf{X_1}$.
- 2. Εύρεση της κατάλληλης κατεύθυνσης αναζήτησης $\mathbf{S_i}$ (ξεκινώντας με i=1), η οποία οδηγεί προς το βέλτιστο.
- 3. Εύρεση του κατάλληλου μήκους βήματος λ_i^* προς την κατεύθυνση $\mathbf{S_i}$.
- 4. Υπολογισμός του νέου σημείου $\mathbf{X}_{i+1} = \mathbf{X}_i + \lambda_i^* \mathbf{S}_i$
- 5. Έλεγχος του $\mathbf{X}_{i+1}$ αν είναι βέλτιστο. Αν είναι τότε ολοκληρώνεται η διαδικασία. Αλλιώς τίθεται i = i + 1 και επαναλαμβάνεται η διαδικασία στο βήμα 2.

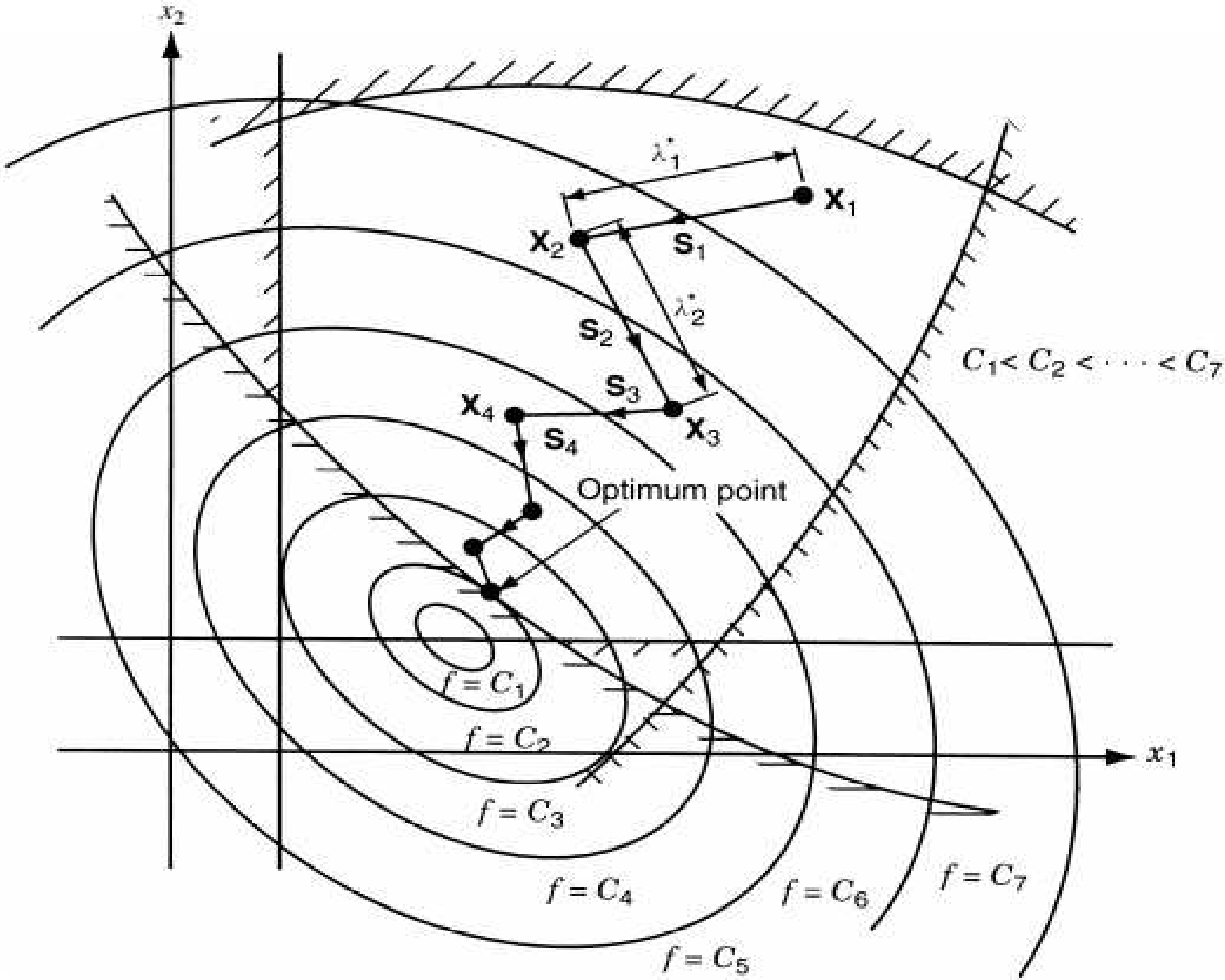
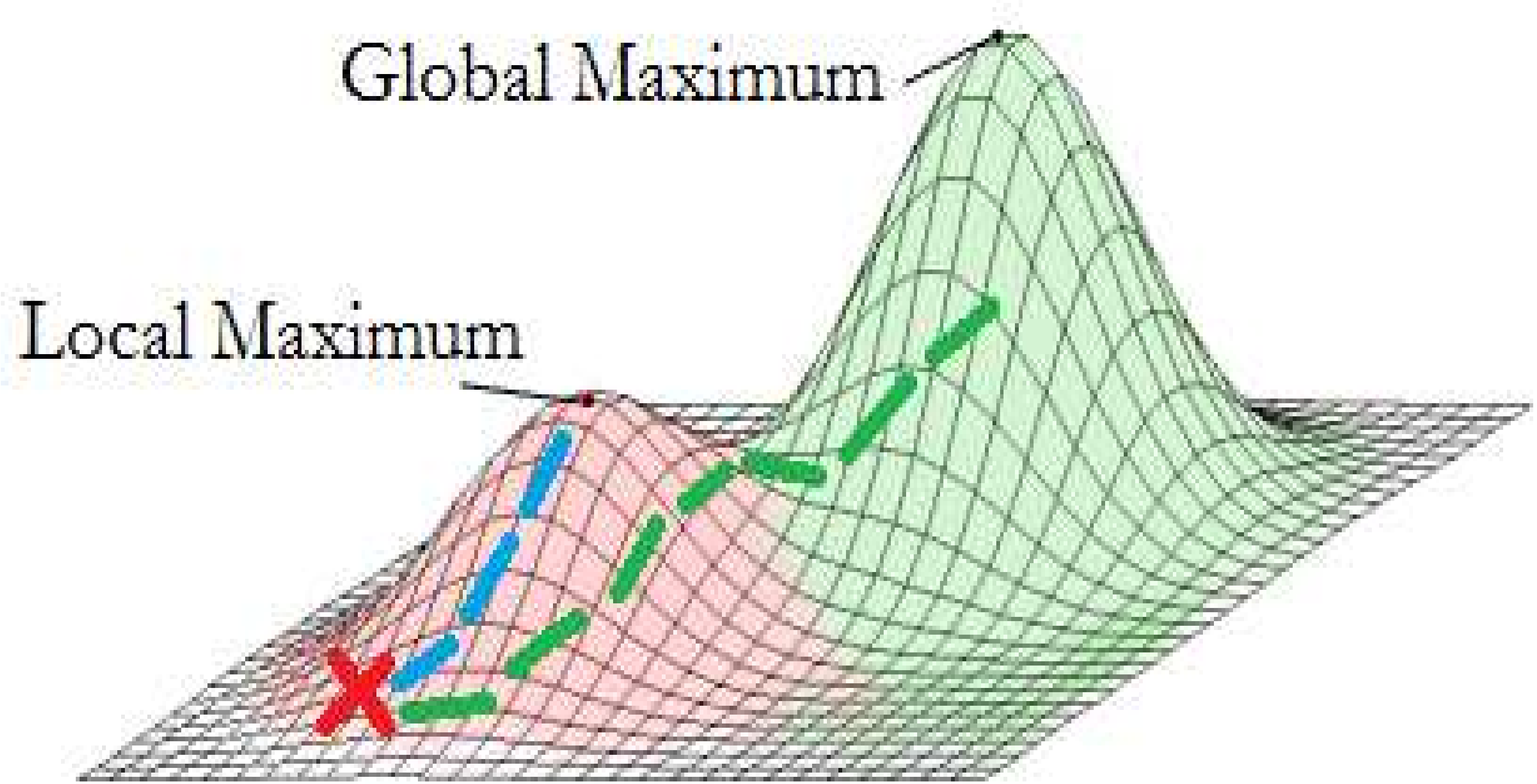


Figure 5.3 Iterative process of optimization.


Global Maximum
Local Maximum

- Η επαναληπτική διαδικασία των διαδοχικών βημάτων προς κατεύθυνση $\mathbf{S}_i$ και μήκος βήματος λ_i^* είναι κατάλληλη τόσο για προβλήματα με περιορισμούς όσο και για προβλήματα χωρίς περιορισμούς.
- Η απόδοση των αντίστοιχων μεθόδων εξαρτάται από την απόδοση των μεθόδων εκτίμησης της κατεύθυνσης $\mathbf{S}_i$ και του μήκους βήματος λ_i^*.
- Η συγκεκριμένη διάλεξη θα εστιάσει στις μεθόδους εκτίμησης του μήκους βήματος λ_i^*.
- Οι επόμενες 2 διαλέξεις θα αφιερωθούν στις μεθόδους εύρεσης της κατεύθυνσης $\mathbf{S}_i$.

Εύρεση του κατάλληλου λ_i^*

- Έστω $f(\mathbf{X})$ η αντικειμενική συνάρτηση που απαιτεί ελαχιστοποίηση.
- Θέλουμε να βρούμε το λ_i^* , το οποίο ελαχιστοποιεί τον επόμενο υπολογισμό $f(\mathbf{X}_{i+1})=f(\mathbf{X}_i+\lambda_i\mathbf{S}_i)$
- Το υφιστάμενο σημείο $\mathbf{X}_i$ και η κατεύθυνση $\mathbf{S}_i$ είναι καθορισμένα με συγκεκριμένες τιμές.
- Επομένως το πρόβλημα απλοποιείται στη μορφή $f(\mathbf{X}_{i+1})=f(\lambda_i)$
- Αφού υπάρχει μόνο μία μεταβλητή (το λ_i) το πρόβλημα είναι *μονοδιάστατο*. Υπάρχουν πολλές μέθοδοι επίλυσης μονοδιάστατων προβλημάτων βελτιστοποίησης.

Μέθοδοι επίλυσης μονοδιάστατων προβλημάτων βελτιστοποίησης

Table 5.1 One-dimensional Minimization Methods

- Analytical methods (differential calculus methods)
- Numerical methods
  - Elimination methods
    - Unrestricted search
    - Exhaustive search
    - Dichotomous search
    - Fibonacci method
    - Golden section method
  - Interpolation methods
    - Requiring no derivatives (quadratic)
    - Requiring derivatives
      - Cubic
      - Direct root
        - Newton
        - Quasi-Newton
        - Secant

Αναλυτικές vs Αριθμητικές

- Στις πρώτες διαλέξεις παρουσιάστηκε η αναλυτική επίλυση προβλημάτων βελτιστοποίησης με τη χρήση του διαφορικού λογισμού για συναρτήσεις που είναι συνεχείς και διπλά παραγωγίσιμες. Ο υπολογισμός της τιμής της αντικειμενικής συνάρτησης είναι το τελευταίο βήμα της διαδικασίας. Πρώτα καθορίζονται οι βέλτιστες τιμές των μεταβλητών απόφασης και έπειτα υπολογίζεται η τιμή της αντικειμενικής συνάρτησης.
- Στην αριθμητική προσέγγιση ακολουθείται αντίθετη διαδικασία. Πρώτα υπολογίζεται η τιμή της αντικειμενικής συνάρτησης για διάφορους συνδυασμούς των μεταβλητών απόφασης. Έπειτα εξάγονται συμπεράσματα ως προς τη βέλτιστη λύση.

Σχόλια

- Οι αριθμητικές μέθοδοι χωρίζονται σε 2 κατηγορίες: τις μεθόδους απαλοιφής και τις μεθόδους παρεμβολής.
- Οι μέθοδοι απαλοιφής μπορούν να χρησιμοποιηθούν και για συναρτήσεις που δεν είναι συνεχείς.
- Οι τετραγωνικές και οι κυβικές μέθοδοι παρεμβολής περιλαμβάνουν πολυονομικές προσεγγίσεις μιας δεδομένης συνάρτησης.

A *unimodal function* is one that has only one peak (maximum) or valley (minimum) in a given interval. Thus 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). This can be stated mathematically as follows:

> A function $f(x)$ is unimodal if (*i*) $x_1 < x_2 < x^*$ implies that $f(x_2) < f(x_1)$, and (ii) $x_2 > x_1 > x^*$ implies that $f(x_1) < f(x_2)$, where x^* is the minimum point.

Some examples of unimodal functions are shown in Fig. 5.4. Thus a unimodal function can be a nondifferentiable or even a discontinuous function. If a function is known to be unimodal in a given range, the interval in which the minimum lies can be narrowed down provided that the function values are known at two different points in the range.

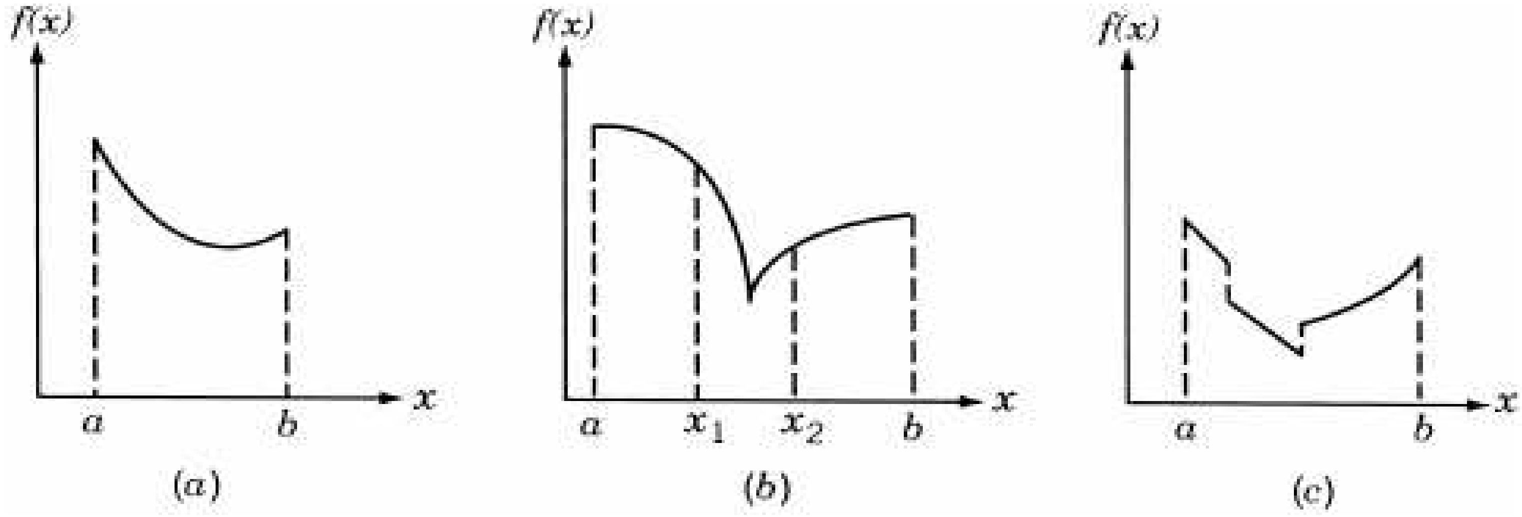


Figure 5.4 Unimodal function.

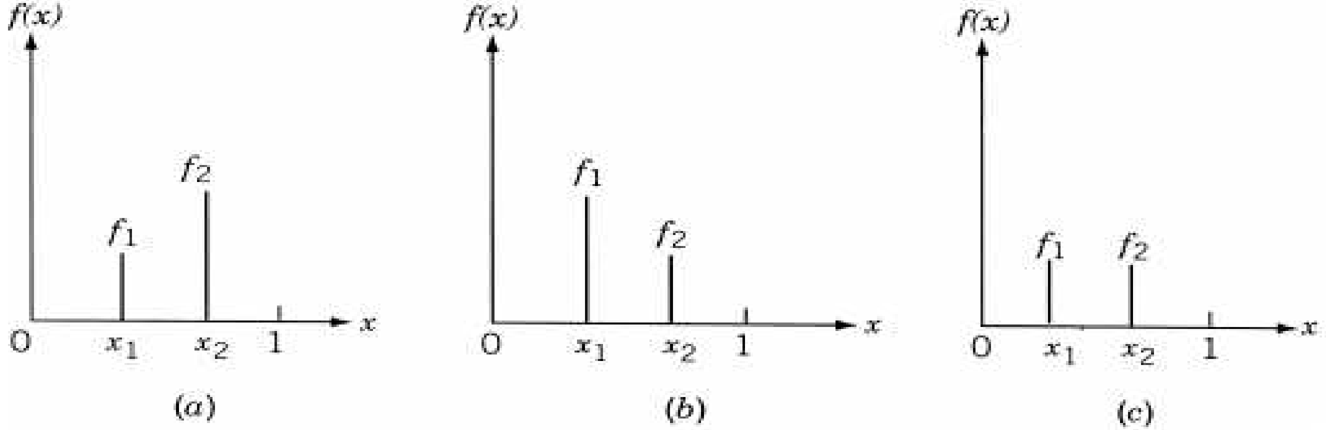


Figure 5.5 Outcome of first two experiments: (*a*) $f_1 < f_2$; (*b*) $f_1 > f_2$; (*c*) $f_1 = f_2$.

For example, consider the normalized interval [0, 1] and two function evaluations within the interval as shown in Fig. 5.5. There are three possible outcomes, namely, $f_1 < f_2$, $f_1 > f_2$, or $f_1 = f_2$. If the outcome is that $f_1 < f_2$, the minimizing x cannot lie to the right of x_2. Thus that part of the interval $[x_2, 1]$ can be discarded and a new smaller interval of uncertainty, $[0, x_2]$, results as shown in Fig. 5.5*a*. If $f(x_1) > f(x_2)$, the interval $[0, x_1]$ can be discarded to obtain a new smaller interval of uncertainty, $[x_1, 1]$ (Fig. 5.5*b*), while if $f(x_1) = f(x_2)$, intervals $[0, x_1]$ and $[x_2, 1]$ can both be discarded to obtain the new interval of uncertainty as $[x_1, x_2]$ (Fig. 5.5*c*). Further, if one of the original experiments† remains within the new interval, as will be the situation in Fig. 5.5*a* and *b*, only one other experiment need be placed within the new interval in order that the process be repeated. In situations such as Fig. 5.5*c*, two more experiments are to be placed in the new interval in order to find a reduced interval of uncertainty.

The assumption of unimodality is made in all the elimination techniques. If a function is known to be *multimodal* (i.e., having several valleys or peaks), the range of the function can be subdivided into several parts and the function treated as a unimodal function in each part.

Μέθοδοι απαλοιφής

Μέθοδος σταθερού βήματος

- Η πιο βασική μέθοδος είναι να χρησιμοποιηθεί σταθερό μήκος βήματος και να μετακινηθεί η αναζήτηση από το αρχικό σημείο προς την επιθυμητή κατεύθυνση (θετική ή αρνητική).
- Το μήκος βήματος πρέπει να είναι σχετικά μικρό ανάλογα με την επιθυμητή ακρίβεια των αποτελεσμάτων.
- Αυτή η μέθοδος είναι απλή στην εφαρμογή, αλλά δεν είναι αποδοτική για αρκετές περιπτώσεις.

Περιγραφή μεθόδου σταθερού βήματος

1. Start with an initial guess point, say, x_1.
2. Find $f_1 = f(x_1)$.
3. Assuming a step size s, find $x_2 = x_1 + s$.
4. Find $f_2 = f(x_2)$.
5. If $f_2 < f_1$, and if the problem is one of minimization, the assumption of unimodality indicates that the desired minimum cannot lie at $x < x_1$. Hence the search can be continued further along points $x_3, x_4, \ldots$ using the unimodality assumption while testing each pair of experiments. This procedure is continued until a point, $x_i = x_1 + (i-1)s$, shows an increase in the function value.
6. The search is terminated at x_i, and either x_{i-1} or x_i can be taken as the optimum point.
7. Originally, if $f_2 > f_1$, the search should be carried in the reverse direction at points $x_{-2}, x_{-3}, \ldots$, where $x_{-j} = x_1 - (j-1)s$.
8. If $f_2 = f_1$, the desired minimum lies in between x_1 and x_2, and the minimum point can be taken as either x_1 or x_2.
9. If it happens that both f_2 and f_{-2} are greater than f_1, it implies that the desired minimum will lie in the double interval $x_{-2} < x < x_2$.

Σχόλια για τη μέθοδο σταθερού βήματος

- Είναι απλή στην εφαρμογή μέθοδος.
- Ο σημαντικός περιορισμός εφαρμογής της μεθόδου προκύπτει από την απεριόριστη περιοχή στην οποία μπορεί να υφίσταται η βέλτιστη λύση.
- Π.χ. ας υποθέσουμε ότι το βέλτιστο σημείο βρίσκεται στη θέση $x_{opt} = 50\,000$. Αφού δεν γνωρίζουμε τη θέση του εξαρχής θέτουμε ως αρχικό σημείο το $x = 0$ και μήκος βήματος $s = 0.01$.Αυτό σημαίνει ότι απαιτούνται 5 000 001 υπολογισμοί για την εύρεση του βέλτιστου.

Μέθοδος επιταχυνόμενου μήκους βήματος

- Μια προφανή βελτίωση της μεθόδου σταθερού βήματος μπορεί να επιτευχθεί αυξάνοντας το μήκος βήματος έως ότου περιοριστεί η θέση της βέλτιστης λύσης.
- Μια απλή μέθοδος προτείνει το διπλασιασμό του μήκους βήματος έως ότου σταματήσει να βελτιώνεται η τιμή της αντικειμενικής συνάρτησης. Αρκετές ακόμη βελτιώσεις της μεθόδου έχουν προταθεί. Μια δυνατότητα είναι η μείωση του μήκους βήματος κατόπιν του περιορισμού του βέλτιστου μεταξύ 2 τιμών (x_{i-1} , x_i). Ξεκινώντας είτε από το x_{i-1} είτε από το x_i μπορεί να συνεχιστεί η διαδικασία έως ότου η θέση του βέλτιστου περιοριστεί σε πολύ μικρή περιοχή.

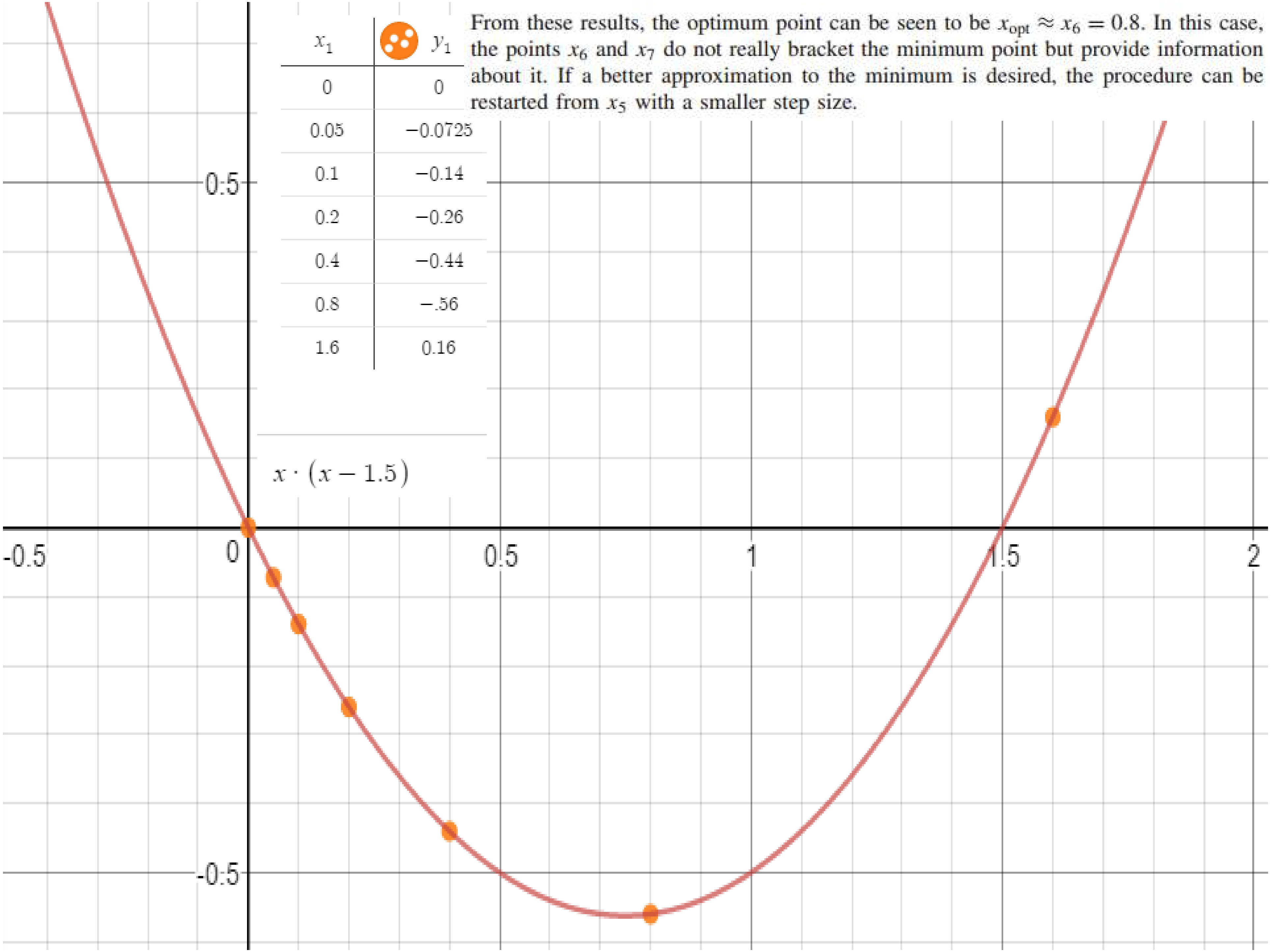
Example 5.3 Find the minimum of $f = x(x - 1.5)$ by starting from 0.0 with an initial step size of 0.05.

SOLUTION The function value at x_1 is $f_1 = 0.0$. If we try to start moving in the negative x direction, we find that $x_{-2} = -0.05$ and $f_{-2} = 0.0775$. Since $f_{-2} > f_1$, the assumption of unimodality indicates that the minimum cannot lie toward the left of x_{-2}. Thus we start moving in the positive x direction and obtain the following results:

i	Value of s	$x_i = x_1 + s$	$f_i = f(x_i)$	Is $f_i > f_{i-1}$?
1	—	0.0	0.0	—
2	0.05	0.05	−0.0725	No
3	0.10	0.10	−0.140	No
4	0.20	0.20	−0.260	No
5	0.40	0.40	−0.440	No
6	0.80	0.80	−0.560	No
7	1.60	1.60	+0.160	Yes

From these results, the optimum point can be seen to be $x_{opt} \approx x_6 = 0.8$. In this case, the points x_6 and x_7 do not really bracket the minimum point but provide information about it. If a better approximation to the minimum is desired, the procedure can be restarted from x_5 with a smaller step size.

From these results, the optimum point can be seen to be $x_{\text{opt}} \approx x_6 = 0.8$. In this case, the points x_6 and x_7 do not really bracket the minimum point but provide information about it. If a better approximation to the minimum is desired, the procedure can be restarted from x_5 with a smaller step size.



Εξαντλητική αναζήτηση (exhaustive search)

The exhaustive search method can be used to solve problems where the interval in which the optimum is known to lie is finite. Let x_s and x_f denote, respectively, the starting and final points of the interval of uncertainty.† The *exhaustive search method* consists of evaluating the objective function at a predetermined number of equally spaced points in the interval (x_s, x_f), and reducing the interval of uncertainty using the assumption of unimodality. Suppose that a function is defined on the interval (x_s, x_f) and let it be evaluated at eight equally spaced interior points x_1 to x_8. Assuming that the function values appear as shown in Fig. 5.6, the minimum point 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.

In general, if the function is evaluated at n equally spaced points in the original interval of uncertainty of length $L_0 = x_f - x_s$, and if the optimum value of the function (among the n function values) turns out to be at point x_j, the final interval of uncertainty

Since the function is evaluated at all n points simultaneously, this method can be called a *simultaneous search method*. This method is relatively inefficient compared to the sequential search methods discussed next, where the information gained from the initial trials is used in placing the subsequent experiments.

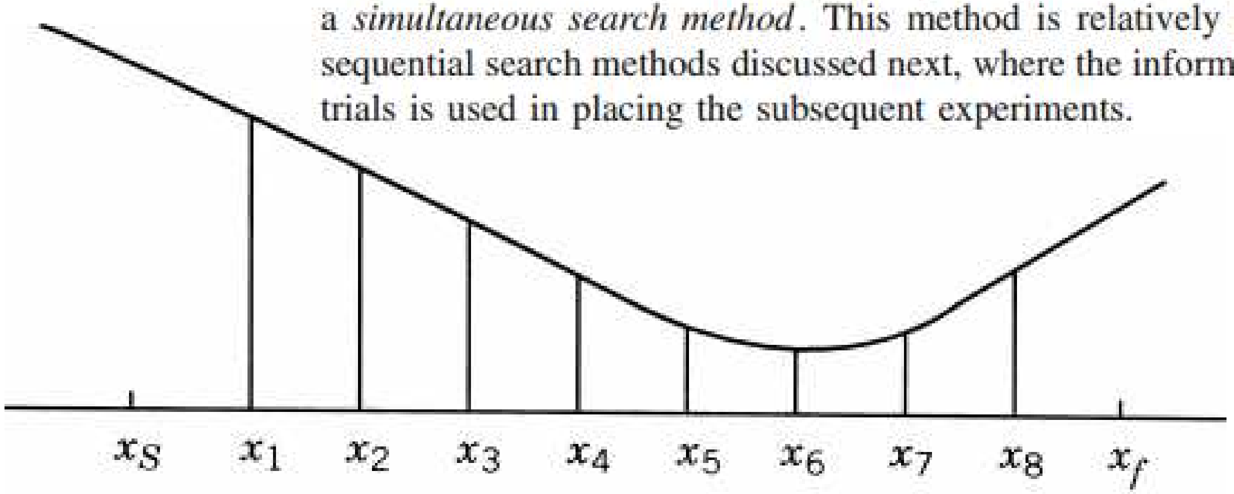


Figure 5.6 Exhaustive search.

Example 5.4 Find the minimum of $f = x(x - 1.5)$ in the interval (0.0, 1.00) to within 10% of the exact value.

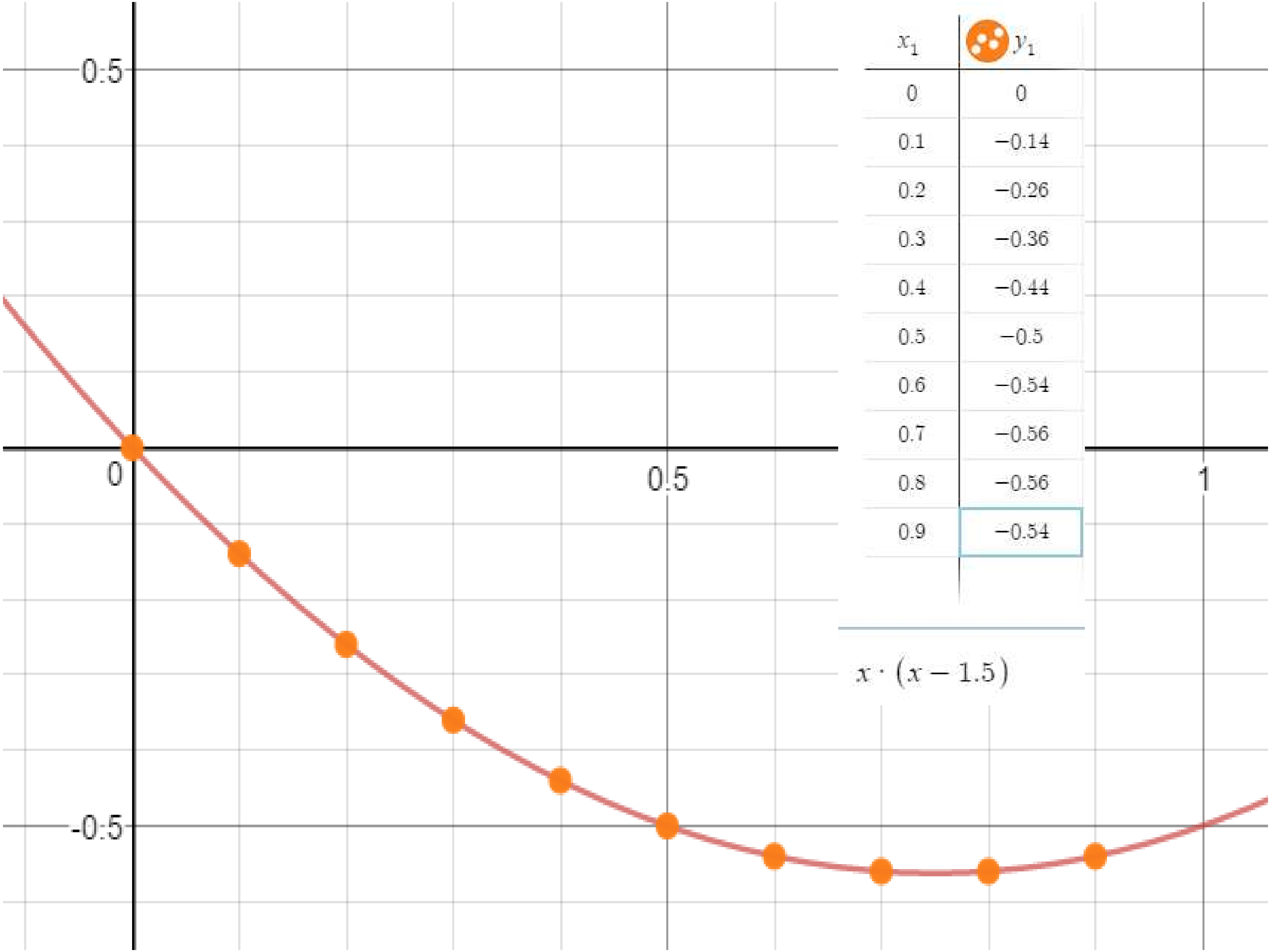
SOLUTION If the middle point of the final interval of uncertainty is taken as the approximate optimum point, the maximum deviation could be $1/(n+1)$ times the initial interval of uncertainty. Thus to find the optimum within 10% of the exact value, we should have

$$\frac{1}{n+1} \le \frac{1}{10} \quad \text{or} \quad n \ge 9$$

By taking $n = 9$, the following function values can be calculated:

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
$f_i = f(x_i)$	−0.14	−0.26	−0.36	−0.44	−0.50	−0.54	−0.56	−0.56	−0.54

Since $x_7 = x_8$, the assumption of unimodality gives the final interval of uncertainty as $L_9 = (0.7, 0.8)$. By taking the middle point of L_9 (i.e., 0.75) as an approximation to the optimum point, we find that it is, in fact, the true optimum point.



x_1	y_1
0	0
0.1	−0.14
0.2	−0.26
0.3	−0.36
0.4	−0.44
0.5	−0.5
0.6	−0.54
0.7	−0.56
0.8	−0.56
0.9	−0.54

Μέθοδοι διαδοχικής αναζήτησης (Sequential search)

- Αναζήτηση διχοτόμησης (dichotomous search)
- Μέθοδος χρυσής τομής (golden section method)
- Μέθοδος Fibonacci

- Σ' αυτές τις μεθόδους το αποτέλεσμα ενός σημείου επηρεάζει τη θέση της επόμενης αναζήτησης.

Αναζήτηση διχοτόμησης (dichotomous search)

In the dichotomous search, two experiments are placed as close as possible at the center of the interval of uncertainty. Based on the relative values of the objective function at the two points, almost half of the interval of uncertainty is eliminated. Let the positions of the two experiments be given by (Fig. 5.7)

$$x_1 = \frac{L_0}{2} - \frac{\delta}{2}$$

$$x_2 = \frac{L_0}{2} + \frac{\delta}{2}$$

where δ is a small positive number chosen so that the two experiments give significantly different results. Then the new interval of uncertainty is given by $(L_0/2 + \delta/2)$. The building block of dichotomous search consists of conducting a pair of experiments at the center of the current interval of uncertainty. The next pair of experiments is, therefore, conducted at the center of the remaining interval of uncertainty. This results in the reduction of the interval of uncertainty by nearly a factor of 2. The intervals of uncertainty at the end of different pairs of experiments are given in the following table:

Number of experiments	2	4	6
Final interval of uncertainty	$\frac{1}{2}(L_0 + \delta)$	$\frac{1}{2}\left(\frac{L_0 + \delta}{2}\right) + \frac{\delta}{2}$	$\frac{1}{2}\left(\frac{L_0 + \delta}{4} + \frac{\delta}{2}\right) + \frac{\delta}{2}$

In general, the final interval of uncertainty after conducting n experiments (n even) is given by

$$L_n = \frac{L_0}{2^{n/2}} + \delta\left(1 - \frac{1}{2^{n/2}}\right) \tag{5.3}$$

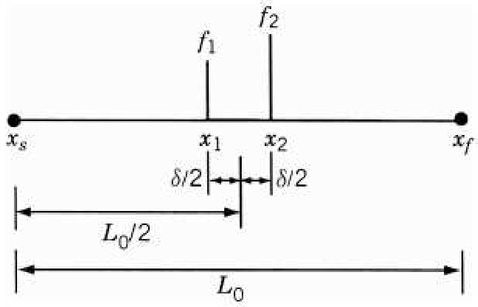


Figure 5.7 Dichotomous search.

Example 5.5 Find the minimum of $f = x(x - 1.5)$ in the interval (0.0, 1.00) to within 10% of the exact value.

SOLUTION The ratio of final to initial intervals of uncertainty is given by [from Eq. (5.3)]

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

where δ is a small quantity, say 0.001, and n is the number of experiments. If the middle point of the final interval is taken as the optimum point, the requirement can be stated as

$$\frac{1}{2}\frac{L_n}{L_0} \leq \frac{1}{10}$$

i.e.,

$$\frac{1}{2^{n/2}} + \frac{\delta}{L_0}\left(1 - \frac{1}{2^{n/2}}\right) \leq \frac{1}{5}$$

Since $\delta = 0.001$ and $L_0 = 1.0$, we have

$$\frac{1}{2^{n/2}} + \frac{1}{1000}\left(1 - \frac{1}{2^{n/2}}\right) \leq \frac{1}{5}$$

i.e.,

$$\frac{999}{1000}\frac{1}{2^{n/2}} \leq \frac{995}{5000} \quad \text{or} \quad 2^{n/2} \geq \frac{999}{199} \simeq 5.0$$

Since n has to be even, this inequality gives the minimum admissible value of n as 6.

The search is made as follows. The first two experiments are made at

$$x_1 = \frac{L_0}{2} - \frac{\delta}{2} = 0.5 - 0.0005 = 0.4995$$

$$x_2 = \frac{L_0}{2} + \frac{\delta}{2} = 0.5 + 0.0005 = 0.5005$$

with the function values given by

$$f_1 = f(x_1) = 0.4995(-1.0005) \simeq -0.49975$$

$$f_2 = f(x_2) = 0.5005(-0.9995) \simeq -0.50025$$

Since $f_2 < f_1$, the new interval of uncertainty will be (0.4995, 1.0). The second pair of experiments is conducted at

$$x_3 = \left(0.4995 + \frac{1.0 - 0.4995}{2}\right) - 0.0005 = 0.74925$$

$$x_4 = \left(0.4995 + \frac{1.0 - 0.4995}{2}\right) + 0.0005 = 0.75025$$

which give the function values as

$$f_3 = f(x_3) = 0.74925(-0.75075) = -0.5624994375$$

$$f_4 = f(x_4) = 0.75025(-0.74975) = -0.5624999375$$

Since $f_3 > f_4$, we delete $(0.4995, x_3)$ and obtain the new interval of uncertainty as

$$(x_3, 1.0) = (0.74925, 1.0)$$

The final set of experiments will be conducted at

$$x_5 = \left(0.74925 + \frac{1.0 - 0.74925}{2}\right) - 0.0005 = 0.874125$$

$$x_6 = \left(0.74925 + \frac{1.0 - 0.74925}{2}\right) + 0.0005 = 0.875125$$

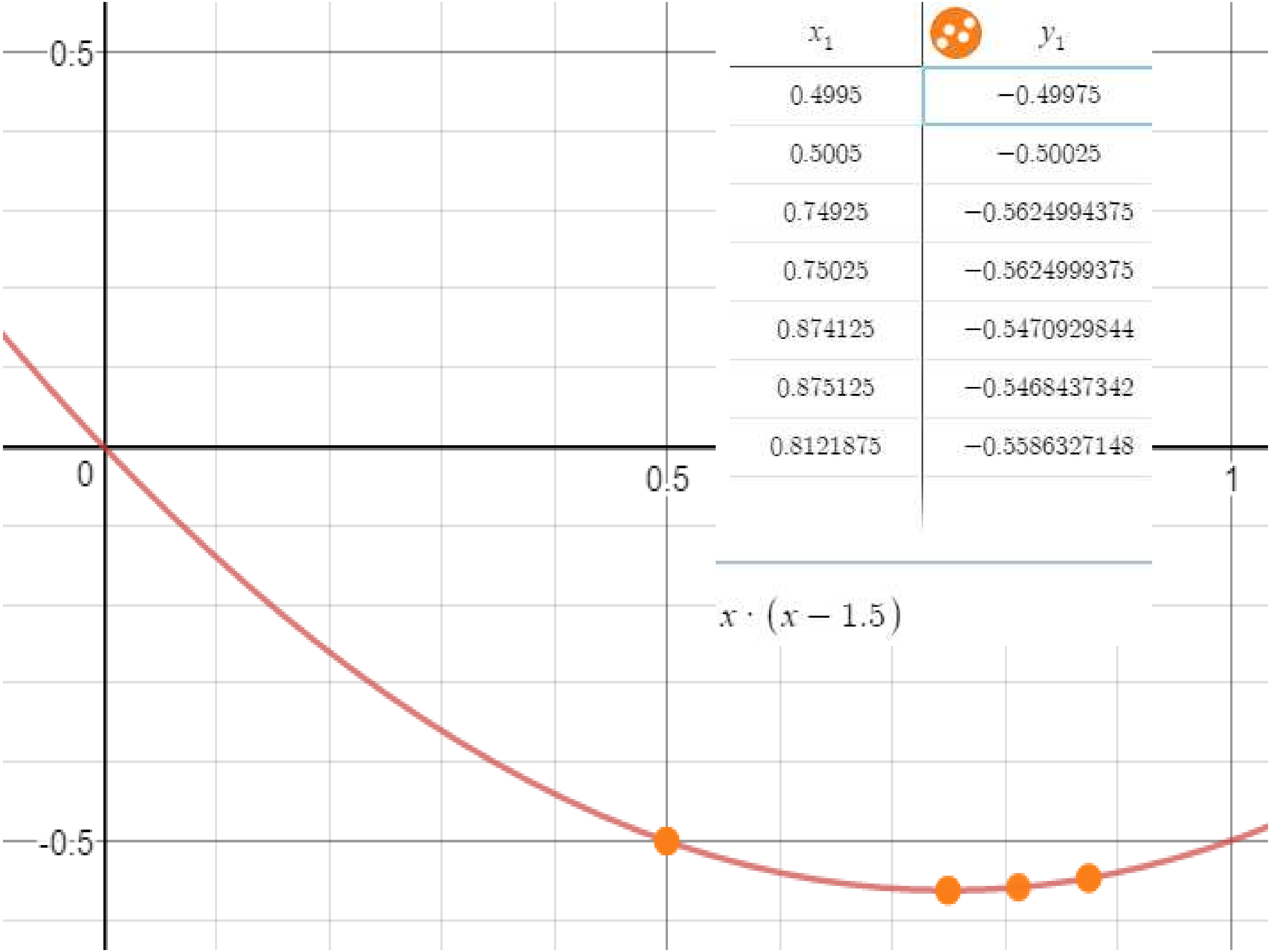
The corresponding function values are

$$f_5 = f(x_5) = 0.874125(-0.625875) = -0.5470929844$$

$$f_6 = f(x_6) = 0.875125(-0.624875) = -0.5468437342$$

Since $f_5 < f_6$, the new interval of uncertainty is given by $(x_3, x_6) = (0.74925, 0.875125)$. The middle point of this interval can be taken as optimum, and hence

$$x_{\text{opt}} \simeq 0.8121875 \quad \text{and} \quad f_{\text{opt}} \simeq -0.5586327148$$



x_1	y_1
0.4995	−0.49975
0.5005	−0.50025
0.74925	−0.5624994375
0.75025	−0.5624999375
0.874125	−0.5470929844
0.875125	−0.5468437342
0.8121875	−0.5586327148

In the *interval halving method*, exactly one-half of the current interval of uncertainty is deleted in every stage. It requires three experiments in the first stage and two experiments in each subsequent stage. The procedure can be described by the following steps:

1. Divide the initial interval of uncertainty $L_0 = [a, b]$ into four equal parts and label the middle point x_0 and the quarter-interval points x_1 and x_2.
2. Evaluate the function $f(x)$ at the three interior points to obtain $f_1 = f(x_1)$, $f_0 = f(x_0)$, and $f_2 = f(x_2)$.
3. (a) If $f_2 > f_0 > f_1$ as shown in Fig. 5.8*a*, delete the interval (x_0, b), label x_1 and x_0 as the new x_0 and b, respectively, and go to step 4.
   (b) If $f_2 < f_0 < f_1$ as shown in Fig. 5.8*b*, delete the interval (a, x_0), label x_2 and x_0 as the new x_0 and a, respectively, and go to step 4.
   (c) If $f_1 > f_0$ and $f_2 > f_0$ as shown in Fig. 5.8*c*, delete both the intervals (a, x_1) and (x_2, b), label x_1 and x_2 as the new a and b, respectively, and go to step 4.
4. Test whether the new interval of uncertainty, $L = b - a$, satisfies the convergence criterion $L \leq \varepsilon$, where ε is a small quantity. If the convergence criterion is satisfied, stop the procedure. Otherwise, set the new $L_0 = L$ and go to step 1.

Remarks:

1. In this method, the function value at the middle point of the interval of uncertainty, f_0, will be available in all the stages except the first stage.
2. The interval of uncertainty remaining at the end of n experiments ($n \geq 3$ and odd) is given by

$$L_n = \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \tag{5.4}$$

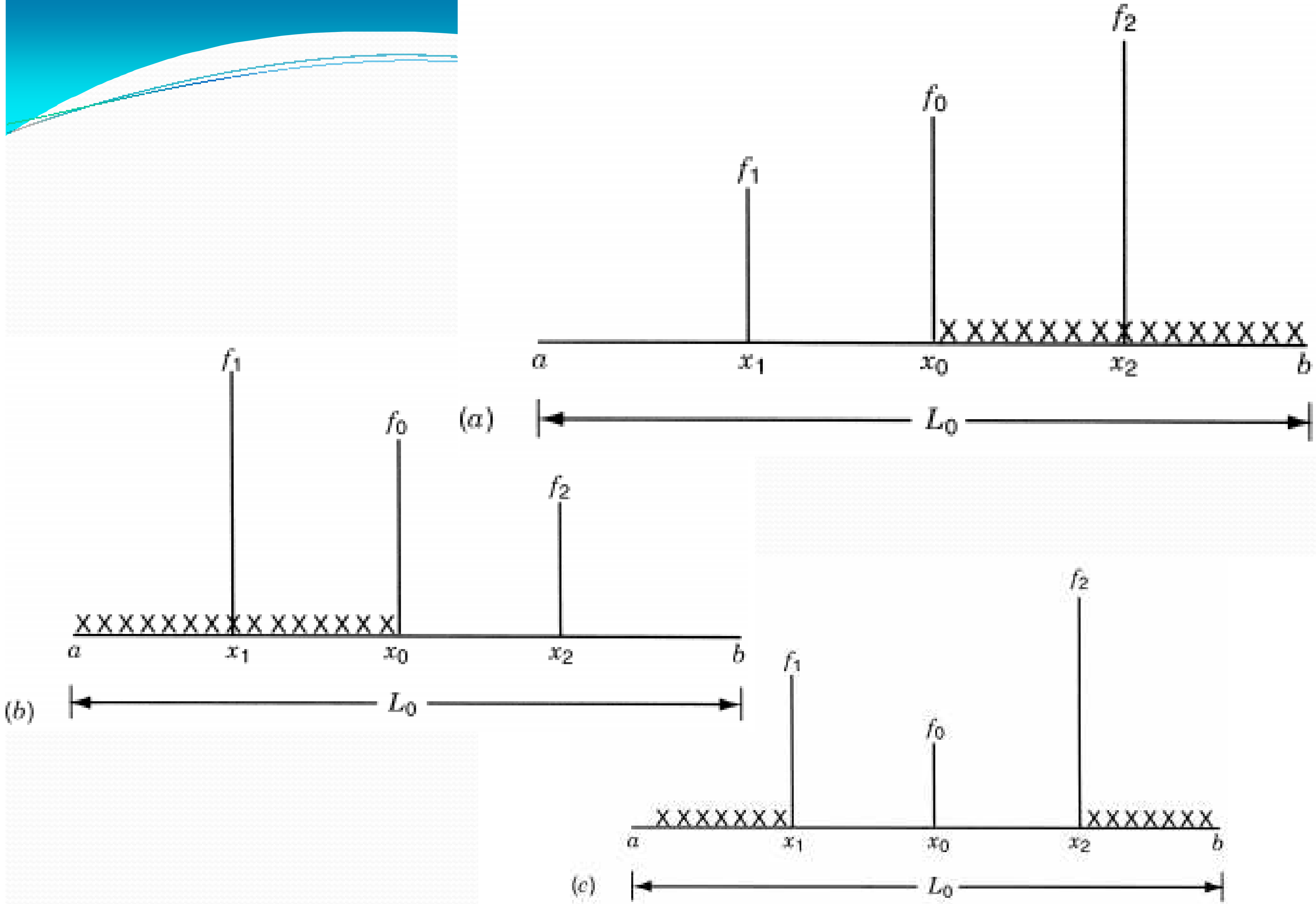


Figure 5.8 Possibilities in the interval halving method: (*a*) $f_2 > f_0 > f_1$; (*b*) $f_1 > f_0 > f_2$; (*c*) $f_1 > f_0$ and $f_2 > f_0$.

Example 5.6 Find the minimum of $f = x(x - 1.5)$ in the interval (0.0, 1.0) 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

$$\frac{1}{2}L_n \le \frac{L_0}{10} \quad \text{or} \quad \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \le \frac{L_0}{5} \tag{E$_1$}$$

Since $L_0 = 1$, Eq. (E_1) gives

$$\frac{1}{2^{(n-1)/2}} \le \frac{1}{5} \quad \text{or} \quad 2^{(n-1)/2} \ge 5 \tag{E$_2$}$$

Since n has to be odd, inequality (E_2) gives the minimum permissible value of n as 7. With this value of $n = 7$, the search is conducted as follows. The first three experiments are placed at one-fourth points of the interval $L_0 = [a = 0, b = 1]$ as

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

$$x_0 = 0.50, \qquad f_0 = 0.50(-1.00) = -0.5000$$

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

Since $f_1 > f_0 > f_2$, we delete the interval $(a, x_0) = (0.0, 0.5)$, label x_2 and x_0 as the new x_0 and a so that $a = 0.5$, $x_0 = 0.75$, and $b = 1.0$. By dividing the new interval of uncertainty, $L_3 = (0.5, 1.0)$ into four equal parts, we obtain

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

$$x_0 = 0.750, \qquad f_0 = 0.750(-0.750) = -0.562500$$

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

Since $f_1 > f_0$ and $f_2 > f_0$, we delete both the intervals (a, x_1) and (x_2, b), and label x_1, x_0, and x_2 as the new a, x_0, and b, respectively. Thus the new interval of uncertainty will be $L_5 = (0.625, 0.875)$. Next, this interval is divided into four equal parts to obtain

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

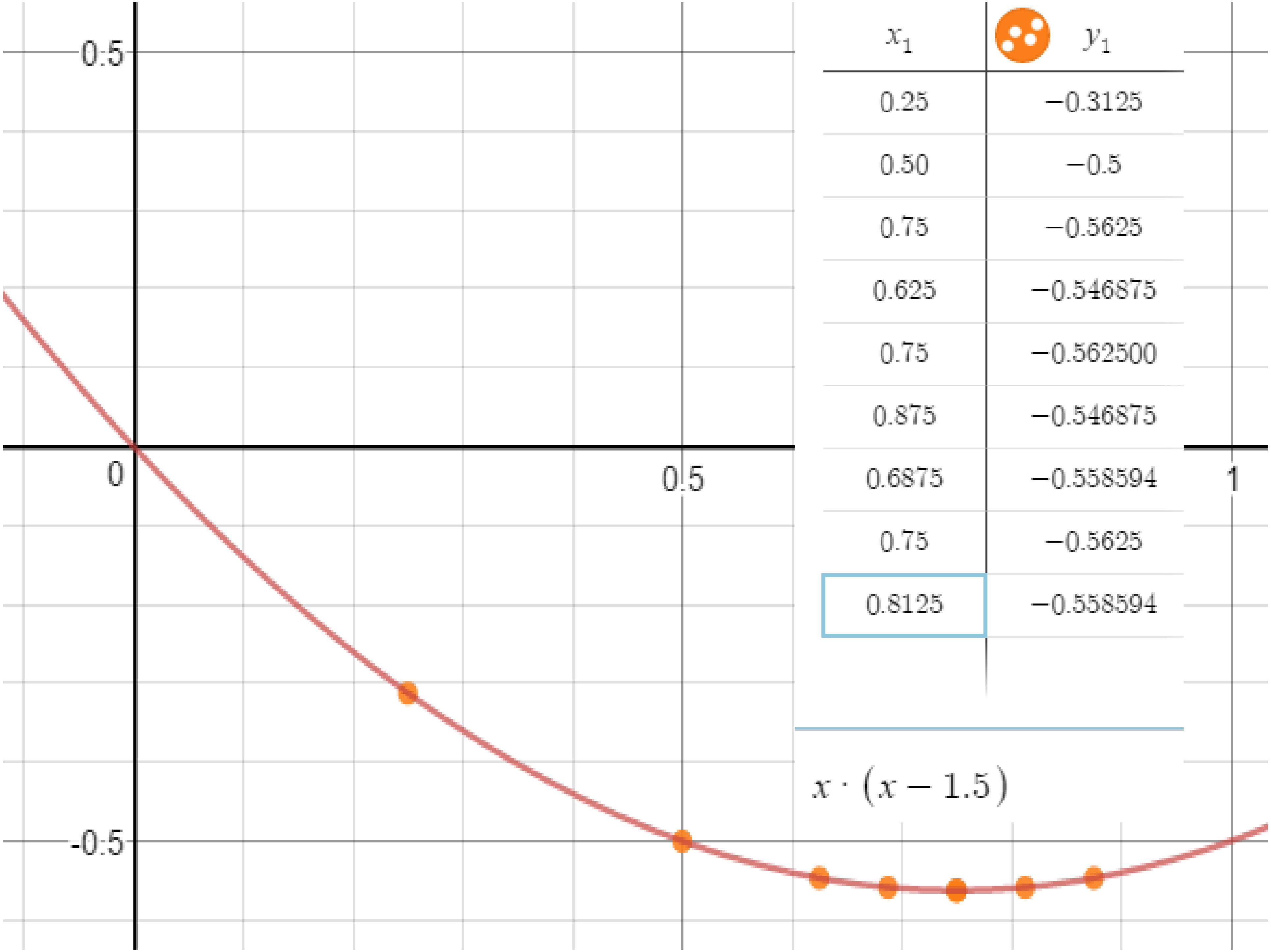
$$x_0 = 0.75, \qquad f_0 = 0.75(-0.75) = -0.5625$$

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

Again we note that $f_1 > f_0$ and $f_2 > f_0$ and hence we delete both the intervals (a, x_1) and (x_2, b) to obtain the new interval of uncertainty as $L_7 = (0.6875, 0.8125)$. By taking the middle point of this interval (L_7) as optimum, we obtain

$$x_{\text{opt}} \approx 0.75 \quad \text{and} \quad f_{\text{opt}} \approx -0.5625$$

(This solution happens to be the exact solution in this case.)



x_1	y_1
0.25	−0.3125
0.50	−0.5
0.75	−0.5625
0.625	−0.546875
0.75	−0.562500
0.875	−0.546875
0.6875	−0.558594
0.75	−0.5625
0.8125	−0.558594

Μέθοδος Fibonacci

As stated earlier, the *Fibonacci method* can be used to find the minimum of a function of one variable even if the function is not continuous. This method, like many other elimination methods, has the following limitations:

1. The initial interval of uncertainty, in which the optimum lies, has to be known.
2. The function being optimized has to be unimodal in the initial interval of uncertainty.
3. The exact optimum cannot be located in this method. Only an interval known as the *final interval of uncertainty* will be known. The final interval of uncertainty can be made as small as desired by using more computations.
4. The number of function evaluations to be used in the search or the resolution required has to be specified beforehand.

This method makes use of the sequence of Fibonacci numbers, $\{F_n\}$, for placing the experiments. These numbers are defined as

$$F_0 = F_1 = 1$$

$$F_n = F_{n-1} + F_{n-2}, \qquad n = 2, 3, 4, \ldots$$

which yield the sequence 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ...

Procedure. Let L_0 be the initial interval of uncertainty defined by $a \le x \le b$ and n be the total number of experiments to be conducted. Define

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 \tag{5.5}$$

and place the first two experiments at points x_1 and x_2, which are located at a distance of L_2^* from each end of L_0.[†] This gives[‡]

$$\begin{aligned} x_1 &= a + L_2^* = a + \frac{F_{n-2}}{F_n} L_0 \\ x_2 &= b - L_2^* = b - \frac{F_{n-2}}{F_n} L_0 = a + \frac{F_{n-1}}{F_n} L_0 \end{aligned} \tag{5.6}$$

Discard part of the interval by using the unimodality assumption. Then there remains a smaller interval of uncertainty L_2 given by[§]

$$L_2 = L_0 - L_2^* = L_0 \left(1 - \frac{F_{n-2}}{F_n}\right) = \frac{F_{n-1}}{F_n} L_0 \tag{5.7}$$

and with one experiment left in it. This experiment will be at a distance of

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 = \frac{F_{n-2}}{F_{n-1}} L_2 \tag{5.8}$$

from one end and

$$L_2 - L_2^* = \frac{F_{n-3}}{F_n} L_0 = \frac{F_{n-3}}{F_{n-1}} L_2 \tag{5.9}$$

from the other end. Now place the third experiment in the interval L_2 so that the current two experiments are located at a distance of

$$L_3^* = \frac{F_{n-3}}{F_n} L_0 = \frac{F_{n-3}}{F_{n-1}} L_2 \tag{5.10}$$

from each end of the interval L_2. Again the unimodality property will allow us to reduce the interval of uncertainty to L_3 given by

$$L_3 = L_2 - L_3^* = L_2 - \frac{F_{n-3}}{F_{n-1}} L_2 = \frac{F_{n-2}}{F_{n-1}} L_2 = \frac{F_{n-2}}{F_n} L_0 \tag{5.11}$$

This process of discarding a certain interval and placing a new experiment in the remaining interval can be continued, so that the location of the jth experiment and the interval of uncertainty at the end of j experiments are, respectively, given by

$$L_j^* = \frac{F_{n-j}}{F_{n-(j-2)}} L_{j-1} \tag{5.12}$$

$$L_j = \frac{F_{n-(j-1)}}{F_n} L_0 \tag{5.13}$$

The ratio of the interval of uncertainty remaining after conducting j of the n predetermined experiments to the initial interval of uncertainty becomes

$$\frac{L_j}{L_0} = \frac{F_{n-(j-1)}}{F_n} \tag{5.14}$$

and for $j = n$, we obtain

$$\frac{L_n}{L_0} = \frac{F_1}{F_n} = \frac{1}{F_n} \tag{5.15}$$

The ratio L_n/L_0 will permit us to determine n, the required number of experiments, to achieve any desired accuracy in locating the optimum point. Table 5.2 gives the reduction ratio in the interval of uncertainty obtainable for different number of experiments.

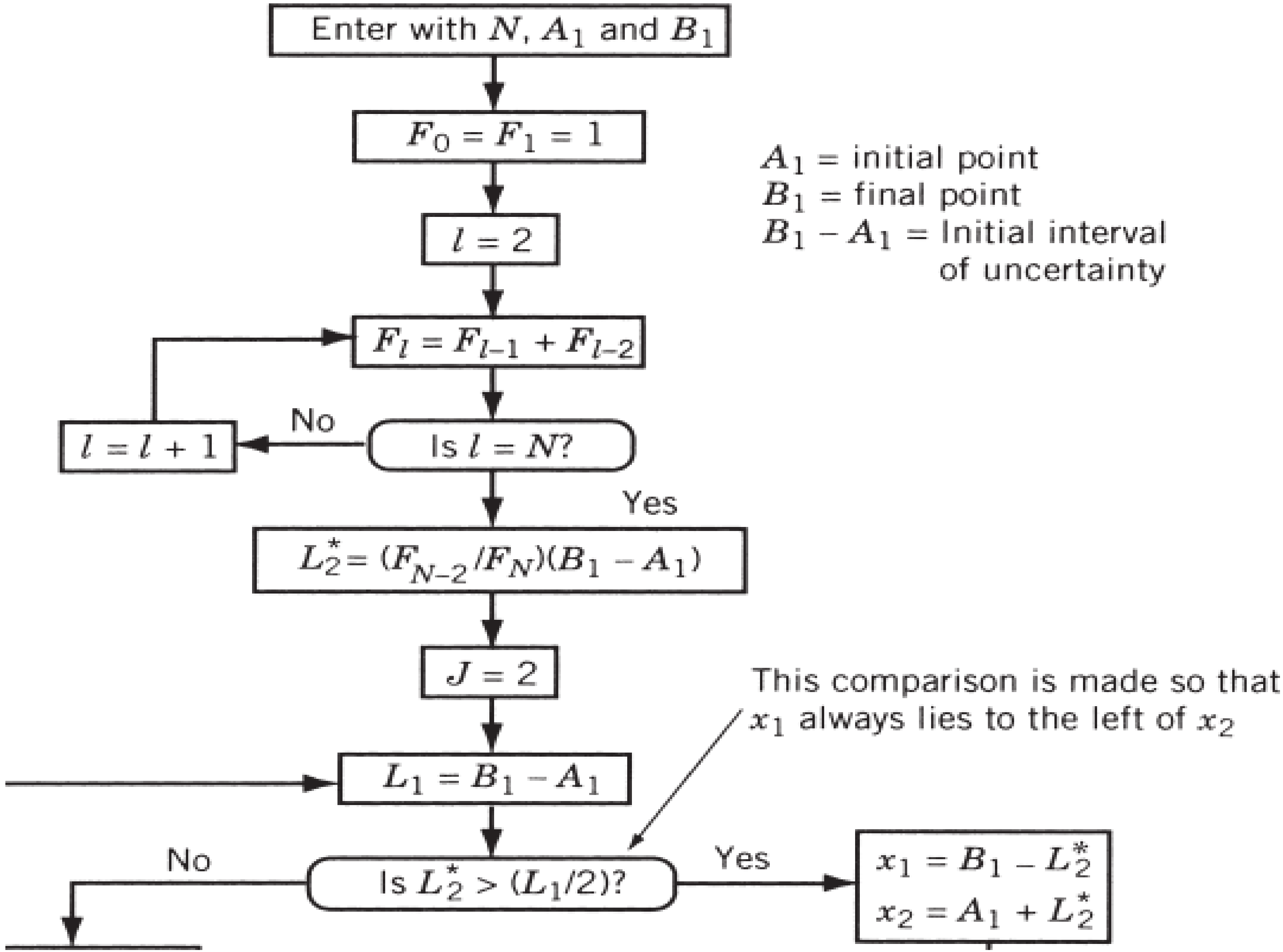
Table 5.2 Reduction Ratios

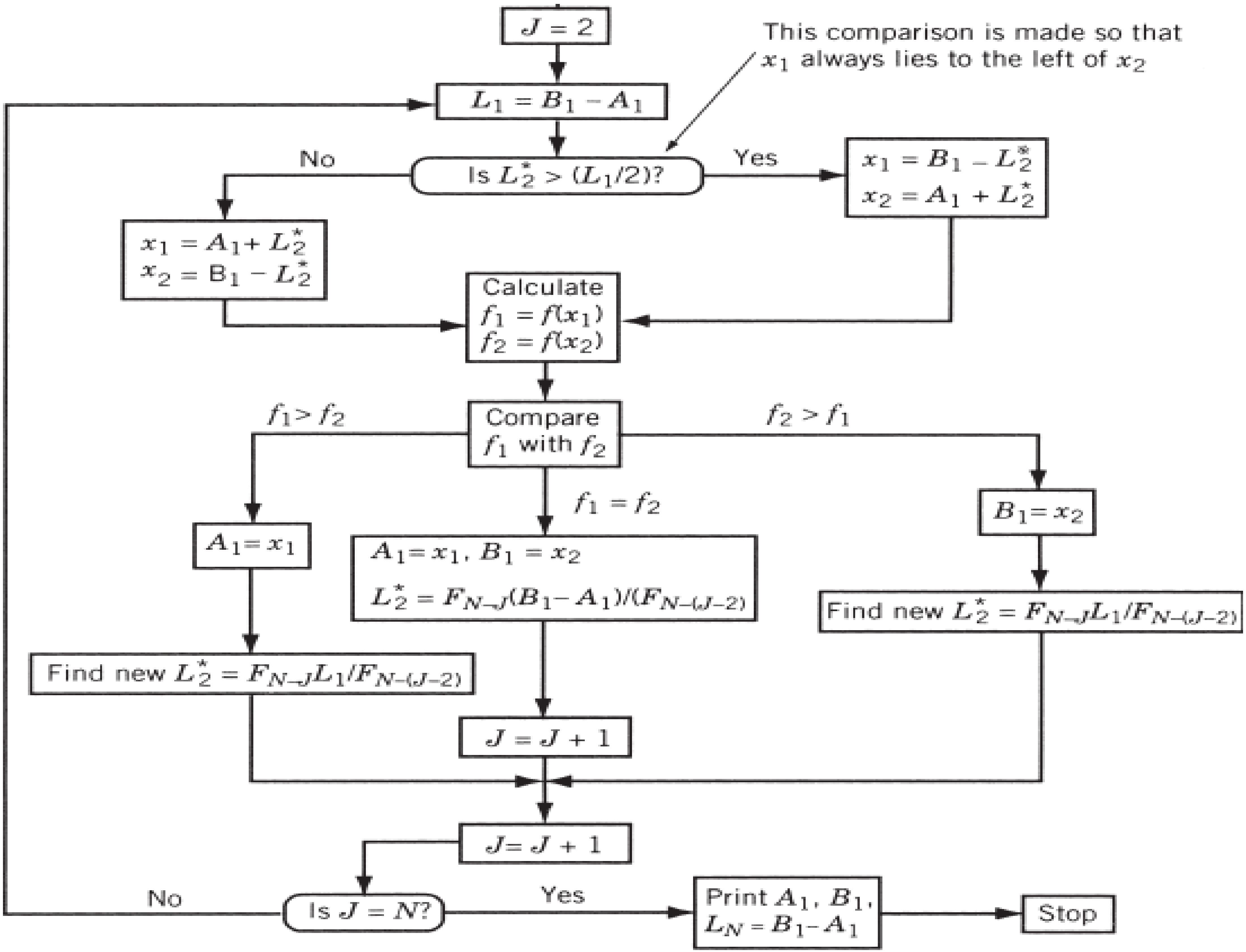
Value of n	Fibonacci number, F_n	Reduction ratio, L_n/L_0
0	1	1.0
1	1	1.0
2	2	0.5
3	3	0.3333
4	5	0.2
5	8	0.1250
6	13	0.07692
7	21	0.04762
8	34	0.02941
9	55	0.01818
10	89	0.01124
11	144	0.006944
12	233	0.004292
13	377	0.002653
14	610	0.001639
15	987	0.001013
16	1,597	0.0006406
17	2,584	0.0003870
18	4,181	0.0002392
19	6,765	0.0001479
20	10,946	0.00009135

Position of the Final Experiment. In this method the last experiment has to be placed with some care. Equation (5.12) gives

$$\frac{L_n^*}{L_{n-1}} = \frac{F_0}{F_2} = \frac{1}{2} \quad \text{for} \quad \text{all } n \tag{5.16}$$

Thus after conducting $n - 1$ experiments and discarding the appropriate interval in each step, the remaining interval will contain one experiment precisely at its middle point. However, the final experiment, namely, the nth experiment, is also to be placed at the center of the present interval of uncertainty. That is, the position of the nth experiment will be same as that of $(n - 1)$th one, and this is true for whatever value we choose for n. Since no new information can be gained by placing the nth experiment exactly at the same location as that of the $(n - 1)$th experiment, we place the nth experiment very close to the remaining valid experiment, as in the case of the dichotomous search method. This enables us to obtain the final interval of uncertainty to within $\frac{1}{2}L_{n-1}$. A flowchart for implementing the Fibonacci method of minimization is given in Fig. 5.9.


Enter with N, A_1 and B_1
$F_0 = F_1 = 1$
A_1 = initial point
B_1 = final point
$B_1 - A_1$ = Initial interval of uncertainty
$l = 2$
$F_l = F_{l-1} + F_{l-2}$
No
$l = l + 1$
Is $l = N$?
Yes
$L_2^* = (F_{N-2}/F_N)(B_1 - A_1)$
$J = 2$
This comparison is made so that x_1 always lies to the left of x_2
$L_1 = B_1 - A_1$
No
Is $L_2^* > (L_1/2)$?
Yes
$x_1 = B_1 - L_2^*$
$x_2 = A_1 + L_2^*$



J = 2
This comparison is made so that
x1 always lies to the left of x2
L1 = B1 − A1
No
Is L*2 > (L1/2)?
Yes
x1 = B1 − L*2
x2 = A1 + L*2
x1 = A1 + L*2
x2 = B1 − L*2
Calculate
f1 = f(x1)
f2 = f(x2)
f1 > f2
Compare
f1 with f2
f2 > f1
f1 = f2
B1 = x2
A1 = x1
A1 = x1, B1 = x2
L*2 = FN−J(B1 − A1)/(FN−(J−2)
Find new L*2 = FN−JL1/FN−(J−2)
Find new L*2 = FN−JL1/FN−(J−2)
J = J + 1
J = J + 1
No
Is J = N?
Yes
Print A1, B1,
LN = B1 − A1
Stop

Example 5.7 Minimize $f(x) = 0.65 - [0.75/(1 + x^2)] - 0.65x \tan^{-1}(1/x)$ in the interval [0,3] by the Fibonacci method using $n = 6$. (Note that this objective is equivalent to the one stated in Example 5.2.)

SOLUTION Here $n = 6$ and $L_0 = 3.0$, which yield

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 = \frac{5}{13}(3.0) = 1.153846$$

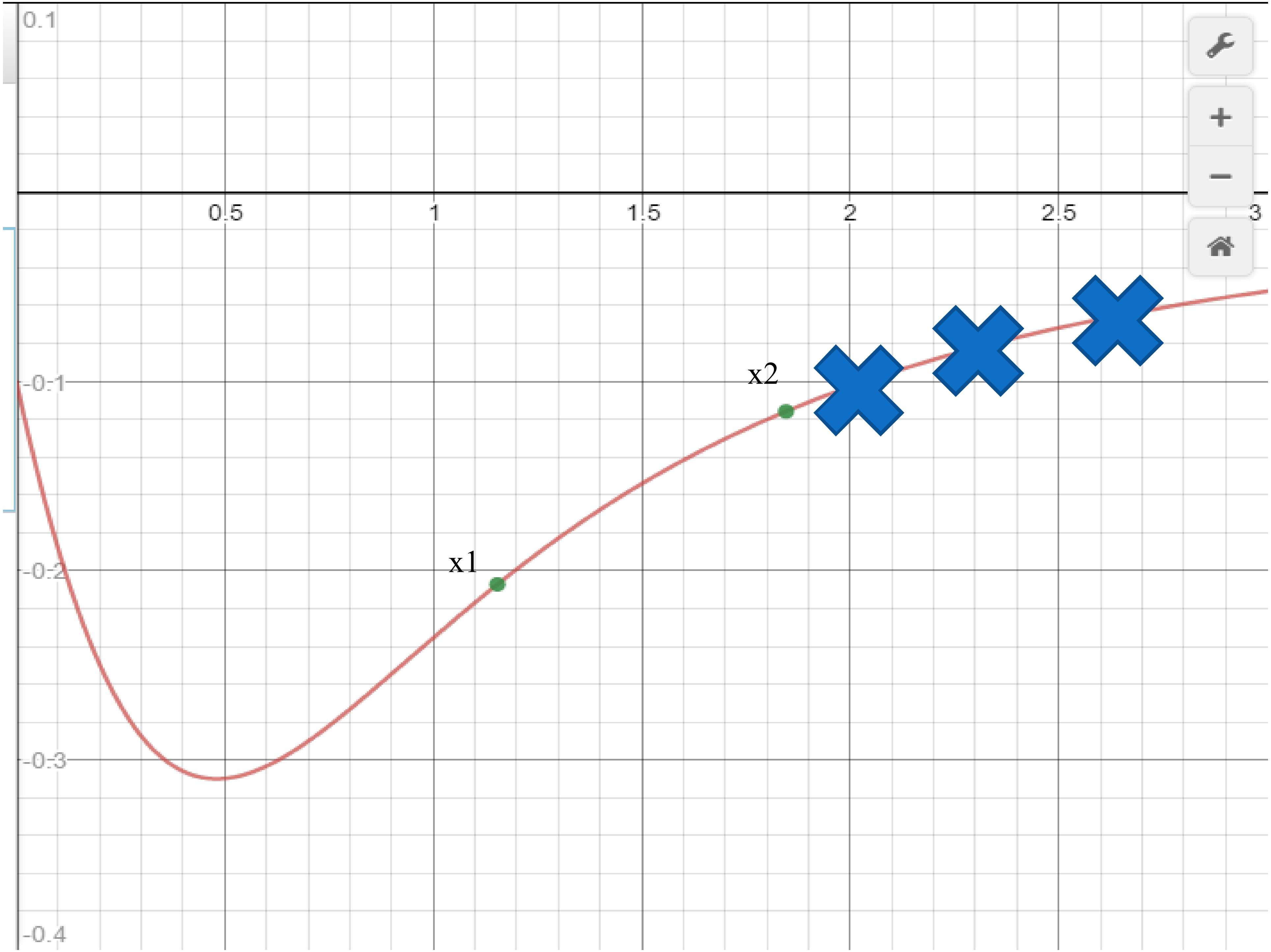
Thus the positions of the first two experiments are given by $x_1 = 1.153846$ and $x_2 = 3.0 - 1.153846 = 1.846154$ with $f_1 = f(x_1) = -0.207270$ and $f_2 = f(x_2) = -0.115843$. Since f_1 is less than f_2, we can delete the interval $[x_2, 3.0]$ by using the unimodality assumption (Fig. 5.10*a*). The third experiment is placed at $x_3 = 0 + (x_2 - x_1) = 1.846154 - 1.153846 = 0.692308$, with the corresponding function value of $f_3 = -0.291364$.

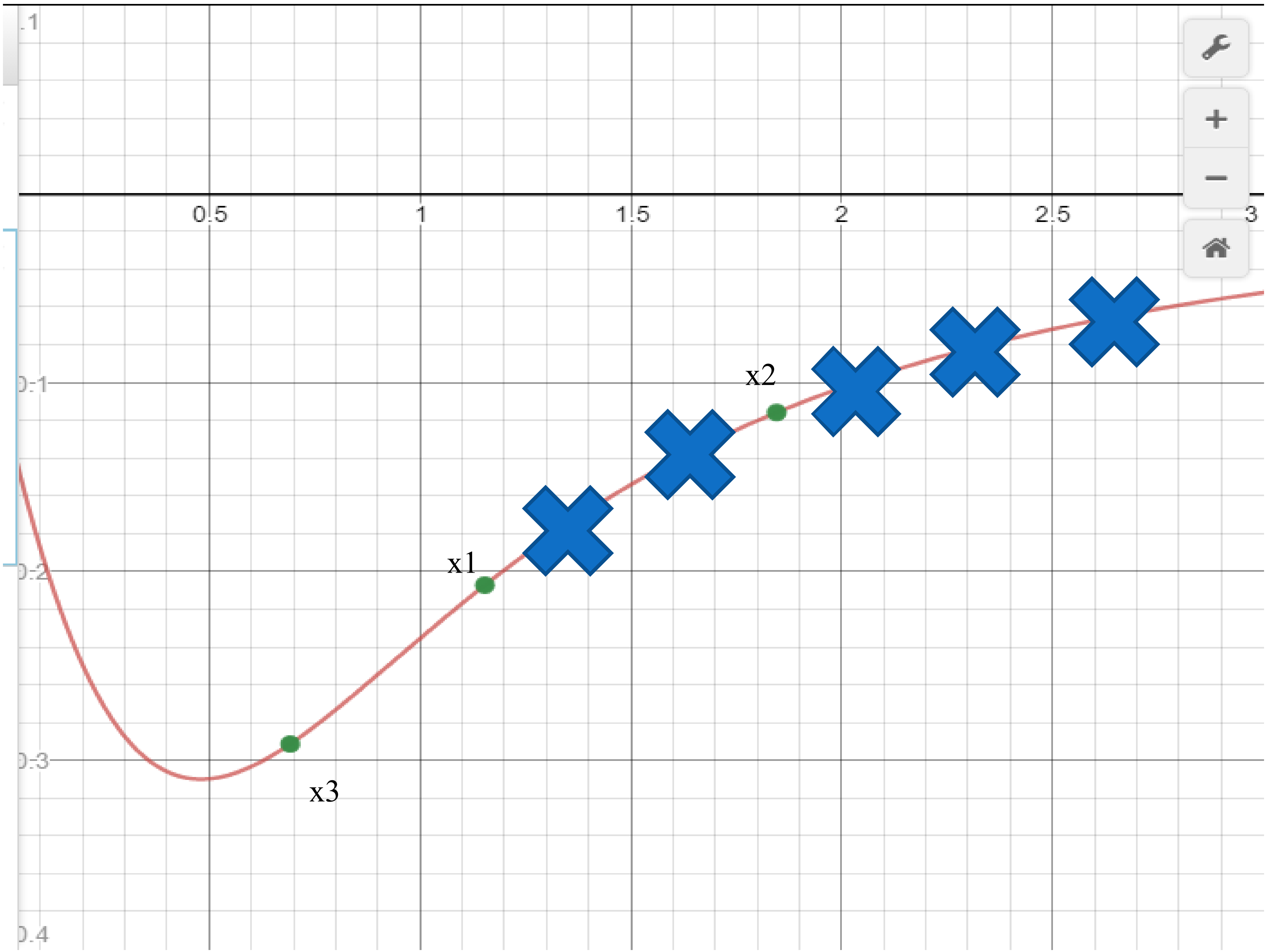
Since $f_1 > f_3$, we delete the interval $[x_1, x_2]$ (Fig. 5.10*b*). The next experiment is located at $x_4 = 0 + (x_1 - x_3) = 1.153846 - 0.692308 = 0.461538$ with $f_4 = -0.309811$. Nothing that $f_4 < f_3$, we delete the interval $[x_3, x_1]$ (Fig. 5.10*c*). The location of the next experiment can be obtained as $x_5 = 0 + (x_3 - x_4) = 0.692308 - 0.461538 = 0.230770$ with the corresponding objective function value of $f_5 = -0.263678$. Since $f_5 > f_4$, we delete the interval $[0, x_5]$ (Fig. 5.10*d*). The final experiment is positioned at $x_6 = x_5 + (x_3 - x_4) = 0.230770 + (0.692308 - 0.461538) = 0.461540$ with $f_6 = -0.309810$. (Note that, theoretically, the value of x_6 should be same as that of x_4; however, it is slightly different from x_4, due to round-off error).

Since $f_6 > f_4$, we delete the interval $[x_6, x_3]$ and obtain the final interval of uncertainty as $L_6 = [x_5, x_6] = [0.230770, 0.461540]$ (Fig. 5.10*e*). The ratio of the final to the initial interval of uncertainty is

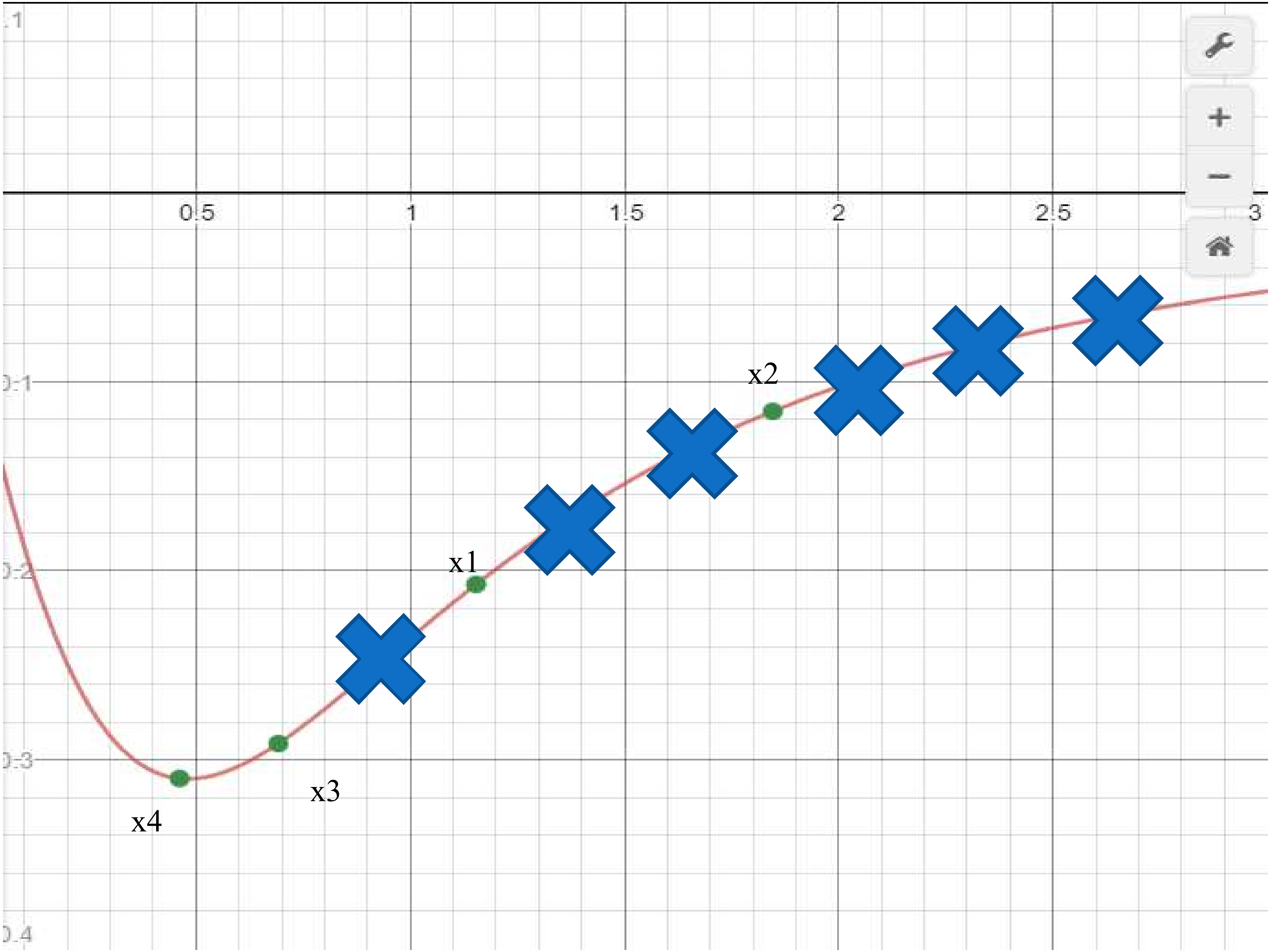
$$\frac{L_6}{L_0} = \frac{0.461540 - 0.230770}{3.0} = 0.076923$$

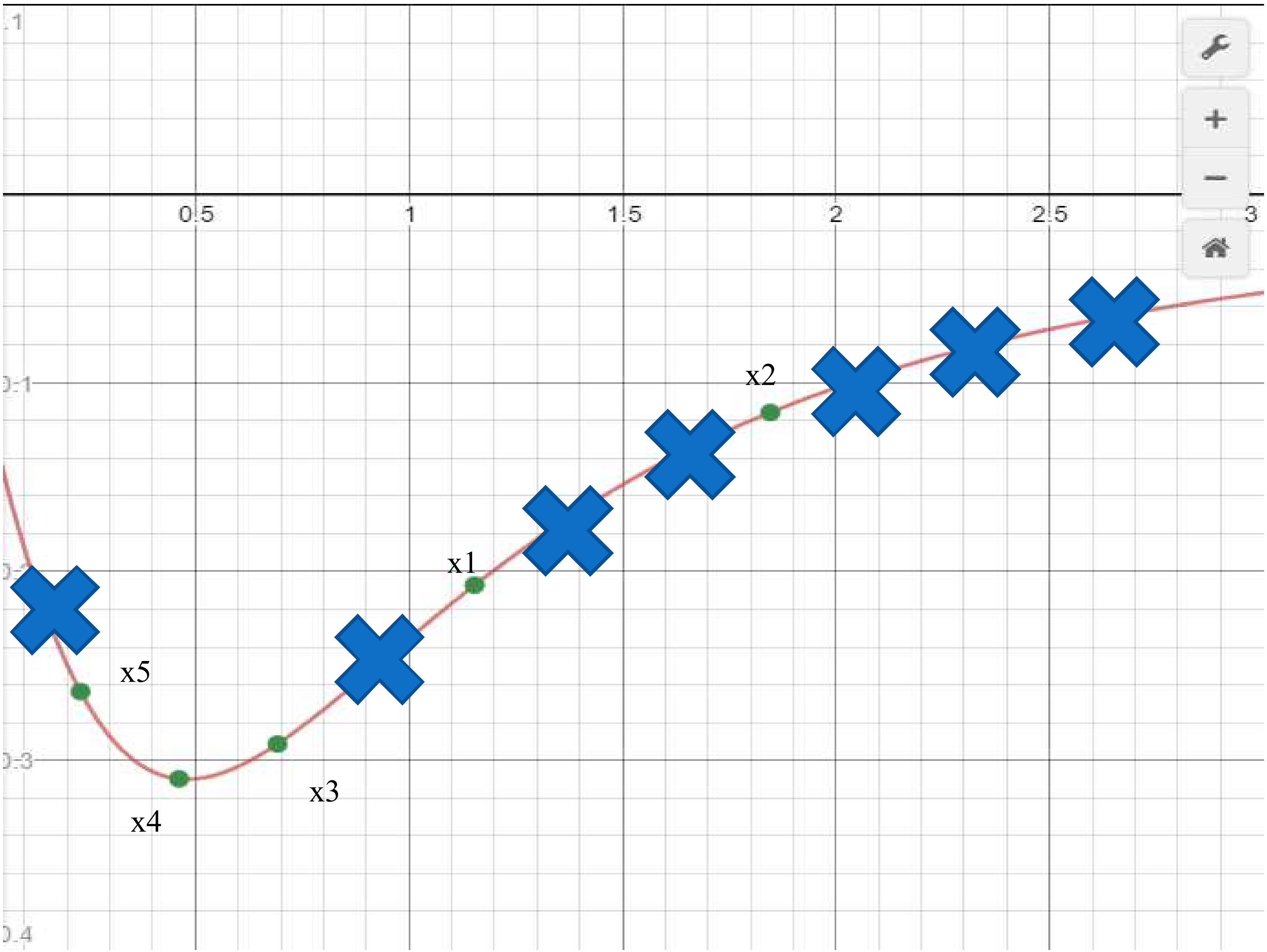
This value can be compared with Eq. (5.15), which states that if n experiments ($n = 6$) are planned, a resolution no finer than $1/F_n = 1/F_6 = \frac{1}{13} = 0.076923$ can be expected from the method.


0.1
0.5
1
1.5
2
2.5
3
-0.1
-0.2
-0.3
-0.4
x1
x2

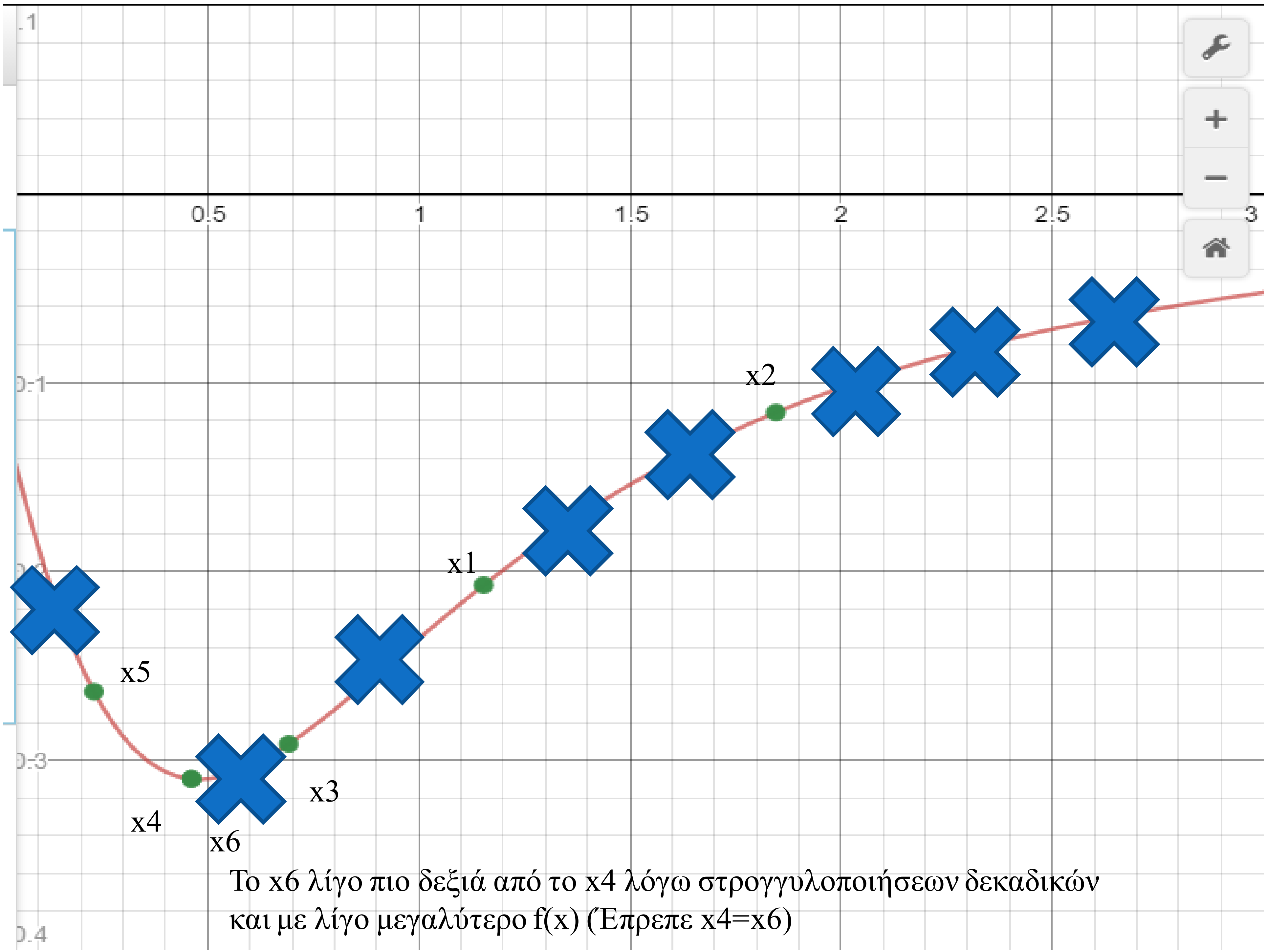


0.5
1
1.5
2
2.5
3
x1
x2
x3


0.5
1
1.5
2
2.5
3
x1
x2
x3
x4



0.5
1
1.5
2
2.5
3
x1
x2
x3
x4
x5



Το x6 λίγο πιο δεξιά από το x4 λόγω στρογγυλοποιήσεων δεκαδικών και με λίγο μεγαλύτερο f(x) (Έπρεπε x4=x6)

Μέθοδος της χρυσής τομής

The *golden section method* is same as the Fibonacci method except that in the Fibonacci method the total number of experiments to be conducted has to be specified before beginning the calculation, whereas this is not required in the golden section method. In the Fibonacci method, the location of the first two experiments is determined by the total number of experiments, N. In the golden section method we start with the assumption that we are going to conduct a large number of experiments. Of course, the total number of experiments can be decided during the computation.

The intervals of uncertainty remaining at the end of different number of experiments can be computed as follows:

$$L_2 = \lim_{N\to\infty} \frac{F_{N-1}}{F_N} L_0 \tag{5.17}$$

$$L_3 = \lim_{N\to\infty} \frac{F_{N-2}}{F_N} L_0 = \lim_{N\to\infty} \frac{F_{N-2}}{F_{N-1}} \frac{F_{N-1}}{F_N} L_0$$

$$\simeq \lim_{N\to\infty} \left(\frac{F_{N-1}}{F_N}\right)^2 L_0 \tag{5.18}$$

This result can be generalized to obtain

$$L_k = \lim_{N \to \infty} \left(\frac{F_{N-1}}{F_N} \right)^{k-1} L_0 \tag{5.19}$$

Using the relation

$$F_N = F_{N-1} + F_{N-2} \tag{5.20}$$

we obtain, after dividing both sides by F_{N-1},

$$\frac{F_N}{F_{N-1}} = 1 + \frac{F_{N-2}}{F_{N-1}} \tag{5.21}$$

By defining a ratio γ as

$$\gamma = \lim_{N \to \infty} \frac{F_N}{F_{N-1}} \tag{5.22}$$

Eq. (5.21) can be expressed as

$$\gamma \simeq \frac{1}{\gamma} + 1$$

that is,

$$\gamma^2 - \gamma - 1 = 0 \tag{5.23}$$

This gives the root $\gamma = 1.618$, and hence Eq. (5.19) yields

$$L_k = \left(\frac{1}{\gamma}\right)^{k-1} L_0 = (0.618)^{k-1} L_0 \tag{5.24}$$

In Eq. (5.18) the ratios F_{N-2}/F_{N-1} and F_{N-1}/F_N have been taken to be same for large values of N. The validity of this assumption can be seen from the following table:

Value of N	2	3	4	5	6	7	8	9	10	∞
Ratio $\frac{F_{N-1}}{F_N}$	0.5	0.667	0.6	0.625	0.6156	0.619	0.6177	0.6181	0.6184	0.618

The ratio γ has a historical background. Ancient Greek architects believed that a building having the sides d and b satisfying the relation

$$\frac{d+b}{d} = \frac{d}{b} = \gamma \tag{5.25}$$

would have the most pleasing properties (Fig. 5.11). The origin of the name, *golden section method*, can also be traced to the Euclid's geometry. In Euclid's geometry, when a line segment is divided into two unequal parts so that the ratio of the whole to the larger part is equal to the ratio of the larger to the smaller, the division is called the golden section and the ratio is called the golden mean.

Procedure. The procedure is same as the Fibonacci method except that the location of the first two experiments is defined by

$$L_2^* = \frac{F_{N-2}}{F_N} L_0 = \frac{F_{N-2}}{F_{N-1}} \frac{F_{N-1}}{F_N} L_0 = \frac{L_0}{\gamma^2} = 0.382 L_0 \tag{5.26}$$

The desired accuracy can be specified to stop the procedure.

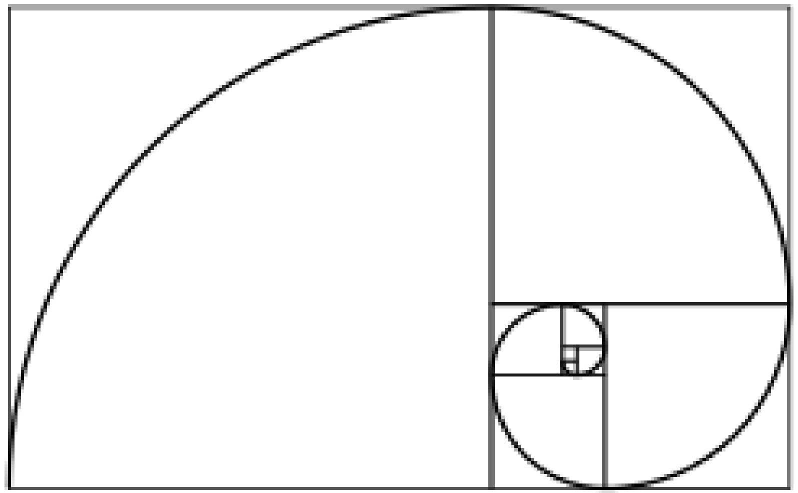
Στα Μαθηματικά και την τέχνη, δύο ποσότητες έχουν αναλογία χρυσής τομής αν ο λόγος του αθροίσματος τους προς τη μεγαλύτερη ποσότητα είναι ίσος με το λόγο της μεγαλύτερης ποσότητας προς τη μικρότερη. Η εικόνα στα δεξιά αναπαριστά τη γεωμετρική ερμηνεία των παραπάνω. Εκφρασμένο αλγεβρικά:

$$\frac{a+b}{a} = \frac{a}{b} \stackrel{\text{def}}{=} \varphi,$$

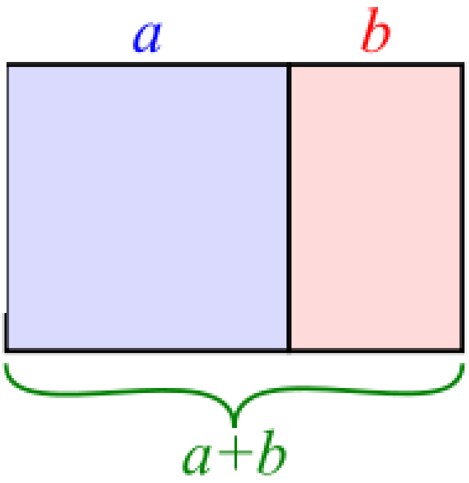
όπου το γράμμα φ αντιπροσωπεύει την χρυσή τομή. Η τιμή του είναι:

$$\varphi = \frac{1+\sqrt{5}}{2} = 1.61803\,39887\ldots.$$

Η χρυσή τομή αναφέρεται επίσης και ως **χρυσός λόγος** ή **χρυσός κανόνας**. Άλλα ονόματα είναι **χρυσή μετριότητα** και **Θεϊκή αναλογία** ενώ στον Ευκλείδη ο όρος ήταν **"άκρος και μέσος λόγος"**.



Μια σπείρα Fibonacci η οποία προσεγγίζει τη χρυσή σπείρα, χρησιμοποιώντας μεγέθη της ακολουθίας Fibonacci έως το 34.



Ένα ορθογώνιο παραλληλόγραμμο με αναλογίες χρυσής τομής, με μεγαλύτερη την πλευρά **a** και μικρότερη την πλευρά **b**, όταν τοποθετείται δίπλα σε ένα τετράγωνο με πλευρές μήκους **a**, θα παραχθεί ένα όμοιο ορθογώνιο παραλληλόγραμμο με αναλογίες χρυσής τομής με μεγαλύτερη πλευρά την **a + b** και μικρότερη την **a**. Αυτό αναπαριστά η σχέση

$$\frac{a+b}{a} = \frac{a}{b} \equiv \varphi.$$

Example 5.8 Minimize the function

$$f(x) = 0.65 - [0.75/(1 + x^2)] - 0.65x \tan^{-1}(1/x)$$

using the golden section method with $n = 6$.

SOLUTION The locations of the first two experiments are defined by $L_2^* = 0.382L_0 = (0.382)(3.0) = 1.1460$. Thus $x_1 = 1.1460$ and $x_2 = 3.0 - 1.1460 = 1.8540$ with $f_1 = f(x_1) = -0.208654$ and $f_2 = f(x_2) = -0.115124$. Since $f_1 < f_2$, we delete the interval $[x_2, 3.0]$ based on the assumption of unimodality and obtain the new interval of uncertainty as $L_2 = [0, x_2] = [0.0, 1.8540]$. The third experiment is placed at $x_3 = 0 + (x_2 - x_1) = 1.8540 - 1.1460 = 0.7080$. Since $f_3 = -0.288943$ is smaller than $f_1 = -0.208654$, we delete the interval $[x_1, x_2]$ and obtain the new interval of uncertainty as $[0.0, x_1] = [0.0, 1.1460]$. The position of the next experiment is given by $x_4 = 0 + (x_1 - x_3) = 1.1460 - 0.7080 = 0.4380$ with $f_4 = -0.308951$.

Since $f_4 < f_3$, we delete $[x_3, x_1]$ and obtain the new interval of uncertainty as $[0, x_3] = [0.0, 0.7080]$. The next experiment is placed at $x_5 = 0 + (x_3 - x_4) = 0.7080 - 0.4380 = 0.2700$. Since $f_5 = -0.278434$ is larger than $f_4 = -0.308951$, we delete the interval $[0, x_5]$ and obtain the new interval of uncertainty as $[x_5, x_3] = [0.2700, 0.7080]$. The final experiment is placed at $x_6 = x_5 + (x_3 - x_4) = 0.2700 + (0.7080 - 0.4380) = 0.5400$ with $f_6 = -0.308234$. Since $f_6 > f_4$, we delete the interval $[x_6, x_3]$ and obtain the final interval of uncertainty as $[x_5, x_6] = [0.2700, 0.5400]$. Note that this final interval of uncertainty is slightly larger than the one found in the Fibonacci method, [0.461540, 0.230770]. The ratio of the final to the initial interval of uncertainty in the present case is

$$\frac{L_6}{L_0} = \frac{0.5400 - 0.2700}{3.0} = \frac{0.27}{3.0} = 0.09$$

Σύγκριση μεθόδων απαλοιφής

The efficiency of an elimination method can be measured in terms of the ratio of the final and the initial intervals of uncertainty, L_n/L_0. The values of this ratio achieved in various methods for a specified number of experiments ($n = 5$ and $n = 10$) are compared in Table 5.3. It can be seen that the Fibonacci method is the most efficient method, followed by the golden section method, in reducing the interval of uncertainty.

A similar observation can be made by considering the number of experiments (or function evaluations) needed to achieve a specified accuracy in various methods. The results are compared in Table 5.4 for maximum permissible errors of 0.1 and 0.01. It can be seen that to achieve any specified accuracy, the Fibonacci method requires the least number of experiments, followed by the golden section method.

Τελικό εύρος ανάλογα με το πλήθος υπολογισμών της αντικειμενικής συνάρτησης

Table 5.3 Final Intervals of Uncertainty

Method	Formula	$n = 5$	$n = 10$
Exhaustive search	$L_n = \frac{2}{n+1} L_0$	$0.33333 L_0$	$0.18182 L_0$
Dichotomous search ($\delta = 0.01$ and $n =$ even)	$L_n = \frac{L_0}{2^{n/2}} + \delta \left(1 - \frac{1}{2^{n/2}}\right)$	$\frac{1}{4} L_0 + 0.0075$ with $n = 4$, $\frac{1}{8} L_0 + 0.00875$ with $n = 6$	$0.03125 L_0 + 0.0096875$
Interval halving ($n \geq 3$ and odd)	$L_n = (\frac{1}{2})^{(n-1)/2} L_0$	$0.25 L_0$	$0.0625 L_0$ with $n = 9$, $0.03125 L_0$ with $n = 11$
Fibonacci	$L_n = \frac{1}{F_n} L_0$	$0.125 L_0$	$0.01124 L_0$
Golden section	$L_n = (0.618)^{n-1} L_0$	$0.1459 L_0$	$0.01315 L_0$

Πλήθος απαιτούμενων υπολογισμών της αντικειμενικής συνάρτησης για δεδομένη ακρίβεια αποτελέσματος

Table 5.4 Number of Experiments for a Specified Accuracy

Method	Error: $\frac{1}{2}\frac{L_n}{L_0} \leq 0.1$	Error: $\frac{1}{2}\frac{L_n}{L_0} \leq 0.01$
Exhaustive search	$n \geq 9$	$n \geq 99$
Dichotomous search ($\delta = 0.01$, $L_0 = 1$)	$n \geq 6$	$n \geq 14$
Interval halving ($n \geq 3$ and odd)	$n \geq 7$	$n \geq 13$
Fibonacci	$n \geq 4$	$n \geq 9$
Golden section	$n \geq 5$	$n \geq 10$

Μέθοδοι παρεμβολής

Μέθοδοι παρεμβολής

The interpolation methods were originally developed as one-dimensional searches within multivariable optimization techniques, and are generally more efficient than Fibonacci-type approaches. The aim of all the one-dimensional minimization methods is to find λ^*, the smallest nonnegative value of λ, for which the function

$$f(\lambda) = f(\mathbf{X} + \lambda \mathbf{S}) \tag{5.27}$$

attains a local minimum. Hence if the original function $f(\mathbf{X})$ is expressible as an explicit function of x_i ($i = 1, 2, \ldots, n$), we can readily write the expression for $f(\lambda) = f(\mathbf{X} + \lambda \mathbf{S})$ for any specified vector $\mathbf{S}$, set

$$\frac{df}{d\lambda}(\lambda) = 0 \tag{5.28}$$

and solve Eq. (5.28) to find λ^* in terms of $\mathbf{X}$ and $\mathbf{S}$. However, in many practical problems, the function $f(\lambda)$ cannot be expressed explicitly in terms of λ (as shown in Example 5.1). In such cases the interpolation methods can be used to find the value of λ^*.

Εύρεση του κατάλληλου λ_i^*

- Έστω f(**X**) η αντικειμενική συνάρτηση που απαιτεί ελαχιστοποίηση.
- Θέλουμε να βρούμε το λ_i^* , το οποίο ελαχιστοποιεί τον επόμενο υπολογισμό $f(\mathbf{X}_{i+1})=f(\mathbf{X}_i+\lambda_i\mathbf{S}_i)$
- Το υφιστάμενο σημείο $\mathbf{X}_i$ και η κατεύθυνση $\mathbf{S}_i$ είναι καθορισμένα με συγκεκριμένες τιμές.
- Επομένως το πρόβλημα απλοποιείται στη μορφή $f(\mathbf{X}_{i+1})=f(\lambda_i)$
- Αφού υπάρχει μόνο μία μεταβλητή (το λ_i) το πρόβλημα είναι *μονοδιάστατο*.

Example 5.9 Derive the one-dimensional minimization problem for the following case:

$$\text{Minimize } f(\mathbf{X}) = (x_1^2 - x_2)^2 + (1 - x_1)^2 \tag{E$_1$}$$

from the starting point $\mathbf{X}_1 = \begin{Bmatrix} -2 \\ -2 \end{Bmatrix}$ along the search direction $\mathbf{S} = \begin{Bmatrix} 1.00 \\ 0.25 \end{Bmatrix}$.

SOLUTION The new design point $\mathbf{X}$ can be expressed as

$$\mathbf{X} = \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \mathbf{X}_1 + \lambda \mathbf{S} = \begin{Bmatrix} -2 + \lambda \\ -2 + 0.25\lambda \end{Bmatrix}$$

By substituting $x_1 = -2 + \lambda$ and $x_2 = -2 + 0.25\lambda$ in Eq. (E$_1$), we obtain f as a function of λ as

$$f(\lambda) = f\begin{pmatrix} -2 + \lambda \\ -2 + 0.25\lambda \end{pmatrix} = [(-2 + \lambda)^2 - (-2 + 0.25\lambda)]^2$$

$$+ [1 - (-2 + \lambda)]^2 = \lambda^4 - 8.5\lambda^3 + 31.0625\lambda^2 - 57.0\lambda + 45.0$$

The value of λ at which $f(\lambda)$ attains a minimum gives λ^*.

In the following sections, we discuss three different interpolation methods with reference to one-dimensional minimization problems that arise during multivariable optimization problems.

Τετραγωνική μέθοδος παρεμβολής

- Αυτή η μέθοδος παρεμβολής χρησιμοποιεί μόνο τις τιμές της συνάρτησης. Επομένως είναι κατάλληλη για την ελαχιστοποίηση του μήκους βήματος λ^* για συναρτήσεις, στις οποίες οι παράγωγοι δεν είναι διαθέσιμοι ή είναι δύσκολο να υπολογιστούν.
- Η μέθοδος προσαρμόζει καμπύλη 2^{ου} βαθμού (τετραγωνική) σε 3 γνωστά σημεία της αντικειμενικής συνάρτησης. Η βέλτιστη θέση στην προσαρμοσμένη καμπύλη υπολογίζεται εύκολα αναλυτικά. Συγκρίνεται η τιμή της προσαρμοσμένης καμπύλης σε σχέση με την τιμή της αντικειμενικής συνάρτησης και αν απέχουν αρκετά η διαδικασία επαναλαμβάνεται μέχρι να συγκλίνουν επαρκώς.
- Η μέθοδος εφαρμόζεται σε 3 στάδια.

Στάδιο 1ο τετραγωνικής μεθόδου παρεμβολής

- Το διάνυσμα **S** (της κατεύθυνσης) κανονικοποιείται, ώστε βήμα μήκους λ=1 να είναι αποδεκτό.

Stage 1. In this stage,† the **S** vector is normalized as follows: Find $\Delta = \max_i |s_i|$, where s_i is the ith component of **S** and divide each component of **S** by Δ. Another method of normalization is to find $\Delta = (s_1^2 + s_2^2 + \cdots + s_n^2)^{1/2}$ and divide each component of **S** by Δ.

- Για μονοδιάστατα προβλήματα δεν απαιτείται.

Στάδιο 2ο τετραγωνικής μεθόδου παρεμβολής

- Επιλογή 3 σημείων για την προσαρμογή καμπύλης 2ου βαθμού της μορφής $h(\lambda) = a + b\lambda + c\lambda^2$
- Για την εφαρμογή απλής διαδικασίας επιλέγονται ως 3 σημεία για λ=0, λ=t και λ=2t, όπου t είναι η προεπιλογή του μήκους βήματος.
- προσαρμόζεται καμπύλη 2ου βαθμού (τετραγωνική) σ' αυτά τα σημεία και υπολογίζεται η βέλτιστη θέση της προσαρμοσμένης καμπύλης

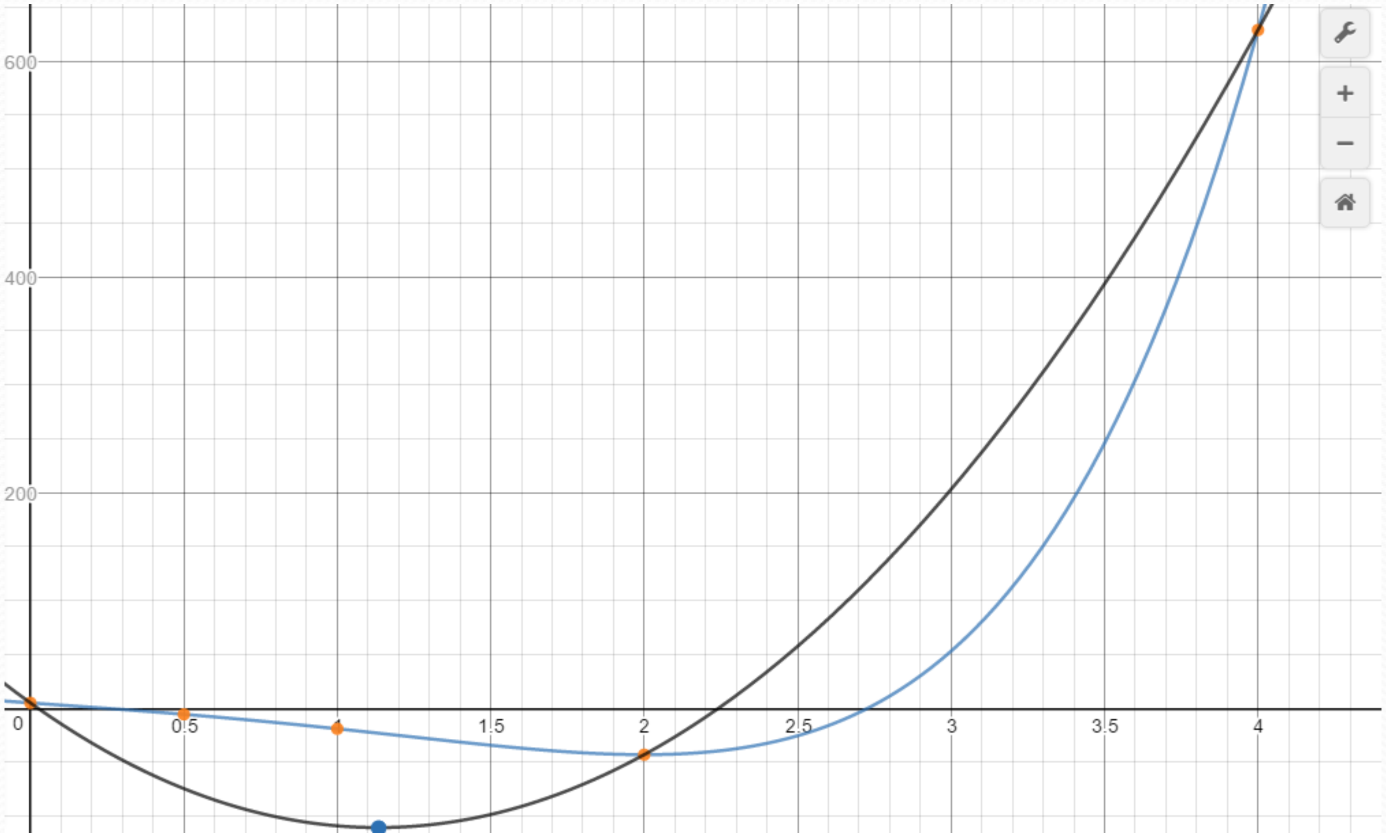
Στάδιο 3ο τετραγωνικής μεθόδου παρεμβολής

- Ελέγχεται η σύγκλιση.
- Συγκρίνεται η τιμή της προσαρμοσμένης καμπύλης σε σχέση με την τιμή της αντικειμενικής συνάρτησης.
- Αν απέχουν αρκετά η διαδικασία επαναλαμβάνεται μέχρι να συγκλίνουν επαρκώς.

- Υπάρχουν διάφοροι τρόποι εκτίμησης της σύγκλισης που θα αναφερθούν παρακάτω.

Υπολογισμός της καμπύλης προσαρμογής 2ου βαθμού

- Στο 2ο στάδιο υπολογίζεται η καμπύλη 2ου βαθμού που θα περνάει από τα 3 σημεία και θα προσεγγίζει την αντικειμενική συνάρτηση. Αυτό γίνεται σύμφωνα με τους τύπους που προκύπτουν από τη διαδικασία που περιγράφεται στη συνέχεια.



Stage 2. Let

$$h(\lambda) = a + b\lambda + c\lambda^2 \tag{5.29}$$

be the quadratic function used for approximating the function $f(\lambda)$. It is worth noting at this point that a quadratic is the lowest-order polynomial for which a finite minimum can exist. The necessary condition for the minimum of $h(\lambda)$ is that

$$\frac{dh}{d\lambda} = b + 2c\lambda = 0$$

that is,

$$\tilde{\lambda}^* = -\frac{b}{2c} \tag{5.30}$$

The sufficiency condition for the minimum of $h(\lambda)$ is that

$$\left.\frac{d^2h}{d\lambda^2}\right|_{\tilde{\lambda}^*} > 0$$

that is,

$$c > 0 \tag{5.31}$$

To evaluate the constants $a, b,$ and c in Eq. (5.29), we need to evaluate the function $f(\lambda)$ at three points. Let $\lambda = A, \lambda = B$, and $\lambda = C$ be the points at which the function $f(\lambda)$ is evaluated and let f_A, f_B, and f_C be the corresponding function values, that is,

$$f_A = a + bA + cA^2$$

$$f_B = a + bB + cB^2$$

$$f_C = a + bC + cC^2 \tag{5.32}$$

The solution of Eqs. (5.32) gives

$$a = \frac{f_A BC(C - B) + f_B CA(A - C) + f_C AB(B - A)}{(A - B)(B - C)(C - A)} \tag{5.33}$$

$$b = \frac{f_A(B^2 - C^2) + f_B(C^2 - A^2) + f_C(A^2 - B^2)}{(A - B)(B - C)(C - A)} \tag{5.34}$$

$$c = -\frac{f_A(B - C) + f_B(C - A) + f_C(A - B)}{(A - B)(B - C)(C - A)} \tag{5.35}$$

From Eqs. (5.30), (5.34), and (5.35), the minimum of $h(\lambda)$ can be obtained as

$$\tilde{\lambda}^* = \frac{-b}{2c} = \frac{f_A(B^2 - C^2) + f_B(C^2 - A^2) + f_C(A^2 - B^2)}{2[f_A(B - C) + f_B(C - A) + f_C(A - B)]} \tag{5.36}$$

provided that c, as given by Eq. (5.35), is positive.

To start with, for simplicity, the points A, B, and C can be chosen as 0, t, and $2t$, respectively, where t is a preselected trial step length. By this procedure, we can save one function evaluation since $f_A = f(\lambda = 0)$ is generally known from the previous iteration (of a multivariable search). For this case, Eqs. (5.33) to (5.36) reduce to

$$a = f_A \tag{5.37}$$

$$b = \frac{4f_B - 3f_A - f_C}{2t} \tag{5.38}$$

$$c = \frac{f_C + f_A - 2f_B}{2t^2} \tag{5.39}$$

$$\tilde{\lambda}^* = \frac{4f_B - 3f_A - f_C}{4f_B - 2f_C - 2f_A} t \tag{5.40}$$

Οι παραπάνω συντελεστές καθορίζουν την καμπύλη προσαρμογής:

$$h(\lambda) = a + b\lambda + c\lambda^2$$

provided that

$$c = \frac{f_C + f_A - 2f_B}{2t^2} > 0 \tag{5.41}$$

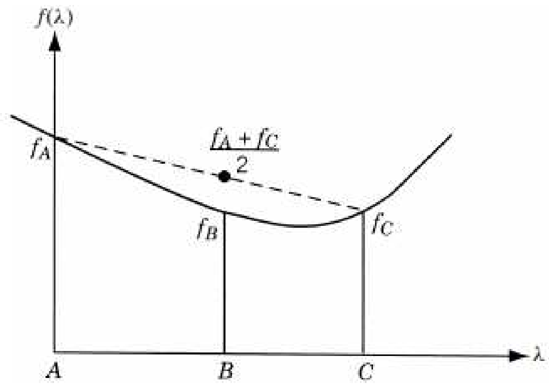


Figure 5.12 f_B smaller than $(f_A + f_C)/2$.

The inequality (5.41) can be satisfied if

$$\frac{f_A + f_C}{2} > f_B \tag{5.42}$$

(i.e., the function value f_B should be smaller than the average value of f_A and f_C). This can be satisfied if f_B lies below the line joining f_A and f_C as shown in Fig. 5.12.

The following procedure can be used not only to satisfy the inequality (5.42) but also to ensure that the minimum $\tilde{\lambda}^*$ lies in the interval $0 < \tilde{\lambda}^* < 2t$.

1. Assuming that $f_A = f(\lambda = 0)$ and the initial step size t_0 are known, evaluate the function f at $\lambda = t_0$ and obtain $f_1 = f(\lambda = t_0)$. The possible outcomes are shown in Fig. 5.13.
2. If $f_1 > f_A$ is realized (Fig. 5.13*c*), set $f_C = f_1$ and evaluate the function f at $\lambda = t_0/2$ and $\tilde{\lambda}^*$ using Eq. (5.40) with $t = t_0/2$.
3. If $f_1 \le f_A$ is realized (Fig. 5.13*a* or *b*), set $f_B = f_1$, and evaluate the function f at $\lambda = 2t_0$ to find $f_2 = f(\lambda = 2t_0)$. This may result in any one of the situations shown in Fig. 5.14.
4. If f_2 turns out to be greater than f_1 (Fig. 5.14*b* or *c*), set $f_C = f_2$ and compute $\tilde{\lambda}^*$ according to Eq. (5.40) with $t = t_0$.
5. If f_2 turns out to be smaller than f_1, set new $f_1 = f_2$ and $t_0 = 2t_0$, and repeat steps 2 to 4 until we are able to find $\tilde{\lambda}^*$.

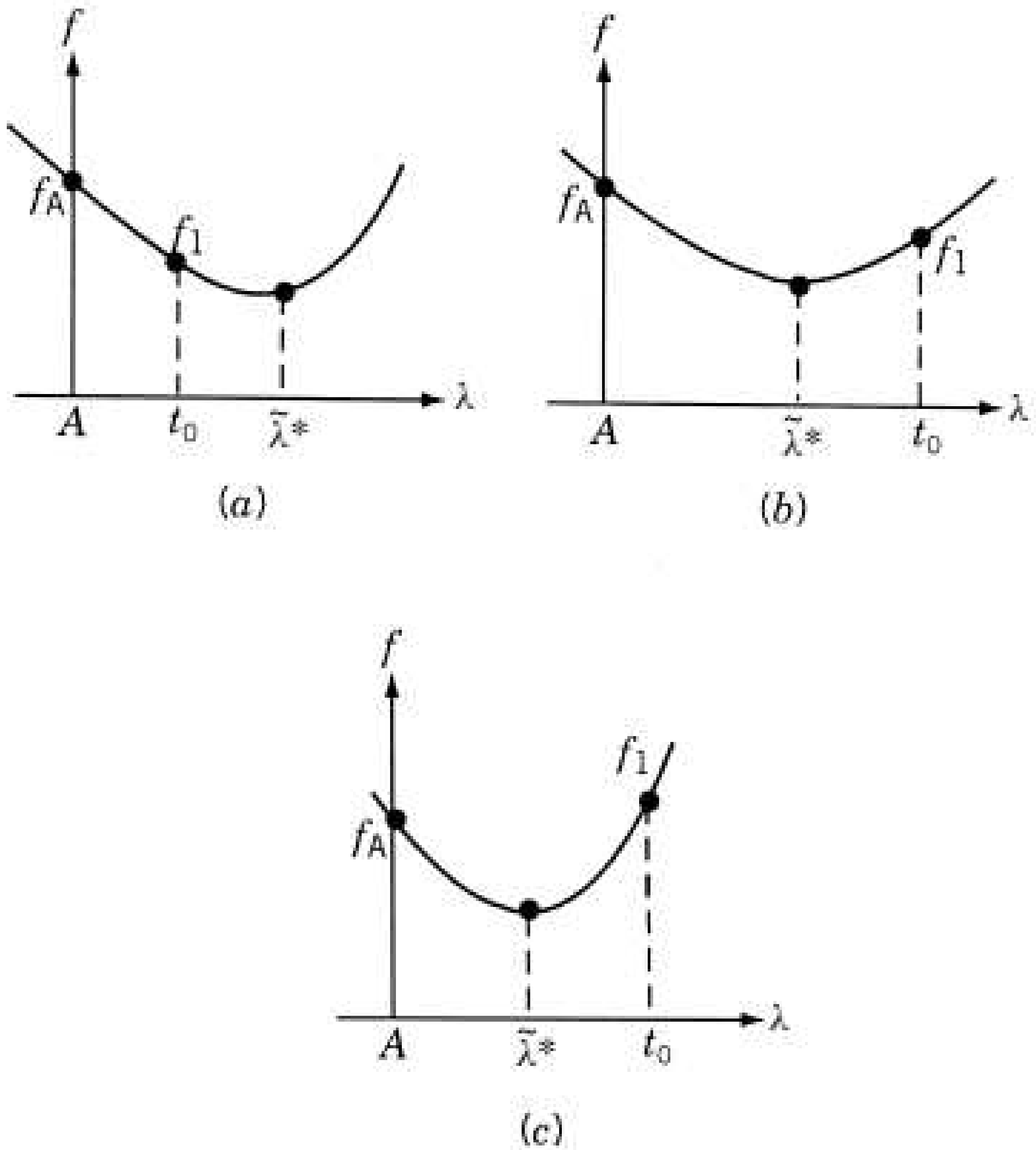


Figure 5.13 Possible outcomes when the function is evaluated at $\lambda = t_0$: (*a*) $f_1 < f_A$ and $t_0 < \tilde{\lambda}^*$; (*b*) $f_1 < f_A$ and $t_0 > \tilde{\lambda}^*$; (*c*) $f_1 > f_A$ and $t_0 > \tilde{\lambda}^*$.

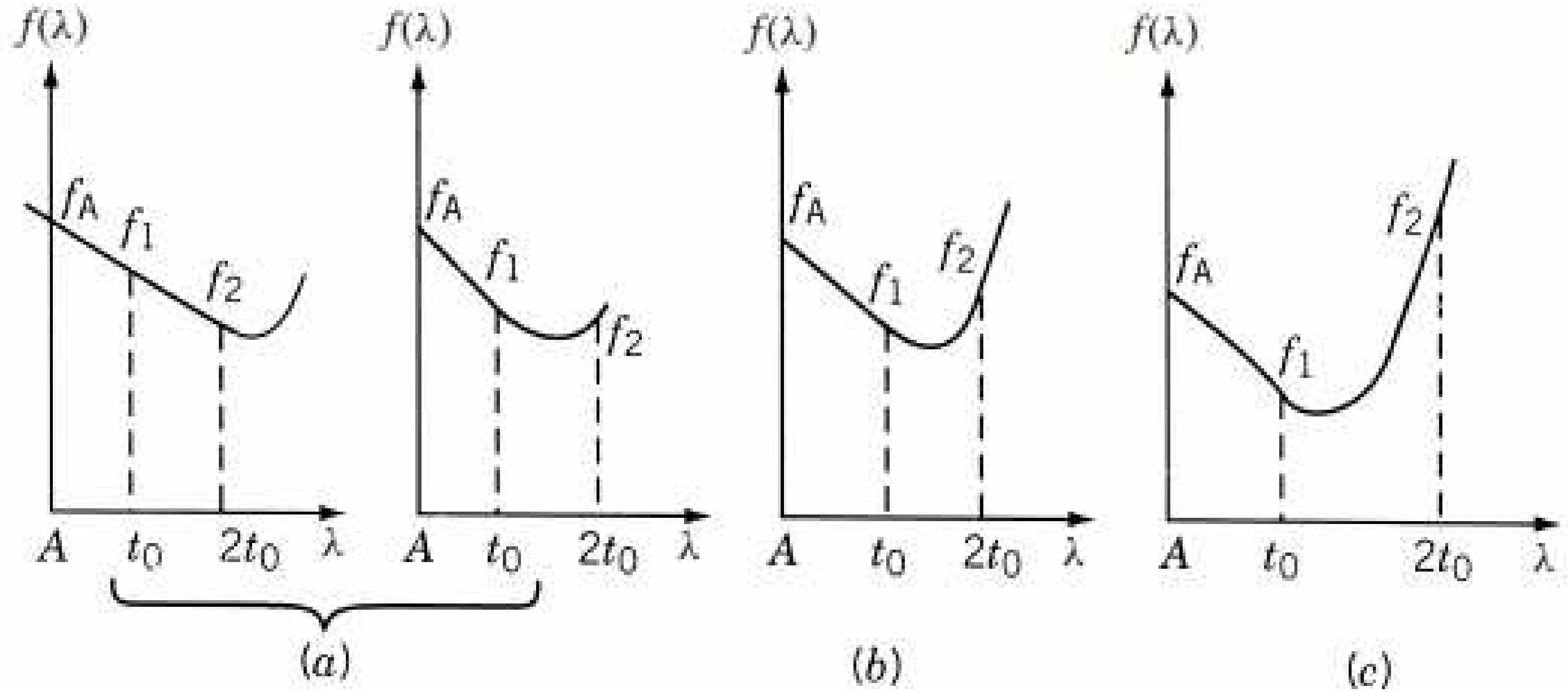


Figure 5.14 Possible outcomes when function is evaluated at $\lambda = t_0$ and $2t_0$: (a) $f_2 < f_1$ and $f_2 < f_A$; (b) $f_2 < f_A$ and $f_2 > f_1$; (c) $f_2 > f_A$ and $f_2 > f_1$.

Σύγκλιση βέλτιστου

- Στο 3ο στάδιο ελέγχεται η σύγκλιση.
- Μπορούν να γίνουν διάφορες δοκιμασίες π.χ.
- Έλεγχος του αποτελέσματος της προσαρμοσμένης καμπύλης σε σχέση με την τιμή της αντικειμενικής συνάρτησης στο ίδιο σημείο αν διαφέρουν λιγότερο από κάποιο κριτήριο ε_1:

$$\left| \frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)} \right| \leq \varepsilon_1$$

- Εναλλακτικά μπορεί να ελεγχθεί αν η παράγωγος της αντικειμενικής είναι κοντά στο μηδέν. Σ' αυτή τη μέθοδο δεν εκτιμώνται οι παράγωγοι, οπότε μπορεί να χρησιμοποιηθεί ένας τύπος πεπερασμένων διαφορών:

$$\left| \frac{f(\tilde{\lambda}^* + \Delta\tilde{\lambda}^*) - f(\tilde{\lambda}^* - \Delta\tilde{\lambda}^*)}{2\Delta\tilde{\lambda}^*} \right| \leq \varepsilon_2$$

Κατόπιν του ελέγχου σύγκλισης

- Αν το κριτήριο σύγκλισης επαρκεί τότε η επαναληπτική διαδικασία σταματάει.
- Αν δεν συγκλίνει το αποτέλεσμα τότε επιλέγονται τα καλύτερα 3 σημεία και προσαρμόζεται νέα καμπύλη 2^{ου} βαθμού σ’ αυτά.
- Για να επιλεχθούν τα 3 καλύτερα σημεία παρουσιάζονται παρακάτω οι 4 δυνατές περιπτώσεις.
- Έπειτα συνοψίζονται οι κανόνες επιλογής των 3 σημείων σε πίνακα.

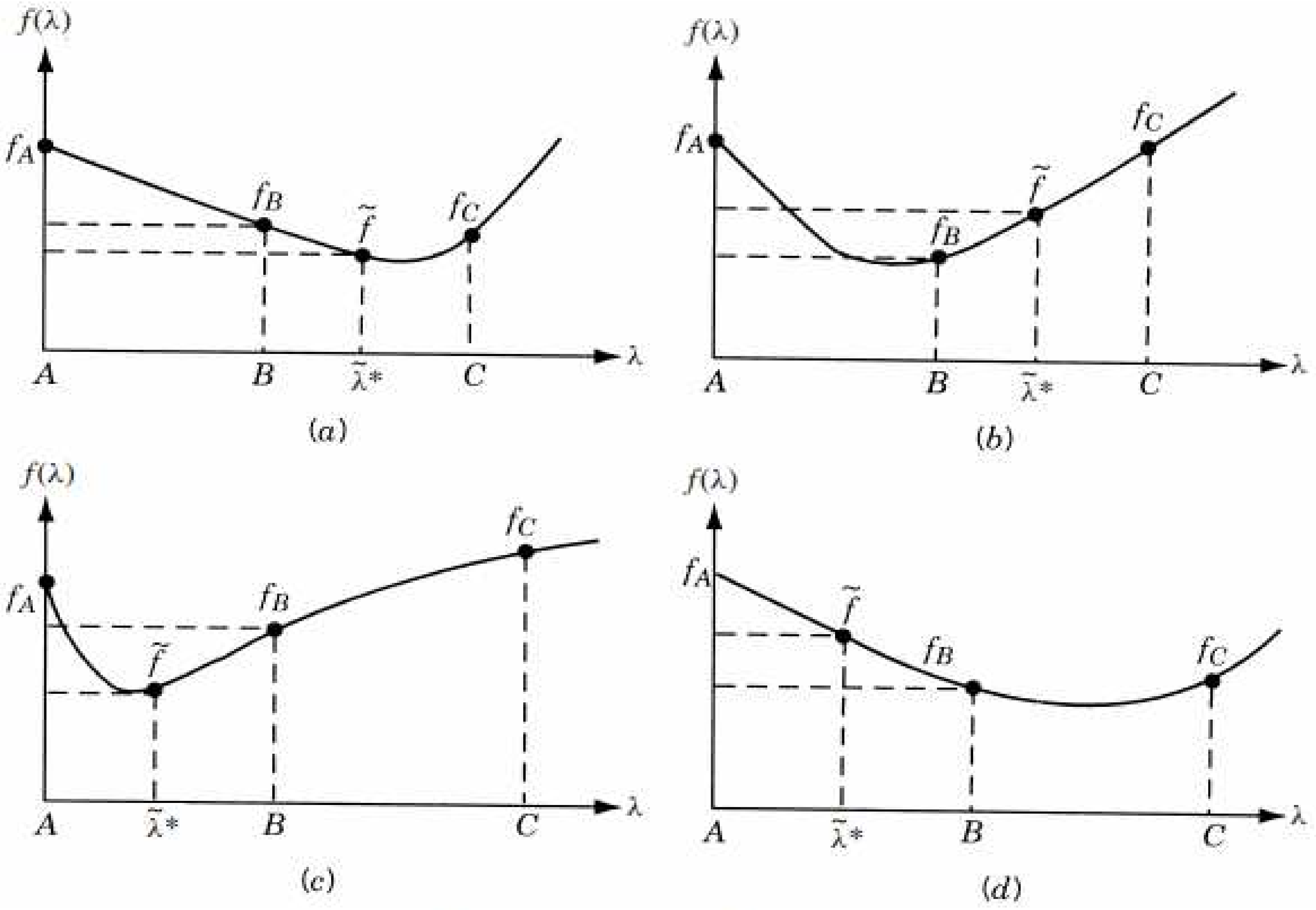


Figure 5.15 Various possibilities for refitting.

- Ανάλογα με τον παρακάτω πίνακα επιλέγονται τα 3 νέα σημεία προσαρμογής:

Table 5.5 Refitting Scheme

		New points for refitting	
Case	Characteristics	New	Old
1	$\tilde{\lambda}^* > B$	A	B
	$\tilde{f} < f_B$	B	$\tilde{\lambda}^*$
		C	C
		Neglect old A	
2	$\tilde{\lambda}^* > B$	A	A
	$\tilde{f} > f_B$	B	B
		C	$\tilde{\lambda}^*$
		Neglect old C	
3	$\tilde{\lambda}^* < B$	A	A
	$\tilde{f} < f_B$	B	$\tilde{\lambda}^*$
		C	B
		Neglect old C	
4	$\tilde{\lambda}^* < B$	A	$\tilde{\lambda}^*$
	$\tilde{f} > f_B$	B	B
		C	C
		Neglect old A	

Example 5.10 Find the minimum of $f = \lambda^5 - 5\lambda^3 - 20\lambda + 5$.

SOLUTION Since this is not a multivariable optimization problem, we can proceed directly to stage 2. Let the initial step size be taken as $t_0 = 0.5$ and $A = 0$.

- Υποτίθεται ότι γνωρίζουμε την κατεύθυνση του ελαχίστου (το **S** υποτίθεται είναι γνωστό)
- Επιλογή αρχικού σημείου για λ=0
- Επιλογή $2^{ου}$ σημείου για $\lambda = t_0 = 0.5$

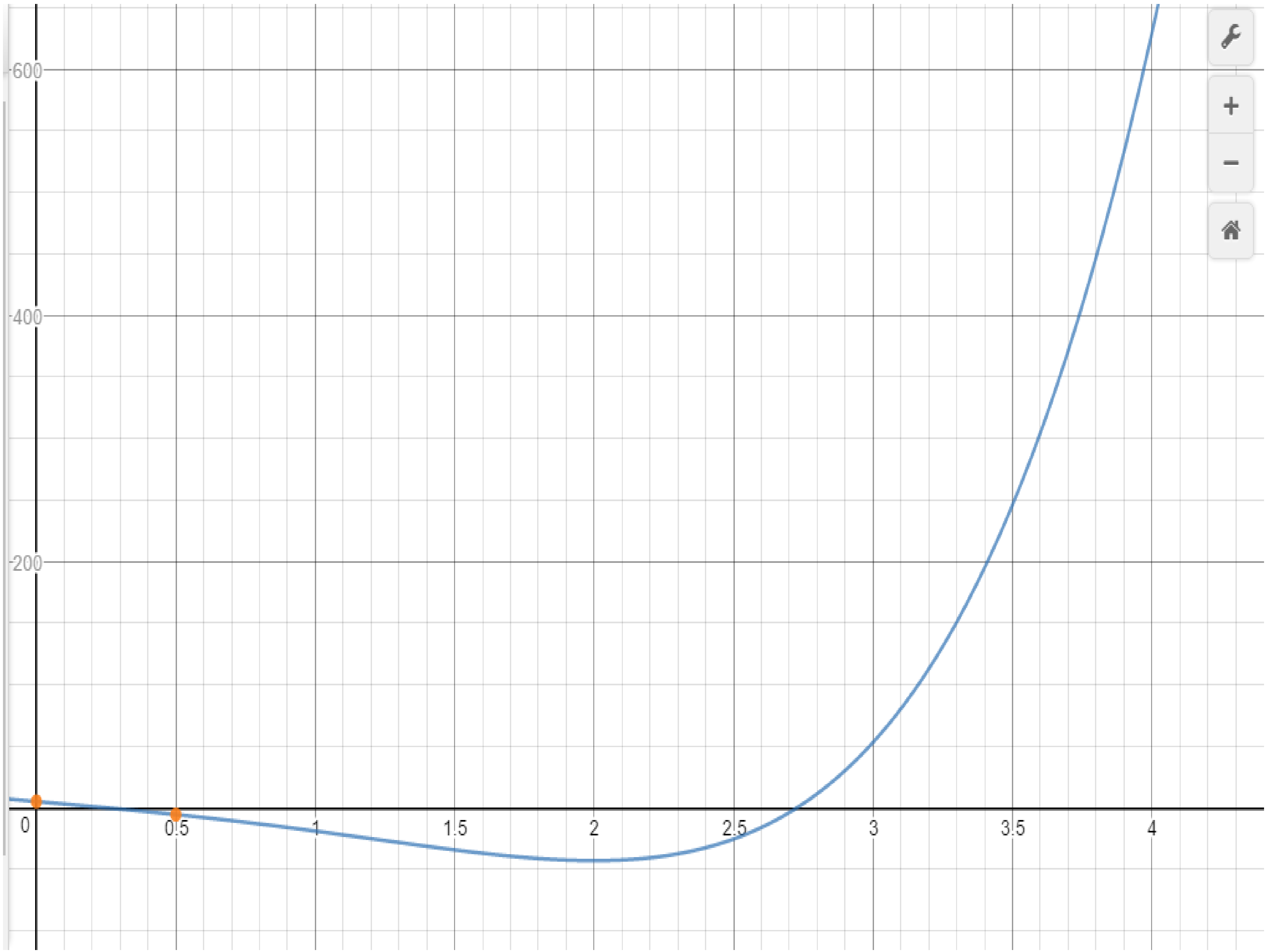
Iteration 1

$$f_A = f(\lambda = 0) = 5$$

$$f_1 = f(\lambda = t_0) = 0.03125 - 5(0.125) - 20(0.5) + 5 = -5.59375$$

Since $f_1 < f_A$, we set $f_B = f_1 = -5.59375$, and find that

$$f_2 = f(\lambda = 2t_0 = 1.0) = -19.0$$


600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4

Example 5.10 Find the minimum of $f = \lambda^5 - 5\lambda^3 - 20\lambda + 5$.

SOLUTION Since this is not a multivariable optimization problem, we can proceed directly to stage 2. Let the initial step size be taken as $t_0 = 0.5$ and $A = 0$.

Iteration 1

$$f_A = f(\lambda = 0) = 5$$

$$f_1 = f(\lambda = t_0) = 0.03125 - 5(0.125) - 20(0.5) + 5 = -5.59375$$

Since $f_1 < f_A$, we set $f_B = f_1 = -5.59375$, and find that

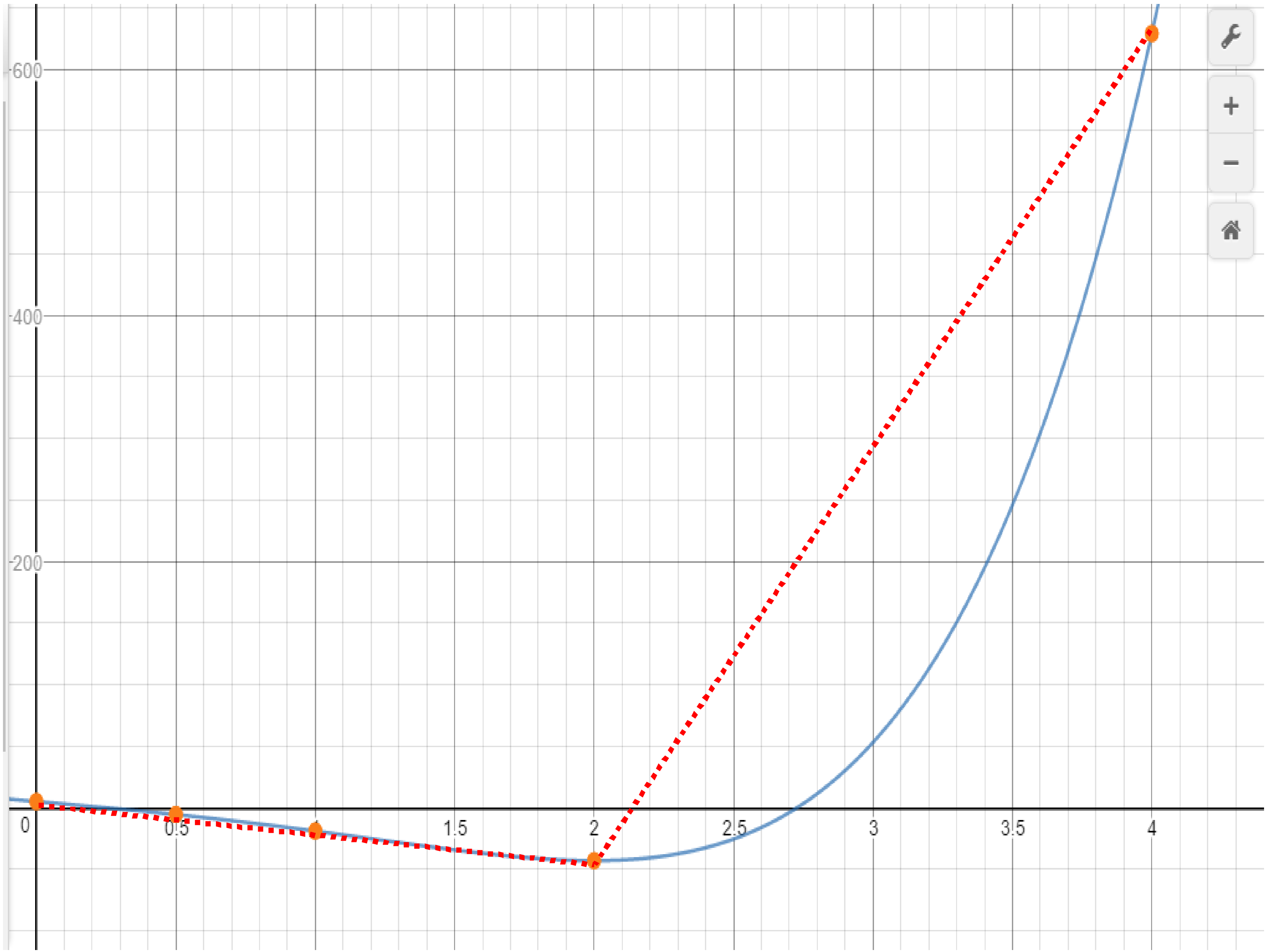
$$f_2 = f(\lambda = 2t_0 = 1.0) = -19.0$$

As $f_2 < f_1$, we set new $t_0 = 1$ and $f_1 = -19.0$. Again we find that $f_1 < f_A$ and hence set $f_B = f_1 = -19.0$, and find that $f_2 = f(\lambda = 2t_0 = 2) = -43$. Since $f_2 < f_1$, we again set $t_0 = 2$ and $f_1 = -43$. As this $f_1 < f_A$, set $f_B = f_1 = -43$ and evaluate $f_2 = f(\lambda = 2t_0 = 4) = 629$. This time $f_2 > f_1$ and hence we set $f_C = f_2 = 629$ and compute $\tilde{\lambda}^*$ from Eq. (5.40) as

$$\tilde{\lambda}^* = \frac{4(-43) - 3(5) - 629}{4(-43) - 2(629) - 2(5)}(2) = \frac{1632}{1440} = 1.135$$

Convergence test: Since $A = 0$, $f_A = 5$, $B = 2$, $f_B = -43$, $C = 4$, and $f_C = 629$, the values of a, b, and c can be found to be

$$a = 5, \quad b = -204, \quad c = 90$$



600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4

Προσαρμογή τετραγωνικής καμπύλης (2ου βαθμού) στα 3 σημεία

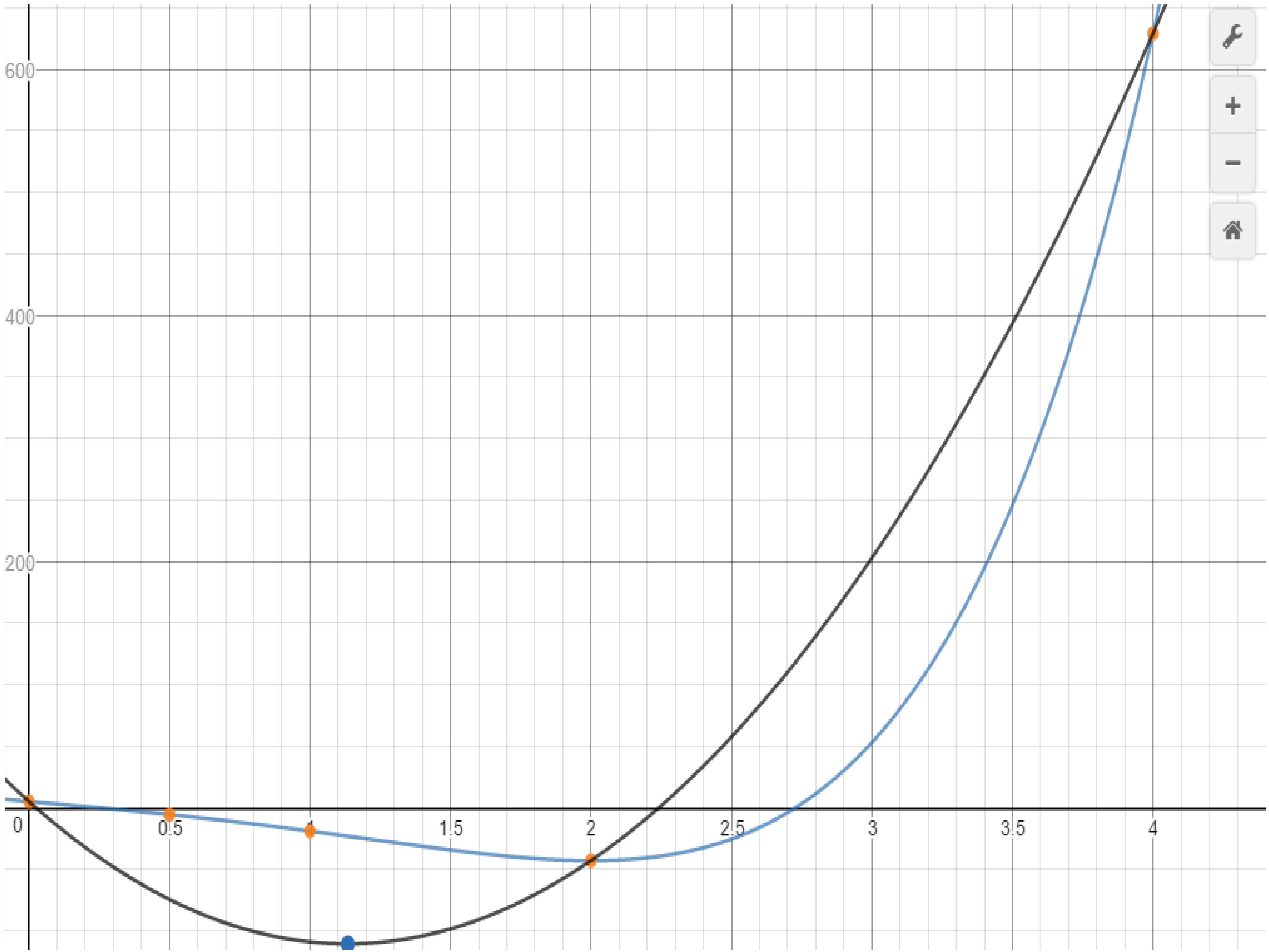
- Χρήση των τύπων για την προσαρμογή καμπύλης και την εύρεση του ελαχίστου της καμπύλης.

$$\tilde{\lambda}^* = \frac{4(-43) - 3(5) - 629}{4(-43) - 2(629) - 2(5)}(2) = \frac{1632}{1440} = 1.135$$

Convergence test: Since $A = 0$, $f_A = 5$, $B = 2$, $f_B = -43$, $C = 4$, and $f_C = 629$, the values of a, b, and c can be found to be

$$a = 5, \quad b = -204, \quad c = 90$$

- Άρα η καμπύλη (2ου βαθμού) που περνά από τα 3 σημεία είναι: $h(\lambda) = 90x^2 - 204x + 5$
- Με ελάχιστο στο $\lambda^* = 1.135$ και $h(\lambda^*) = -110.9$



600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4

Έλεγχος σύγκλισης

$$h(\tilde{\lambda}^*) = h(1.135) = 5 - 204(1.135) + 90(1.135)^2 = -110.9$$

Since

$$\tilde{f} = f(\tilde{\lambda}^*) = (1.135)^5 - 5(1.135)^3 - 20(1.135) + 5.0 = -23.127$$

we have

$$\left|\frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)}\right| = \left|\frac{-116.5 + 23.127}{-23.127}\right| = 3.8$$

As this quantity is very large, convergence is not achieved and hence we have to use *refitting*.

- Η βέλτιστη τιμή της προσαρμοσμένης καμπύλης h(λ) απέχει αρκετά από την τιμή της αντικειμενικής f(λ). Άρα πρέπει να επαναληφθεί η διαδικασία προσαρμογής νέας καμπύλης.


600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4

Επανάληψη προσαρμογής

- Ανάλογα με τον παρακάτω πίνακα επιλέγουμε τα νέα σημεία προσαρμογής:

Table 5.5 Refitting Scheme

Case	Characteristics	New points for refitting: New	New points for refitting: Old
1	$\tilde{\lambda}^* > B$	A	B
	$\tilde{f} < f_B$	B	$\tilde{\lambda}^*$
		C	C
		Neglect old A	
2	$\tilde{\lambda}^* > B$	A	A
	$\tilde{f} > f_B$	B	B
		C	$\tilde{\lambda}^*$
		Neglect old C	
3	$\tilde{\lambda}^* < B$	A	A
	$\tilde{f} < f_B$	B	$\tilde{\lambda}^*$
		C	B
		Neglect old C	
4	$\tilde{\lambda}^* < B$	A	$\tilde{\lambda}^*$
	$\tilde{f} > f_B$	B	B
		C	C
		Neglect old A	

Iteration 2

Since $\tilde{\lambda}^* < B$ and $\tilde{f} > f_B$, we take the new values of A, B, and C as

$$A = 1.135, \qquad f_A = -23.127$$

$$B = 2.0, \qquad f_B = -43.0$$

$$C = 4.0, \qquad f_C = 629.0$$

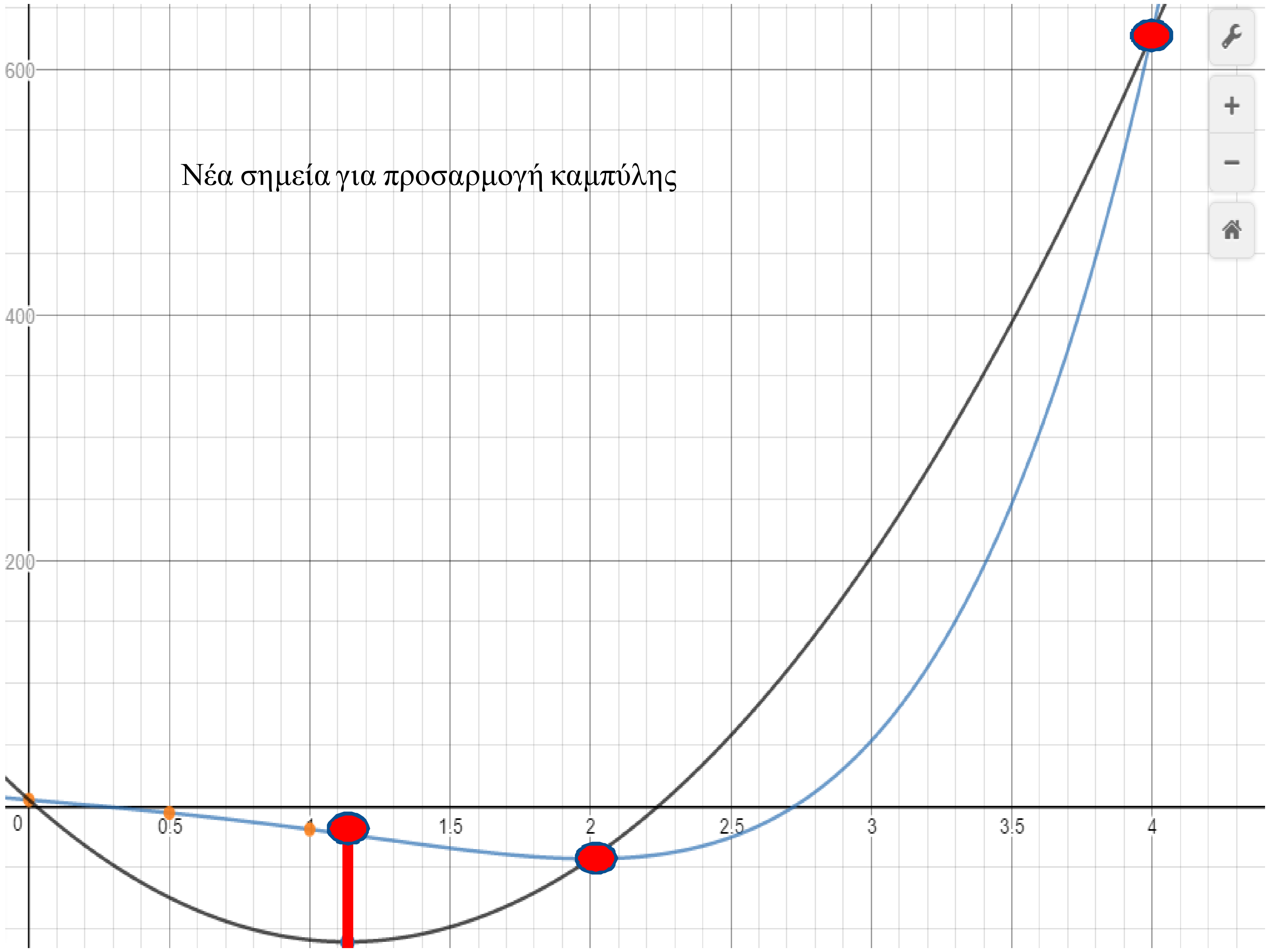
and compute new $\tilde{\lambda}^*$, using Eq. (5.36), as

$$\tilde{\lambda}^* = \frac{\begin{array}{l}(-23.127)(4.0-16.0)+(-43.0)(16.0-1.29)\\ \quad +(629.0)(1.29-4.0)\end{array}}{\begin{array}{l}2[(-23.127)(2.0-4.0)+(-43.0)(4.0-1.135)\\ \quad +(629.0)(1.135-2.0)]\end{array}} = 1.661$$

Convergence test: To test the convergence, we compute the coefficients of the quadratic as

$$a = 288.0, \quad b = -417.0, \quad c = 125.3$$

- Άρα η νέα καμπύλη είναι: $h(\lambda) = 125.3x^2 - 417x + 288$
- και $h(\lambda^* = 1.661) = -59.7$


Νέα σημεία για προσαρμογή καμπύλης
600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4


Νέα σημεία για προσαρμογή καμπύλης
600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4


600
400
200
0
0.5
1
1.5
2
2.5
3
3.5
4

Έλεγχος σύγκλισης

$$\tilde{\lambda}^* = \frac{\begin{array}{c}(-23.127)(4.0-16.0)+(-43.0)(16.0-1.29)\\ +(629.0)(1.29-4.0)\end{array}}{\begin{array}{c}2[(-23.127)(2.0-4.0)+(-43.0)(4.0-1.135)\\ +(629.0)(1.135-2.0)]\end{array}} = 1.661$$

Convergence test: To test the convergence, we compute the coefficients of the quadratic as

$$a = 288.0, \quad b = -417.0, \quad c = 125.3$$

As

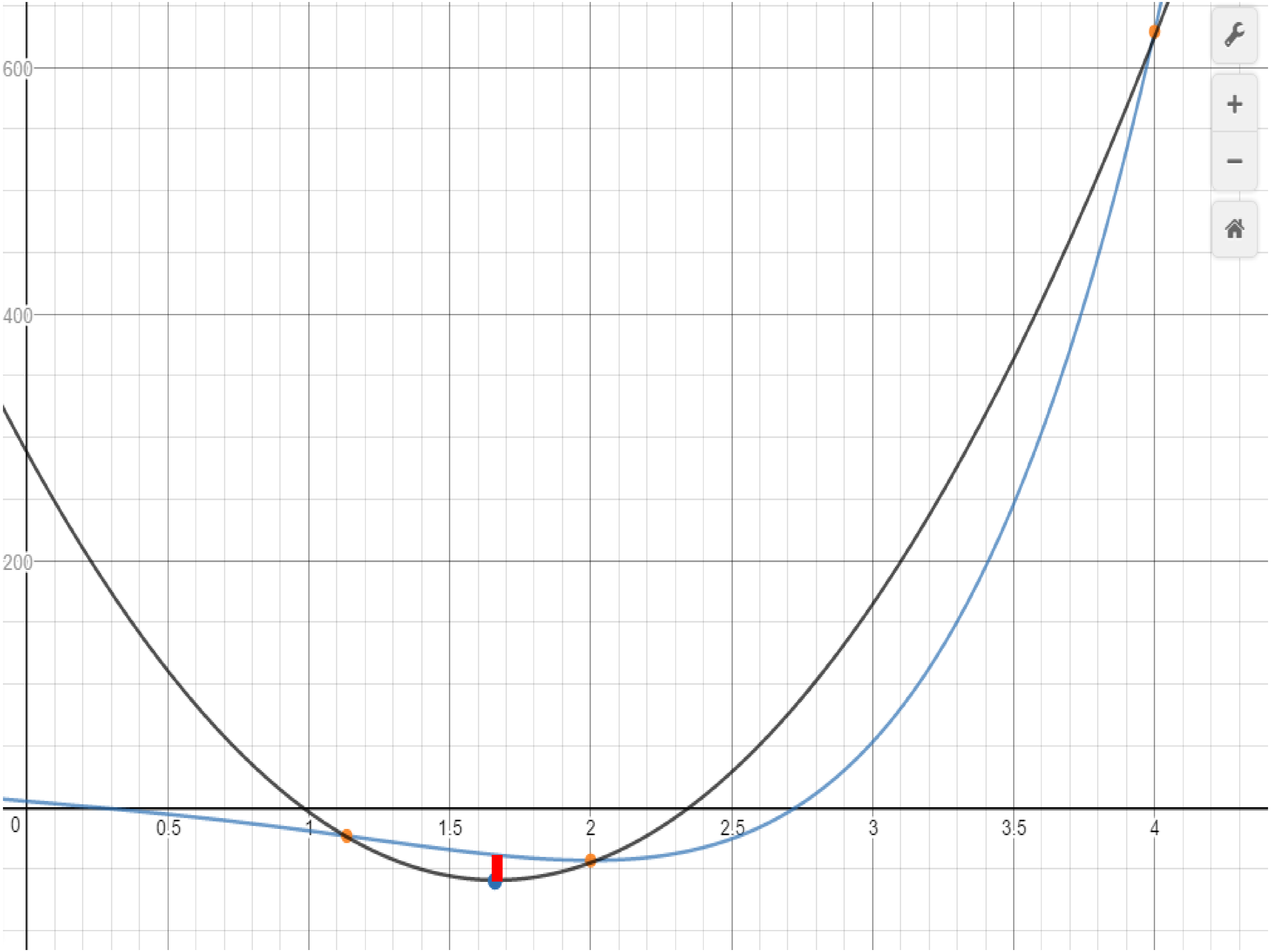
$$h(\tilde{\lambda}^*) = h(1.661) = 288.0 - 417.0(1.661) + 125.3(1.661)^2 = -59.7$$

$$\tilde{f} = f(\tilde{\lambda}^*) = 12.8 - 5(4.59) - 20(1.661) + 5.0 = -38.37$$

we obtain

$$\left|\frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)}\right| = \left|\frac{-59.70 + 38.37}{-38.37}\right| = 0.556$$

Since this quantity is not sufficiently small, we need to proceed to the next refit.


600
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2
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3
3.5
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Κυβική μέθοδος παρεμβολής

- Αυτή η μέθοδος παρεμβολής χρησιμοποιεί τις παραγώγους της συνάρτησης.
- Η μέθοδος προσαρμόζει καμπύλη 3ου βαθμού (κυβική) στην αντικειμενική συνάρτηση.
- Η μέθοδος εφαρμόζεται σε 3 στάδια.

Στάδιο 1ο κυβικής μεθόδου παρεμβολής

- Το διάνυσμα **S** (της κατεύθυνσης) κανονικοποιείται, ώστε βήμα μήκους λ=1 να είναι αποδεκτό.

Stage 1. In this stage,† the **S** vector is normalized as follows: Find $\Delta = \max_i |s_i|$, where s_i is the ith component of **S** and divide each component of **S** by Δ. Another method of normalization is to find $\Delta = (s_1^2 + s_2^2 + \cdots + s_n^2)^{1/2}$ and divide each component of **S** by Δ.

- Για μονοδιάστατα προβλήματα δεν απαιτείται.

Στάδιο 2ο κυβικής μεθόδου παρεμβολής

- Καθορισμός του κάτω και άνω ορίου του βέλτιστου μήκους βήματος λ^*.
- Απαιτείται να βρεθούν 2 σημεία A και B, στα οποία η κλίση df/dλ έχει διαφορετικά πρόσημα.
- Είναι γνωστό ότι $\left.\frac{df}{d\lambda}\right|_{\lambda=0} = \mathbf{S}^T \nabla f(\mathbf{X}) < 0$ αφού το διάνυσμα κατεύθυνσης **S** θεωρείται ότι έχει φορά προς την ελαχιστοποίηση
- Τυπικά επιλέγεται A=0 και επιδιώκεται να βρεθεί λ=B, όπου η κλίση df/dλ είναι θετική. Τίθεται λ ίσο με t_0, $2t_0$, $4t_0$, $8t_0$… έως ότου η παράγωγος να είναι μη αρνητική, όπου t_0 το προκαθορισμένο αρχικό μήκος βήματος.

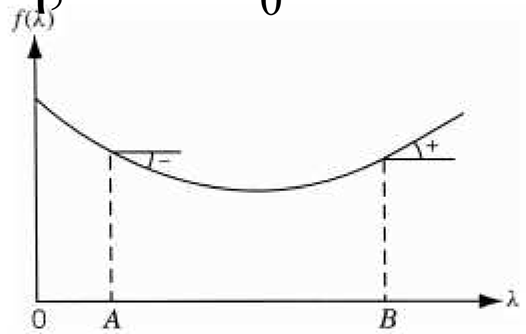


Figure 5.16 Minimum of $f(\lambda)$ lies between A and B.

Στάδιο 3ο κυβικής μεθόδου παρεμβολής

- Επιλογή των οριακών σημείων A και B για την προσαρμογή καμπύλης 3ου βαθμού της μορφής $h(\lambda) = a + b\lambda + c\lambda^2 + \lambda^3$
- προσαρμόζεται καμπύλη 3ου βαθμού (κυβική) σ' αυτά τα σημεία και υπολογίζεται η βέλτιστη θέση της προσαρμοσμένης καμπύλης.

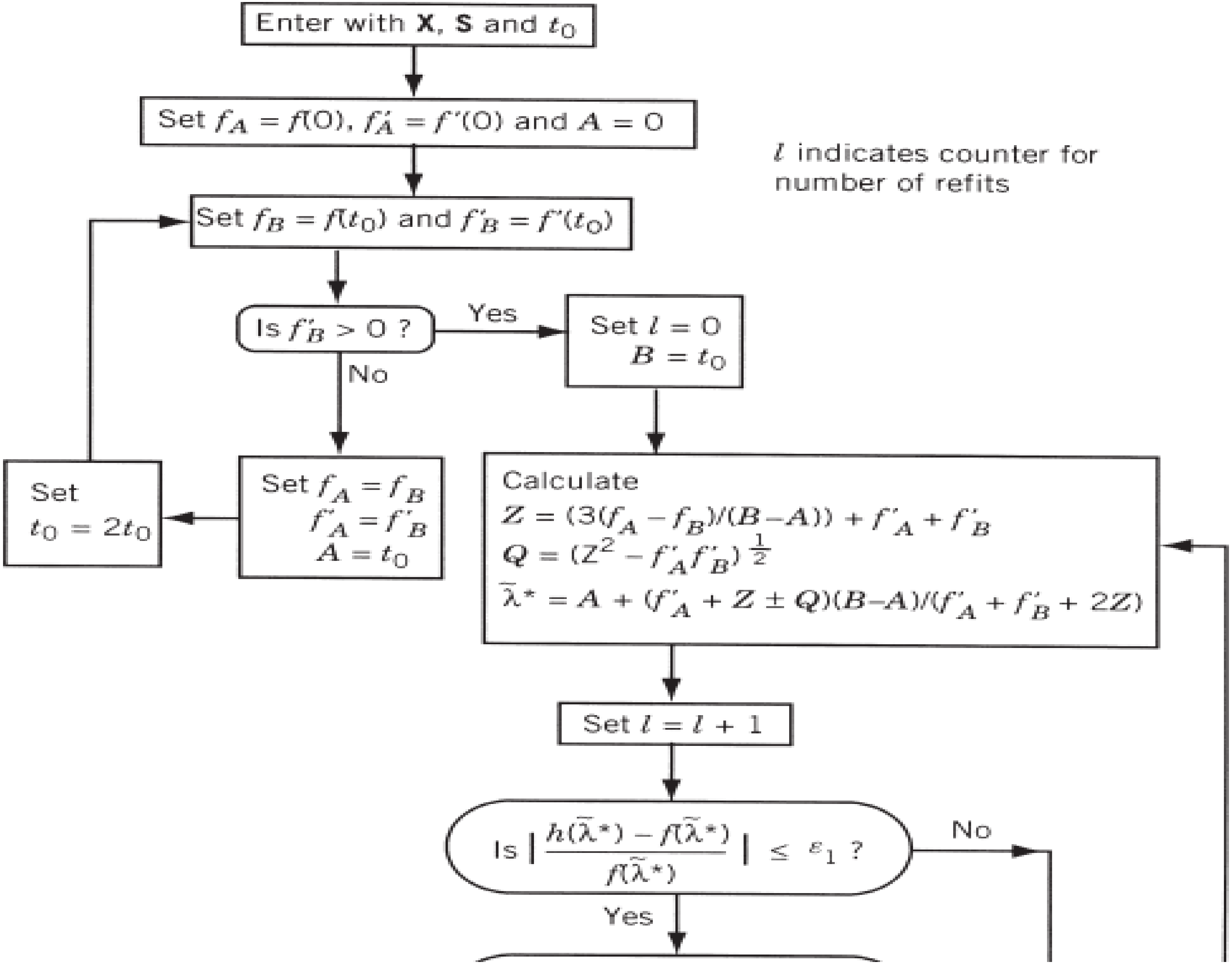
Στάδιο 4ο κυβικής μεθόδου παρεμβολής

- Ελέγχεται η σύγκλιση.
- Συγκρίνεται η τιμή της προσαρμοσμένης καμπύλης σε σχέση με την τιμή της αντικειμενικής συνάρτησης.
- Αν απέχουν αρκετά η διαδικασία επαναλαμβάνεται μέχρι να συγκλίνουν επαρκώς.
- Η εκτίμηση της σύγκλισης υλοποιείται με τα παρακάτω κριτήρια:

$$\left|\frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)}\right| \leq \varepsilon_1 \tag{5.60}$$

$$\left|\frac{df}{d\lambda}\right|_{\tilde{\lambda}^*} = |\mathbf{S}^T \nabla f|_{\tilde{\lambda}^*}| \leq \varepsilon_2 \tag{5.61}$$

- Αν δεν υπάρχει σύγκλιση τότε επιλέγονται τα καλύτερα 2 σημεία μεταξύ των A, B και λ^* και η διαδικασία επαναλαμβάνεται μέχρι να επέλθει σύγκλιση.



Enter with X, S and t_0
Set $f_A = f(0)$, $f'_A = f'(0)$ and $A = 0$
l indicates counter for number of refits
Set $f_B = f(t_0)$ and $f'_B = f'(t_0)$
Is $f'_B > 0$?
Yes
No
Set $l = 0$
$B = t_0$
Set $f_A = f_B$
$f'_A = f'_B$
$A = t_0$
Set
$t_0 = 2t_0$
Calculate
$Z = (3(f_A - f_B)/(B - A)) + f'_A + f'_B$
$Q = (Z^2 - f'_A f'_B)^{\frac{1}{2}}$
$\tilde{\lambda}^* = A + (f'_A + Z \pm Q)(B - A)/(f'_A + f'_B + 2Z)$
Set $l = l + 1$
Is $\left| \frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)} \right| \le \varepsilon_1$?
No
Yes

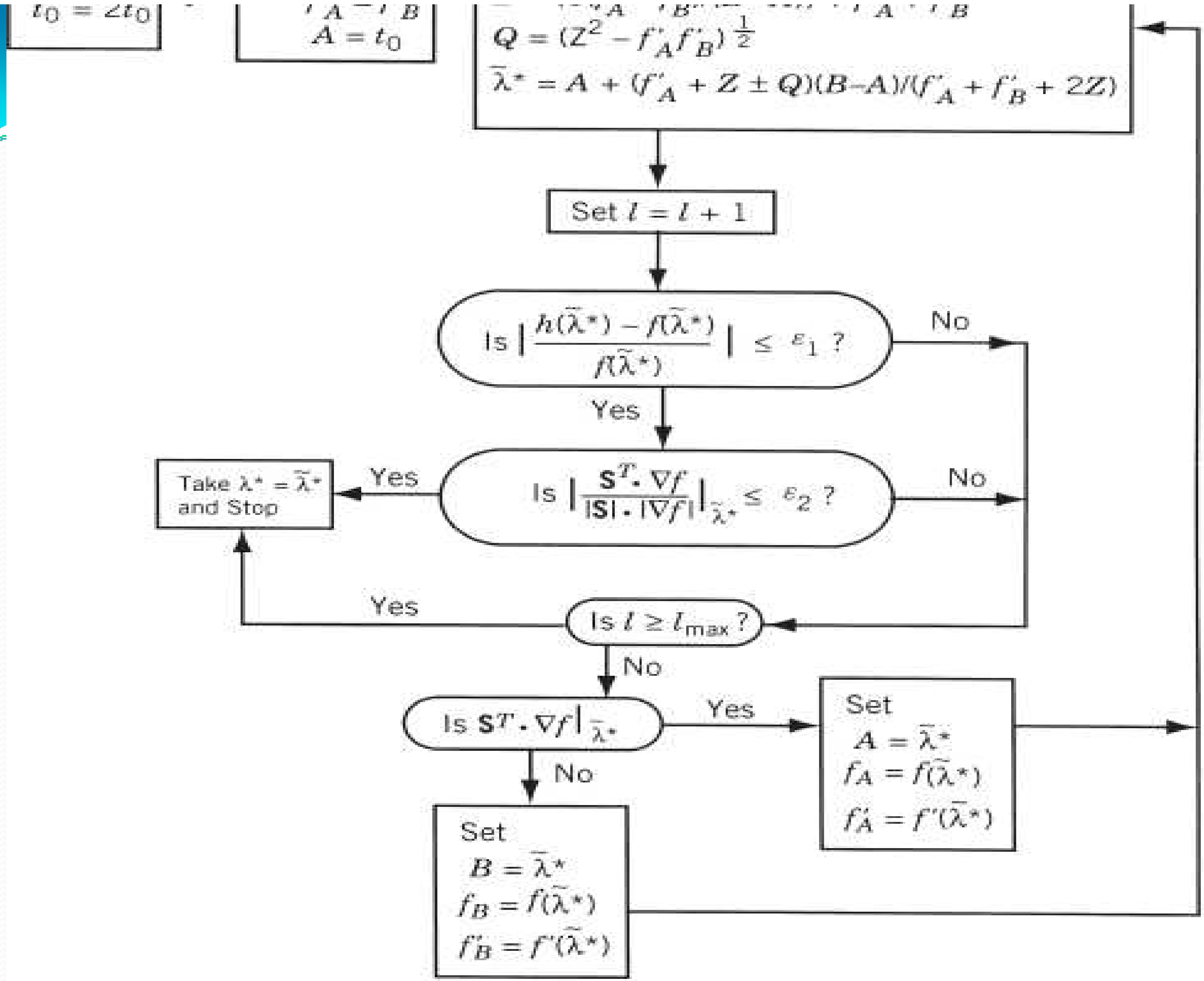


Figure 5.17 Flowchart for cubic interpolation method.

Προσαρμογή της κυβικής συνάρτησης

If the cubic equation

$$h(\lambda) = a + b\lambda + c\lambda^2 + \lambda^3 \tag{5.45}$$

is used to approximate the function $f(\lambda)$ between points A and B, we need to find the values $f_A = f(\lambda = A)$, $f'_A = df/d\lambda(\lambda = A)$, $f_B = f(\lambda = B)$, and $f'_B = df/d\lambda(\lambda = B)$ in order to evaluate the constants, a, b, c, and d in Eq. (5.45). By assuming that $A \neq 0$, we can derive a general formula for $\tilde{\lambda}^*$. From Eq. (5.45) we have

$$\begin{aligned} f_A &= a + bA + cA^2 + dA^3 \\ f_B &= a + bB + cB^2 + dB^3 \\ f'_A &= b + 2cA + 3dA^2 \\ f'_B &= b + 2cB + 3dB^2 \end{aligned} \tag{5.46}$$

Equations (5.46) can be solved to find the constants as

$$a = f_A - bA - cA^2 - dA^3 \tag{5.47}$$

with

$$b = \frac{1}{(A-B)^2}(B^2 f'_A + A^2 f'_B + 2ABZ) \tag{5.48}$$

$$c = -\frac{1}{(A-B)^2}[(A+B)Z + Bf'_A + Af'_B] \tag{5.49}$$

and

$$d = \frac{1}{3(A-B)^2}(2Z + f'_A + f'_B) \tag{5.50}$$

where

$$Z = \frac{3(f_A - f_B)}{B - A} + f'_A + f'_B \tag{5.51}$$

The necessary condition for the minimum of $h(\lambda)$ given by Eq. (5.45) is that

$$\frac{dh}{d\lambda} = b + 2c\lambda + 3d\lambda^2 = 0$$

that is,

$$\tilde{\lambda}^* = \frac{-c \pm (c^2 - 3bd)^{1/2}}{3d} \tag{5.52}$$

The application of the sufficiency condition for the minimum of $h(\lambda)$ leads to the relation

$$\left.\frac{d^2h}{d\lambda^2}\right|_{\tilde{\lambda}^*} = 2c + 6d\tilde{\lambda}^* > 0 \tag{5.53}$$

By substituting the expressions for b, c, and d given by Eqs. (5.48) to (5.50) into Eqs. (5.52) and (5.53), we obtain

$$\tilde{\lambda}^* = A + \frac{f'_A + Z \pm Q}{f'_A + f'_B + 2Z}(B - A) \tag{5.54}$$

where

$$Q = (Z^2 - f'_A f'_B)^{1/2} \tag{5.55}$$

$$\begin{aligned} &2(B - A)(2Z + f'_A + f'_B)(f'_A + Z \pm Q) \\ &\quad -2(B - A)(f'^2_A + Zf'_B + 3Zf'_A + 2Z^2) \\ &\quad -2(B + A)f'_A f'_B > 0 \end{aligned} \tag{5.56}$$

By specializing Eqs. (5.47) to (5.56) for the case where $A = 0$, we obtain

$$a = f_A$$

$$b = f'_A$$

$$c = -\frac{1}{B}(Z + f'_A)$$

$$d = \frac{1}{3B^2}(2Z + f'_A + f'_B)$$

$$\tilde{\lambda}^* = B\frac{f'_A + Z \pm Q}{f'_A + f'_B + 2Z} \tag{5.57}$$

$$Q = (Z^2 - f'_A f'_B)^{1/2} > 0 \tag{5.58}$$

where

$$Z = \frac{3(f_A - f_B)}{B} + f'_A + f'_B \tag{5.59}$$

The two values of $\tilde{\lambda}^*$ in Eqs. (5.54) and (5.57) correspond to the two possibilities for the vanishing of $h'(\lambda)$ [i.e., at a maximum of $h(\lambda)$ and at a minimum]. To avoid imaginary values of Q, we should ensure the satisfaction of the condition

$$Z^2 - f'_A f'_B \geq 0$$

in Eq. (5.55). This inequality is satisfied automatically since A and B are selected such that $f'_A < 0$ and $f'_B \geq 0$. Furthermore, the sufficiency condition (when $A = 0$) requires that $Q > 0$, which is already satisfied. Now we compute $\tilde{\lambda}^*$ using Eq. (5.57) and proceed to the next stage.

Example 5.11 Find the minimum of $f = \lambda^5 - 5\lambda^3 - 20\lambda + 5$ by the cubic interpolation method.

SOLUTION Since this problem has not arisen during a multivariable optimization process, we can skip stage 1. We take $A = 0$ and find that

$$\frac{df}{d\lambda}(\lambda = A = 0) = 5\lambda^4 - 15\lambda^2 - 20\Big|_{\lambda=0} = -20 < 0$$

To find B at which $df/d\lambda$ is nonnegative, we start with $t_0 = 0.4$ and evaluate the derivative at $t_0, 2t_0, 4t_0, \ldots$. This gives

$$f'(t_0 = 0.4) = 5(0.4)^4 - 15(0.4)^2 - 20.0 = -22.272$$

$$f'(2t_0 = 0.8) = 5(0.8)^4 - 15(0.8)^2 - 20.0 = -27.552$$

$$f'(4t_0 = 1.6) = 5(1.6)^4 - 15(1.6)^2 - 20.0 = -25.632$$

$$f'(8t_0 = 3.2) = 5(3.2)^4 - 15(3.2)^2 - 20.0 = 350.688$$

Thus we find that[†]

$$A = 0.0, \qquad f_A = 5.0, \qquad f'_A = -20.0$$

$$B = 3.2, \qquad f_B = 113.0, \qquad f'_B = 350.688$$

$$A < \lambda^* < B$$

Iteration 1

To find the value of $\tilde{\lambda}^*$ and to test the convergence criteria, we first compute Z and Q as

$$Z = \frac{3(5.0 - 113.0)}{3.2} - 20.0 + 350.688 = 229.588$$

$$Q = [229.588^2 + (20.0)(350.688)]^{1/2} = 244.0$$

Hence

$$\tilde{\lambda}^* = 3.2\left(\frac{-20.0 + 229.588 \pm 244.0}{-20.0 + 350.688 + 459.176}\right) = 1.84 \quad \text{or} \quad -0.1396$$

By discarding the negative value, we have

$$\tilde{\lambda}^* = 1.84$$

Convergence criterion: If $\tilde{\lambda}^*$ is close to the true minimum, λ^*, then $f'(\tilde{\lambda}^*) = df(\tilde{\lambda}^*)/d\lambda$ should be approximately zero. Since $f' = 5\lambda^4 - 15\lambda^2 - 20$,

$$f'(\tilde{\lambda}^*) = 5(1.84)^4 - 15(1.84)^2 - 20 = -13.0$$

Convergence criterion: If $\tilde{\lambda}^*$ is close to the true minimum, λ^*, then $f'(\tilde{\lambda}^*) = df(\tilde{\lambda}^*)/d\lambda$ should be approximately zero. Since $f' = 5\lambda^4 - 15\lambda^2 - 20$,

$$f'(\tilde{\lambda}^*) = 5(1.84)^4 - 15(1.84)^2 - 20 = -13.0$$

Since this is not small, we go to the next iteration or refitting. As $f'(\tilde{\lambda}^*) < 0$, we take $A = \tilde{\lambda}^*$ and

$$f_A = f(\tilde{\lambda}^*) = (1.84)^5 - 5(1.84)^3 - 20(1.84) + 5 = -41.70$$

Thus

$$A = 1.84, \qquad f_A = -41.70, \qquad f'_A = -13.0$$

$$B = 3.2, \qquad f_B = 113.0, \qquad f'_B = 350.688$$

$$A < \tilde{\lambda}^* < B$$

Iteration 2

$$Z = \frac{3(-41.7 - 113.0)}{3.20 - 1.84} - 13.0 + 350.688 = -3.312$$

$$Q = [(-3.312)^2 + (13.0)(350.688)]^{1/2} = 67.5$$

Hence

$$\tilde{\lambda}^* = 1.84 + \frac{-13.0 - 3.312 \pm 67.5}{-13.0 + 350.688 - 6.624}(3.2 - 1.84) = 2.05$$

Convergence criterion:

$$f'(\tilde{\lambda}^*) = 5.0(2.05)^4 - 15.0(2.05)^2 - 20.0 = 5.35$$

Since this value is large, we go the next iteration with $B = \tilde{\lambda}^* = 2.05$ [as $f'(\tilde{\lambda}^*) > 0$] and

$$f_B = (2.05)^5 - 5.0(2.05)^3 - 20.0(2.05) + 5.0 = -42.90$$

Thus

$$A = 1.84, \qquad f_A = -41.70, \qquad f'_A = -13.00$$

$$B = 2.05, \qquad f_B = -42.90, \qquad f'_B = 5.35$$

$$A < \lambda^* < B$$

Iteration 3

$$Z = \frac{3.0(-41.70 + 42.90)}{(2.05 - 1.84)} - 13.00 + 5.35 = 9.49$$

$$Q = [(9.49)^2 + (13.0)(5.35)]^{1/2} = 12.61$$

Therefore,

$$\tilde{\lambda}^* = 1.84 + \frac{-13.00 + 9.49 \pm 12.61}{-13.00 + 5.35 + 18.98}(2.05 - 1.84) = 2.0086$$

Convergence criterion:

$$f'(\tilde{\lambda}^*) = 5.0(2.0086)^4 - 15.0(2.0086)^2 - 20.0 = 0.855$$

Assuming that this value is close to zero, we can stop the iterative process and take

$$\lambda^* \simeq \tilde{\lambda}^* = 2.0086$$

DIRECT ROOT METHODS

The necessary condition for $f(\lambda)$ to have a minimum of λ^* is that $f'(\lambda^*) = 0$. The direct root methods seek to find the root (or solution) of the equation, $f'(\lambda) = 0$. Three root-finding methods—the Newton, the quasi-Newton, and the secant methods—are discussed in this section.

Μέθοδος Newton ή Newton-Raphson

Consider the quadratic approximation of the function $f(\lambda)$ at $\lambda = \lambda_i$ using the Taylor's series expansion:

$$f(\lambda) = f(\lambda_i) + f'(\lambda_i)(\lambda - \lambda_i) + \frac{1}{2}f''(\lambda_i)(\lambda - \lambda_i)^2 \tag{5.63}$$

By setting the derivative of Eq. (5.63) equal to zero for the minimum of $f(\lambda)$, we obtain

$$f'(\lambda) = f'(\lambda_i) + f''(\lambda_i)(\lambda - \lambda_i) = 0 \tag{5.64}$$

If λ_i denotes an approximation to the minimum of $f(\lambda)$, Eq. (5.64) can be rearranged to obtain an improved approximation as

$$\lambda_{i+1} = \lambda_i - \frac{f'(\lambda_i)}{f''(\lambda_i)} \tag{5.65}$$

Thus the *Newton method*, Eq. (5.65), is equivalent to using a quadratic approximation for the function $f(\lambda)$ and applying the necessary conditions. The iterative process given by Eq. (5.65) can be assumed to have converged when the derivative, $f'(\lambda_{i+1})$, is close to zero:

$$|f'(\lambda_{i+1})| \leq \varepsilon \tag{5.66}$$

where ε is a small quantity. The convergence process of the method is shown graphically in Fig. 5.18*a*.

Remarks:

1. The Newton method was originally developed by Newton for solving nonlinear equations and later refined by Raphson, and hence the method is also known as *Newton–Raphson method* in the literature of numerical analysis.
2. The method requires both the first- and second-order derivatives of $f(\lambda)$.
3. If $f''(\lambda_i) \neq 0$ [in Eq. (5.65)], the Newton iterative method has a powerful (fastest) convergence property, known as *quadratic convergence*.[†]
4. If the starting point for the iterative process is not close to the true solution λ^*, the Newton iterative process might diverge as illustrated in Fig. 5.18*b*.

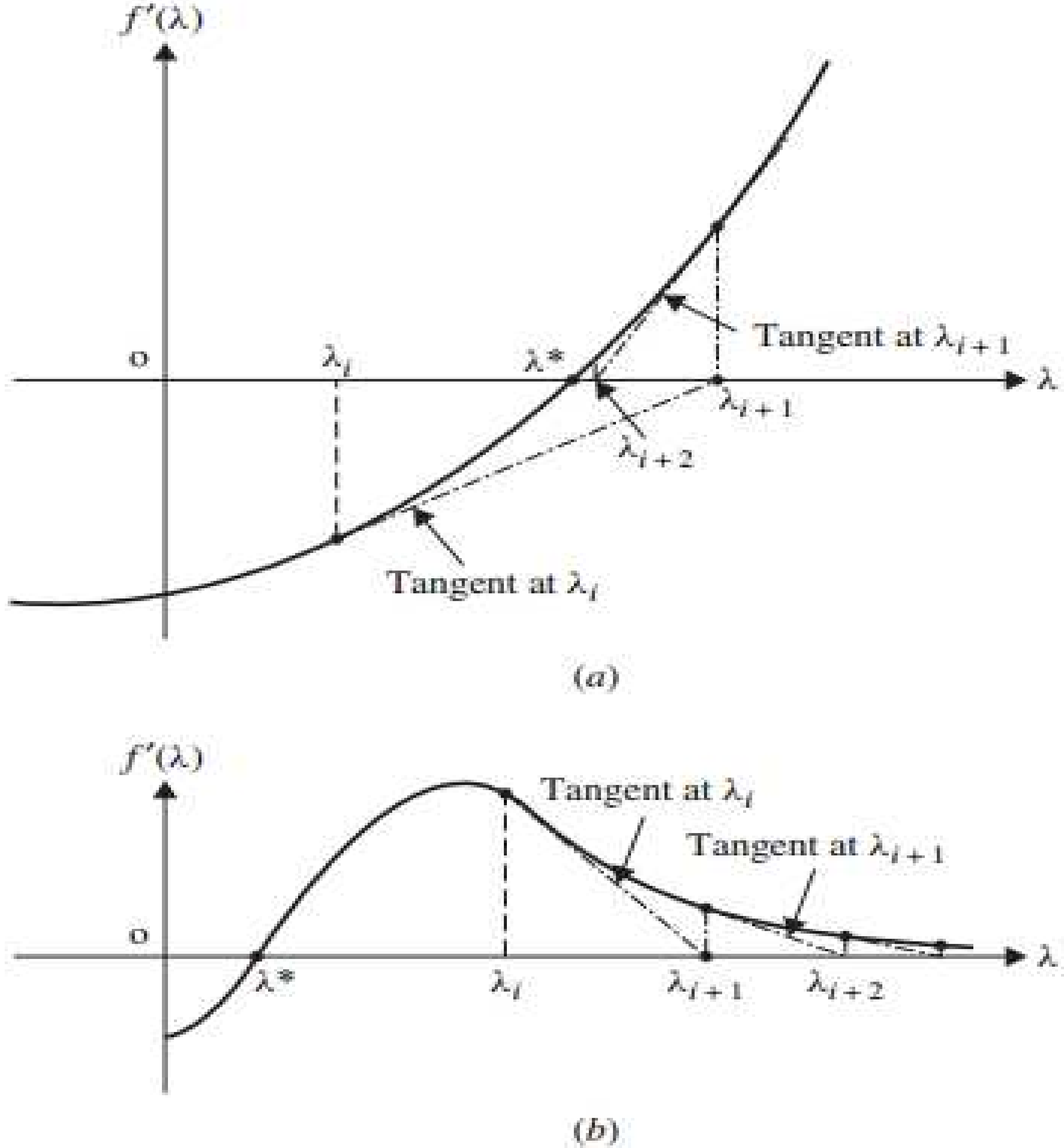


Figure 5.18 Iterative process of Newton method: (*a*) convergence; (*b*) divergence.

Example 5.12 Find the minimum of the function

$$f(\lambda) = 0.65 - \frac{0.75}{1+\lambda^2} - 0.65\lambda \tan^{-1}\frac{1}{\lambda}$$

using the Newton–Raphson method with the starting point $\lambda_1 = 0.1$. Use $\varepsilon = 0.01$ in Eq. (5.66) for checking the convergence.

SOLUTION The first and second derivatives of the function $f(\lambda)$ are given by

$$f'(\lambda) = \frac{1.5\lambda}{(1+\lambda^2)^2} + \frac{0.65\lambda}{1+\lambda^2} - 0.65\tan^{-1}\frac{1}{\lambda}$$

$$f''(\lambda) = \frac{1.5(1-3\lambda^2)}{(1+\lambda^2)^3} + \frac{0.65(1-\lambda^2)}{(1+\lambda^2)^2} + \frac{0.65}{1+\lambda^2} = \frac{2.8-3.2\lambda^2}{(1+\lambda^2)^3}$$

Iteration 1

$$\lambda_1 = 0.1, \quad f(\lambda_1) = -0.188197, \quad f'(\lambda_1) = -0.744832, \quad f''(\lambda_1) = 2.68659$$

$$\lambda_2 = \lambda_1 - \frac{f'(\lambda_1)}{f''(\lambda_1)} = 0.377241$$

Convergence check: $|f'(\lambda_2)| = |-0.138230| > \varepsilon$.

Iteration 2

$$f(\lambda_2) = -0.303279, \quad f'(\lambda_2) = -0.138230, \quad f''(\lambda_2) = 1.57296$$

$$\lambda_3 = \lambda_2 - \frac{f'(\lambda_2)}{f''(\lambda_2)} = 0.465119$$

Convergence check: $|f'(\lambda_3)| = |-0.0179078| > \varepsilon$.

Iteration 3

$$f(\lambda_3) = -0.309881, \quad f'(\lambda_3) = -0.0179078, \quad f''(\lambda_3) = 1.17126$$

$$\lambda_4 = \lambda_3 - \frac{f'(\lambda_3)}{f''(\lambda_3)} = 0.480409$$

Convergence check: $|f'(\lambda_4)| = |-0.0005033| < \varepsilon$.

Since the process has converged, the optimum solution is taken as $\lambda^* \approx \lambda_4 = 0.480409$.

Μέθοδος Quasi-Newton

If the function being minimized $f(\lambda)$ is not available in closed form or is difficult to differentiate, the derivatives $f'(\lambda)$ and $f''(\lambda)$ in Eq. (5.65) can be approximated by the finite difference formulas as

$$f'(\lambda_i) = \frac{f(\lambda_i + \Delta\lambda) - f(\lambda_i - \Delta\lambda)}{2\Delta\lambda} \tag{5.67}$$

$$f''(\lambda_i) = \frac{f(\lambda_i + \Delta\lambda) - 2f(\lambda_i) + f(\lambda_i - \Delta\lambda)}{\Delta\lambda^2} \tag{5.68}$$

where $\Delta\lambda$ is a small step size. Substitution of Eqs. (5.67) and (5.68) into Eq. (5.65) leads to

$$\lambda_{i+1} = \lambda_i - \frac{\Delta\lambda[f(\lambda_i + \Delta\lambda) - f(\lambda_i - \Delta\lambda)]}{2[f(\lambda_i + \Delta\lambda) - 2f(\lambda_i) + f(\lambda_i - \Delta\lambda)]} \tag{5.69}$$

The iterative process indicated by Eq. (5.69) is known as the *quasi-Newton method*. To test the convergence of the iterative process, the following criterion can be used:

$$|f'(\lambda_{i+1})| = \left| \frac{f(\lambda_{i+1} + \Delta\lambda) - f(\lambda_{i+1} - \Delta\lambda)}{2\Delta\lambda} \right| \le \varepsilon \tag{5.70}$$

where a central difference formula has been used for evaluating the derivative of f and ε is a small quantity.

Remarks:

1. The central difference formulas have been used in Eqs. (5.69) and (5.70). However, the forward or backward difference formulas can also be used for this purpose.
2. Equation (5.69) requires the evaluation of the function at the points $\lambda_i + \Delta\lambda$ and $\lambda_i - \Delta\lambda$ in addition to λ_i in each iteration.

Example 5.13 Find the minimum of the function

$$f(\lambda) = 0.65 - \frac{0.75}{1+\lambda^2} - 0.65\lambda \tan^{-1}\frac{1}{\lambda}$$

using quasi-Newton method with the starting point $\lambda_1 = 0.1$ and the step size $\Delta\lambda = 0.01$ in central difference formulas. Use $\varepsilon = 0.01$ in Eq. (5.70) for checking the convergence.

SOLUTION

Iteration 1

$$\lambda_1 = 0.1, \quad \Delta\lambda = 0.01, \quad \varepsilon = 0.01, \quad f_1 = f(\lambda_1) = -0.188197,$$

$$f_1^+ = f(\lambda_1 + \Delta\lambda) = -0.195512, \quad f_1^- = f(\lambda_1 - \Delta\lambda) = -0.180615$$

$$\lambda_2 = \lambda_1 - \frac{\Delta\lambda(f_1^+ - f_1^-)}{2(f_1^+ - 2f_1 + f_1^-)} = 0.377882$$

Convergence check:

$$|f'(\lambda_2)| = \left|\frac{f_2^+ - f_2^-}{2\Delta\lambda}\right| = 0.137300 > \varepsilon$$

Iteration 2

$$f_2 = f(\lambda_2) = -0.303368, \quad f_2^+ = f(\lambda_2 + \Delta\lambda) = -0.304662,$$

$$f_2^- = f(\lambda_2 - \Delta\lambda) = -0.301916$$

$$\lambda_3 = \lambda_2 - \frac{\Delta\lambda(f_2^+ - f_2^-)}{2(f_2^+ - 2f_2 + f_2^-)} = 0.465390$$

Convergence check:

$$|f'(\lambda_3)| = \left|\frac{f_3^+ - f_3^-}{2\Delta\lambda}\right| = 0.017700 > \varepsilon$$

Iteration 3

$$f_3 = f(\lambda_3) = -0.309885, \quad f_3^+ = f(\lambda_3 + \Delta\lambda) = -0.310004,$$

$$f_3^- = f(\lambda_3 - \Delta\lambda) = -0.309650$$

$$\lambda_4 = \lambda_3 - \frac{\Delta\lambda(f_3^+ - f_3^-)}{2(f_3^+ - 2f_3 + f_3^-)} = 0.480600$$

Convergence check:

$$|f'(\lambda_4)| = \left|\frac{f_4^+ - f_4^-}{2\Delta\lambda}\right| = 0.000350 < \varepsilon$$

Since the process has converged, we take the optimum solution as $\lambda^* \approx \lambda_4 = 0.480600$.

Μέθοδος Secant

The secant method uses an equation similar to Eq. (5.64) as

$$f'(\lambda) = f'(\lambda_i) + s(\lambda - \lambda_i) = 0 \tag{5.71}$$

where s is the slope of the line connecting the two points $(A, f'(A))$ and $(B, f'(B))$, where A and B denote two different approximations to the correct solution, λ^*. The slope s can be expressed as (Fig. 5.19)

$$s = \frac{f'(B) - f'(A)}{B - A} \tag{5.72}$$

Equation (5.71) approximates the function $f'(\lambda)$ between A and B as a linear equation (secant), and hence the solution of Eq. (5.71) gives the new approximation to the root of $f'(\lambda)$ as

$$\lambda_{i+1} = \lambda_i - \frac{f'(\lambda_i)}{s} = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} \tag{5.73}$$

The iterative process given by Eq. (5.73) is known as the *secant method* (Fig. 5.19). Since the secant approaches the second derivative of $f(\lambda)$ at A as B approaches A, the secant method can also be considered as a quasi-Newton method.

the secant method can also be considered as a quasi-Newton method. It can also be considered as a form of elimination technique since part of the interval, (A, λ_{i+1}) in Fig. 5.19, is eliminated in every iteration. The iterative process can be implemented by using the following step-by-step procedure.

1. Set $\lambda_1 = A = 0$ and evaluate $f'(A)$. The value of $f'(A)$ will be negative. Assume an initial trial step length t_0. Set $i = 1$.
2. Evaluate $f'(t_0)$.
3. If $f'(t_0) < 0$, set $A = \lambda_i = t_0$, $f'(A) = f'(t_0)$, new $t_0 = 2t_0$, and go to step 2.
4. If $f'(t_0) \geq 0$, set $B = t_0$, $f'(B) = f'(t_0)$, and go to step 5.
5. Find the new approximate solution of the problem as

$$\lambda_{i+1} = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} \tag{5.74}$$

6. Test for convergence:

$$|f'(\lambda_i + 1)| \leq \varepsilon \tag{5.75}$$

   where ε is a small quantity. If Eq. (5.75) is satisfied, take $\lambda^* \approx \lambda_{i+1}$ and stop the procedure. Otherwise, go to step 7.
7. If $f'(\lambda_{i+1}) \geq 0$, set new $B = \lambda_{i+1}$, $f'(B) = f'(\lambda_{i+1})$, $i = i + 1$, and go to step 5.
8. If $f'(\lambda_{i+1}) < 0$, set new $A = \lambda_{i+1}$, $f'(A) = f'(\lambda_{i+1})$, $i = i + 1$, and go to step 5.

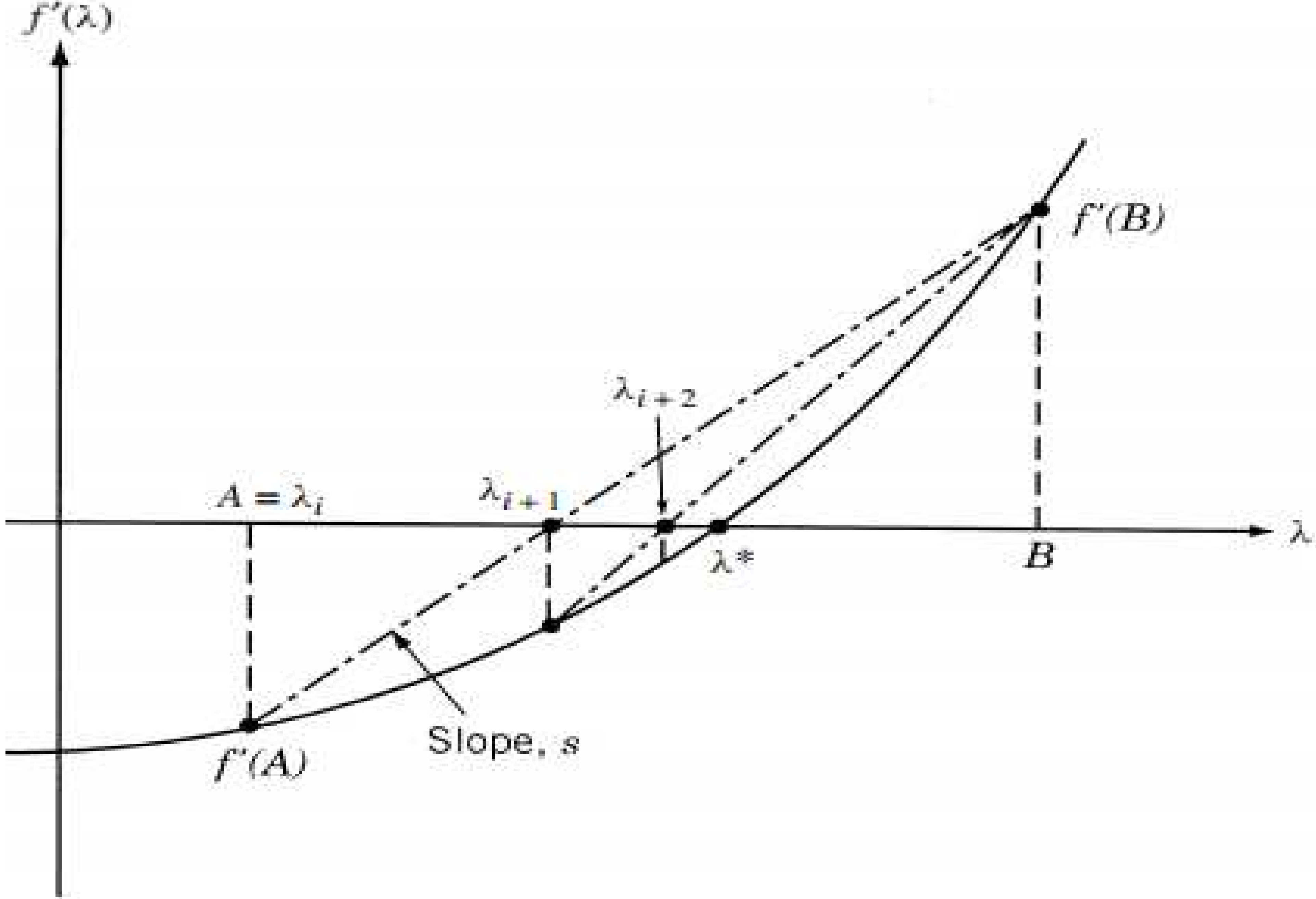


Figure 5.19 Iterative process of the secant method.

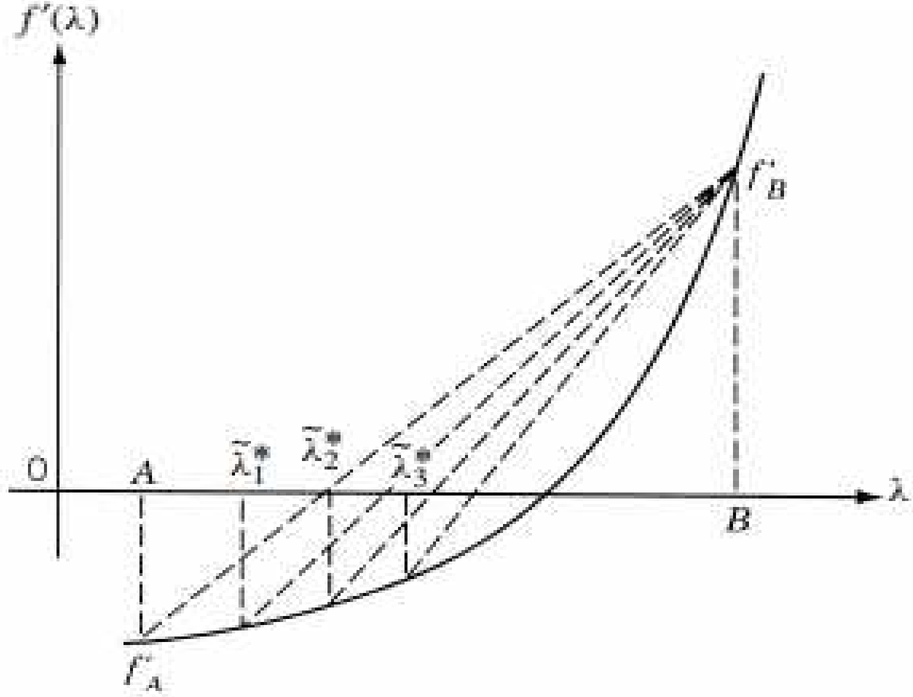


Figure 5.20 Situation when f'_A varies very slowly.

Remarks:

1. The secant method is identical to assuming a linear equation for $f'(\lambda)$. This implies that the original function, $f(\lambda)$, is approximated by a quadratic equation.
2. In some cases we may encounter a situation where the function $f'(\lambda)$ varies very slowly with λ, as shown in Fig. 5.20. This situation can be identified by noticing that the point B remains unaltered for several consecutive refits. Once such a situation is suspected, the convergence process can be improved by taking the next value of λ_{i+1} as $(A + B)/2$ instead of finding its value from Eq. (5.74).

Example 5.14 Find the minimum of the function

$$f(\lambda) = 0.65 - \frac{0.75}{1+\lambda^2} - 0.65\lambda \tan^{-1}\frac{1}{\lambda}$$

using the secant method with an initial step size of $t_0 = 0.1$, $\lambda_1 = 0.0$, and $\varepsilon = 0.01$.

SOLUTION $\lambda_1 = A = 0.0$, $t_0 = 0.1$, $f'(A) = -1.02102$, $B = A + t_0 = 0.1$, $f'(B) = -0.744832$. Since $f'(B) < 0$, we set new $A = 0.1$, $f'(A) = -0.744832$, $t_0 = 2(0.1) = 0.2$, $B = \lambda_1 + t_0 = 0.2$, and compute $f'(B) = -0.490343$. Since $f'(B) < 0$, we set new $A = 0.2$, $f'(A) = -0.490343$, $t_0 = 2(0.2) = 0.4$, $B = \lambda_1 + t_0 = 0.4$, and compute $f'(B) = -0.103652$. Since $f'(B) < 0$, we set new $A = 0.4$, $f'(A) = -0.103652$, $t_0 = 2(0.4) = 0.8$, $B = \lambda_1 + t_0 = 0.8$, and compute $f'(B) = +0.180800$. Since $f'(B) > 0$, we proceed to find λ_2.

Iteration 1

Since $A = \lambda_1 = 0.4$, $f'(A) = -0.103652$, $B = 0.8$, $f'(B) = +0.180800$, we compute

$$\lambda_2 = A - \frac{f'(A)(B-A)}{f'(B) - f'(A)} = 0.545757$$

Convergence check: $|f'(\lambda_2)| = |+0.0105789| > \varepsilon$.

Iteration 2

Since $f'(\lambda_2) = +0.0105789 > 0$, we set new $A = 0.4$, $f'(A) = -0.103652$, $B = \lambda_2 = 0.545757$, $f'(B) = f'(\lambda_2) = +0.0105789$, and compute

$$\lambda_3 = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} = 0.490632$$

Convergence check: $|f'(\lambda_3)| = |+0.00151235| < \varepsilon$.

Since the process has converged, the optimum solution is given by $\lambda^* \approx \lambda_3 = 0.490632$.

Πώς να βελτιωθεί η αποδοτικότητα και η αξιοπιστία των μεθόδων

In some cases, some of the interpolation methods discussed in Sections 5.10 to 5.12 may be very slow to converge, may diverge, or may predict the minimum of the function, $f(\lambda)$, outside the initial interval of uncertainty, especially when the interpolating polynomial is not representative of the variation of the function being minimized. In such cases we can use the Fibonacci or golden section method to find the minimum. In some problems it might prove to be more efficient to combine several techniques. For example, the unrestricted search with an accelerated step size can be used to bracket the minimum and then the Fibonacci or the golden section method can be used to find the optimum point. In some cases the Fibonacci or golden section method can be used in conjunction with an interpolation method.

Σύγκριση μεθόδων

It has been shown in Section 5.9 that the Fibonacci method is the most efficient elimination technique in finding the minimum of a function if the initial interval of uncertainty is known. In the absence of the initial interval of uncertainty, the quadratic interpolation method or the quasi-Newton method is expected to be more efficient when the derivatives of the function are not available. When the first derivatives of the function being minimized are available, the cubic interpolation method or the secant method are expected to be very efficient. On the other hand, if both the first and second derivatives of the function are available, the Newton method will be the most efficient one in finding the optimal step length, λ^*.

In general, the efficiency and reliability of the various methods are problem dependent and any efficient computer program must include many heuristic additions not indicated explicitly by the method. The heuristic considerations are needed to handle multimodal functions (functions with multiple extreme points), sharp variations in the slopes (first derivatives) and curvatures (second derivatives) of the function, and the effects of round-off errors resulting from the precision used in the arithmetic operations. A comparative study of the efficiencies of the various search methods is given in Ref. [5.10].