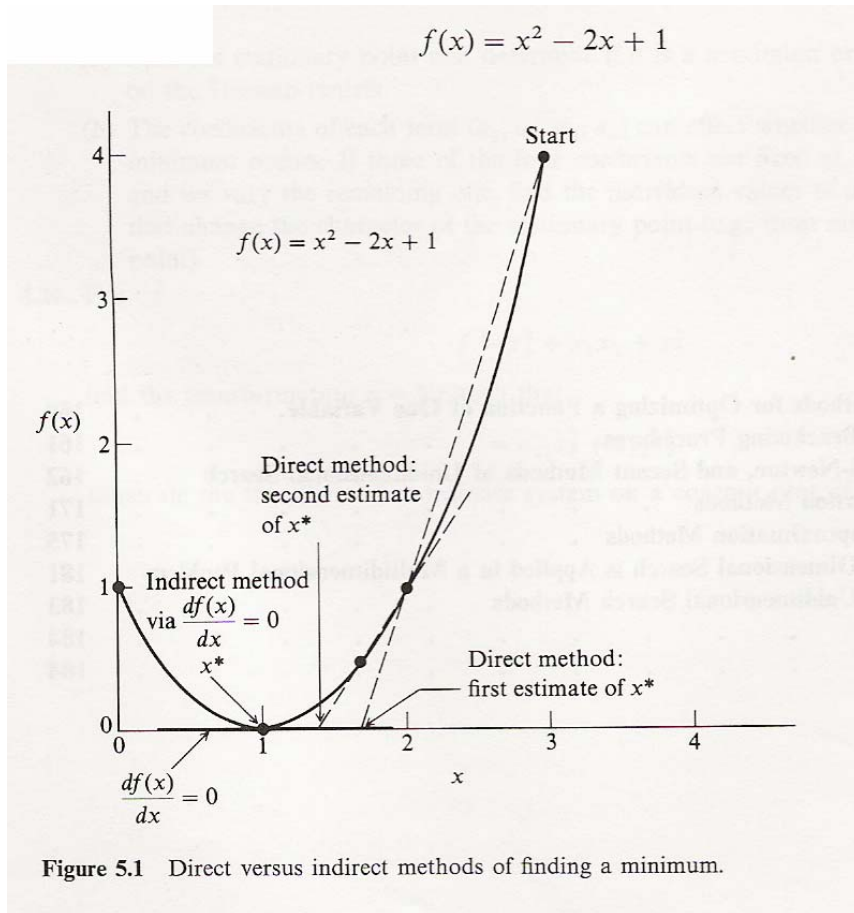


# Optimización de Funciones Irrestringidas



Métodos directos: sólo se usan valores de la función objetivo, se detiene cuando  $f(x^{k+1}) - f(x^k) < \epsilon$

## Métodos Indirectos

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

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

$\vdots$

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

# Método de Newton

$$x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$$

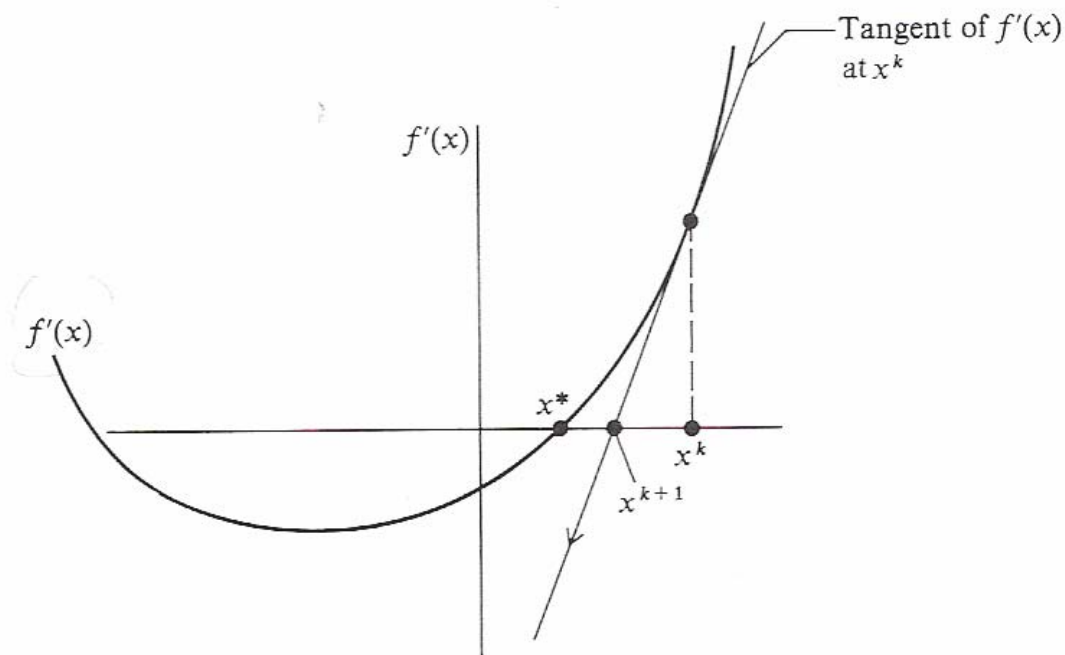


Figure 5.2 Newton's method applied to the solution of  $f'(x) = 0$ .

# Método Quasi Newton

$$x^{k+1} = x^k - \frac{[f(x+h) - f(x-h)]/2h}{[f(x+h) - 2f(x) + f(x-h)]/h^2}$$

# Método de la Secante

$$f'(x^k) + m(x - x^k) = 0$$

$$m = \frac{f'(x^q) - f'(x^p)}{x^q - x^p}$$

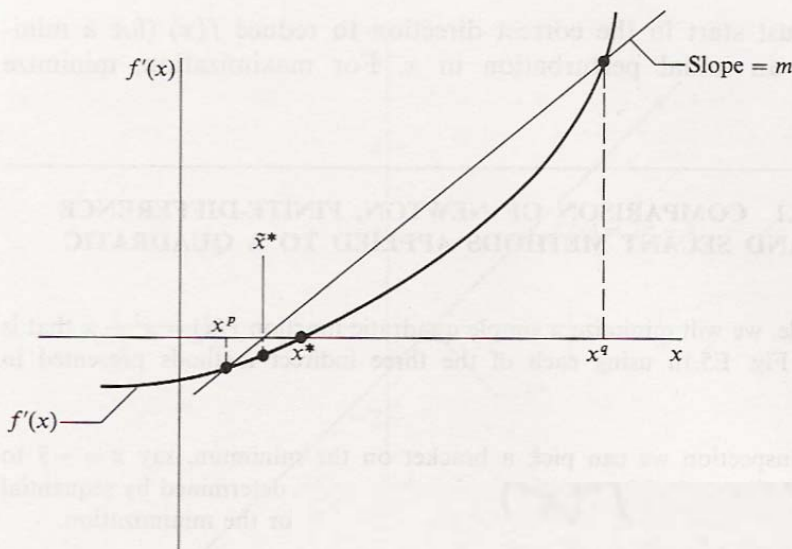
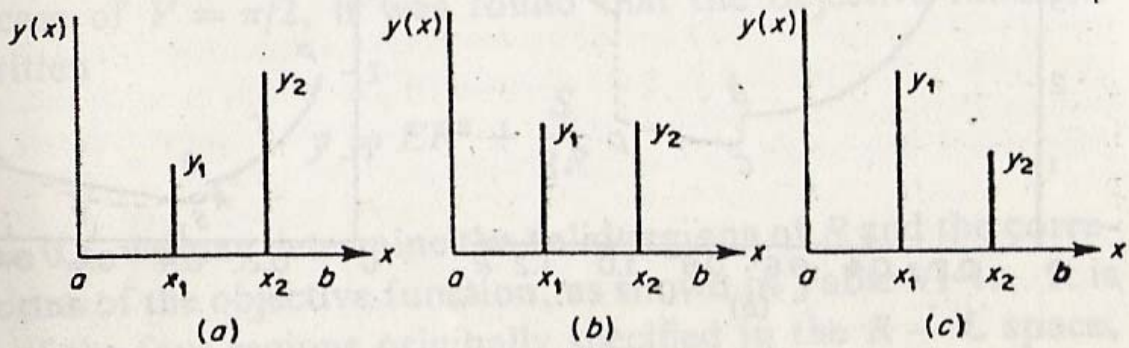


Figure 5.3 Secant method

$$\tilde{x}^* = x^q - \frac{f'(x^q)}{[f'(x^q) - f'(x^p)]/(x^q - x^p)}$$

# Métodos directos ó de eliminación de regiones

Fig. VI-3 Unimodality in numerical search. (a)  $y(x_1) < y(x_2)$ ; (b)  $y(x_1) = y(x_2)$ ; (c)  $y(x_1) > y(x_2)$ .



Funciones Restringidas de una única variable se deben resolver sobre el rango permitido de las variables de la forma

$$x_L \leq x \leq x^L$$

# Método de Búsqueda Preplaneada

$$x_i = a + \frac{i(b-a)}{N+1}$$

where  $i = 1, 2, \dots, N$ .

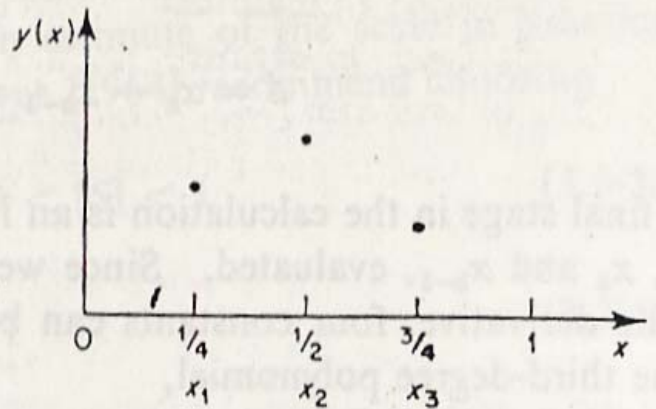


Fig. VI-9 Three-experiment preplanned search.

## Medida de la Efectividad de Búsqueda

$$\alpha = L_N/L_0$$

Sabiendo que  $L_0(1+N)$  es el largo de cada intervalo en el que se dividió  $(a,b)$  inicial

$$\alpha = \frac{L_N}{L_0} = \frac{2}{N+1}$$

$$N \geq \frac{2}{\alpha} - 1 \quad \text{for integer } N$$

# Métodos de Búsqueda Secuencial Uniforme

Se estudia como los resultados de un pequeño conjunto de experimentos influyen en el resultado del próximo conjunto

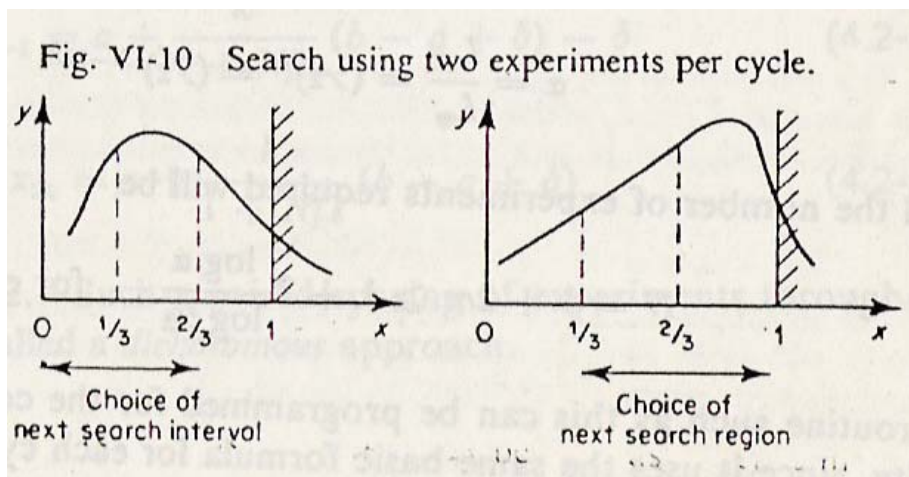
Búsqueda Secuencial con dos experimentos igualmente espaciados por ciclo

$$x_1 = a + \frac{1}{3}L_0 \quad \text{and} \quad x_2 = a + \frac{2}{3}L_0$$

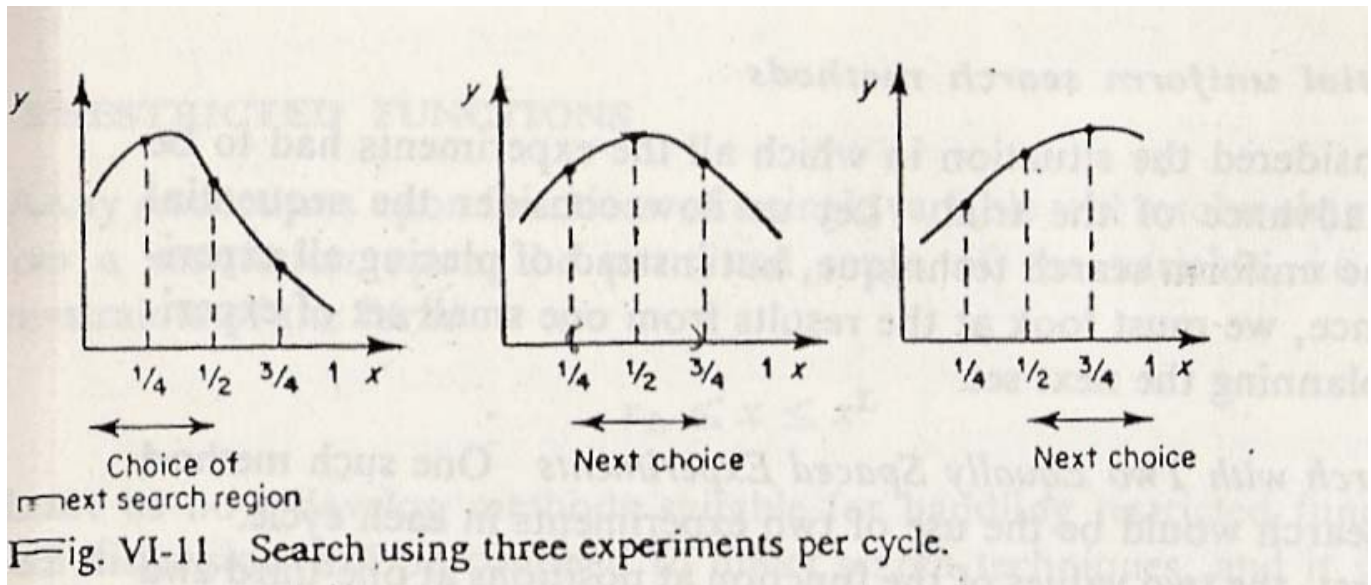
$$L_N = L_{2m} = \left(\frac{2}{3}\right)^m L_0$$

$$\alpha = \frac{L_N}{L_0} = \left(\frac{2}{3}\right)^m = \left(\frac{2}{3}\right)^{N/2}$$

$$N = 2m \geq 2 \frac{\log \alpha}{\log \frac{2}{3}}$$



# Búsqueda Secuencial con Tres experimentos igualmente espaciados por ciclo



$$\alpha = \frac{L_N}{L_0} = \left(\frac{1}{2}\right)^m = \left(\frac{1}{2}\right)^{(N-1)/2}$$

$$N = 1 + 2m \geq 1 + 2 \frac{\log \alpha}{\log \frac{1}{2}}$$

# Búsqueda Secuencial intervalos de medidas irregulares

Búsqueda basada en la Secuencia de los números de Fibonacci

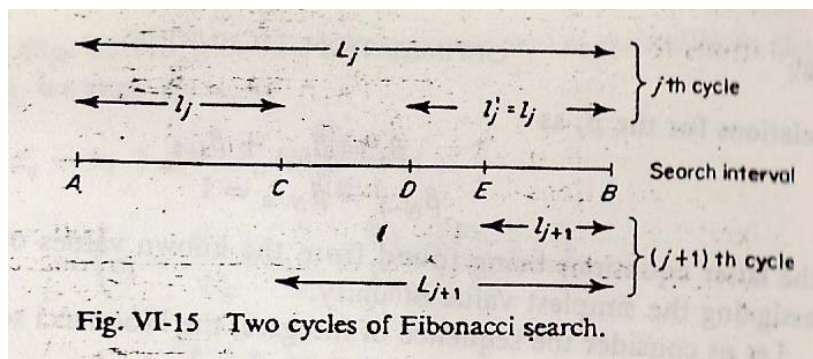


TABLE VI-8 SOME NUMBERS IN THE FIBONACCI SERIES

$n$	$F_n$
0	1
1	1
2	2
3	3
4	5
5	8
6	13
7	21
8	34
9	55
10	89
11	144
12	233
13	377
14	610
15	987
16	1,597
17	2,584
18	4,181
19	6,765
20	10,946



## Step 1 Placing the first two experiments

$$l_1 = \frac{F_{N-2}}{F_N} L_1$$

$$x_1 = a_1 + l_1$$

$$x_2 = b_1 - l_1 = a_1 + L_1 - \left(\frac{F_{N-2}}{F_N}\right)L_1 = a_1 + \frac{F_{N-1}}{F_N} L_1$$

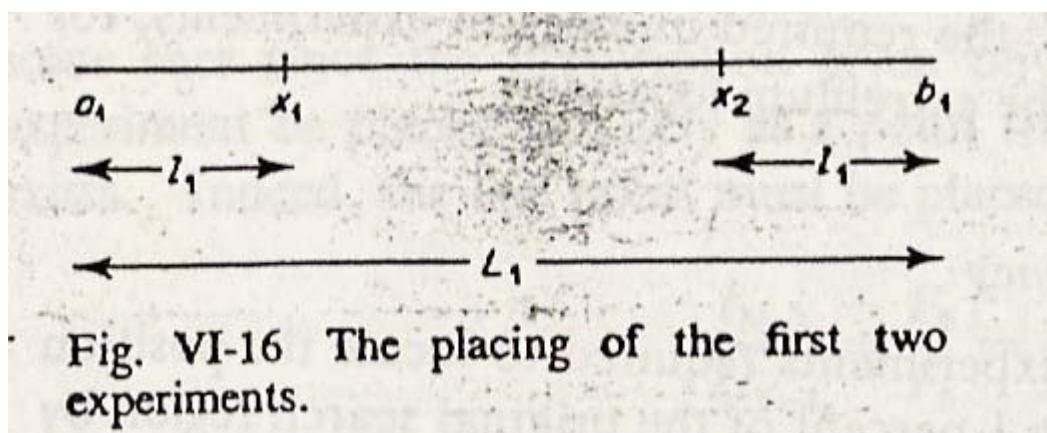


Fig. VI-16 The placing of the first two experiments.

## Step 2 The new subinterval of search

$$L_2 = L_1 - l_1 = b_1 - x_1$$

$$l_k = \frac{F_{N-(k+1)}}{F_{N-(k-1)}} L_k$$

$$L_2 = L_1 - L_1 \frac{F_{N-2}}{F_N} = L_1 \left(1 - \frac{F_{N-2}}{F_N}\right) = L_1 \frac{F_{N-1}}{F_N}$$

**Exactitud de Búsqueda:**

$$\alpha = \frac{1}{F_N}$$

**El experimento final en la búsqueda: F0 / F2=1 / 2**

## Métodos de aproximación polinomial

### Interpolación cuadrática

$$f(x) = a + bx + cx^2$$

$$\tilde{x}^* = -\frac{b}{2c}$$

$$f(x_1) = a + bx_1 + cx_1^2$$

$$f(x_2) = a + bx_2 + cx_2^2$$

$$f(x_3) = a + bx_3 + cx_3^2$$

$$\tilde{x}^* = \frac{1}{2} \left[ \frac{(x_2^2 - x_3^2)f_1 + (x_3^2 - x_1^2)f_2 + (x_1^2 - x_2^2)f_3}{(x_2 - x_3)f_1 + (x_3 - x_1)f_2 + (x_1 - x_2)f_3} \right]$$

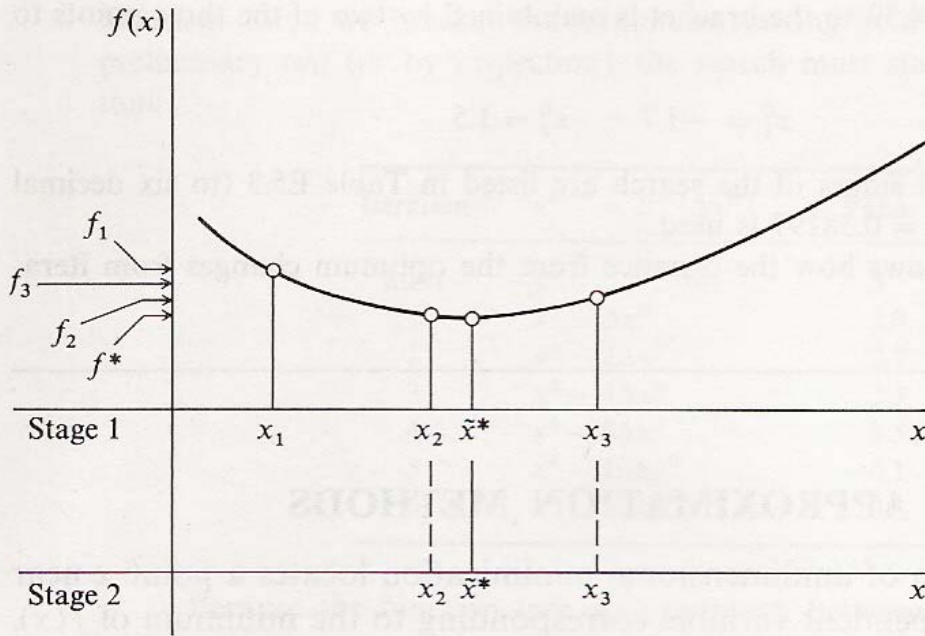


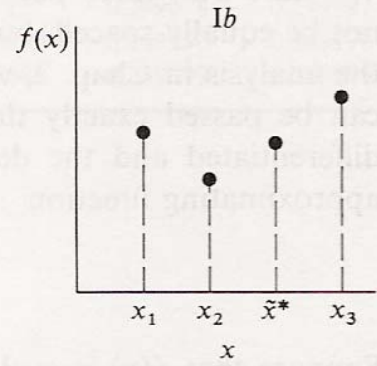
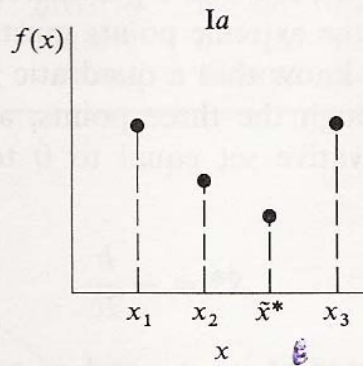
Figure 5.7 Two stages of quadratic interpolation.

I. If  $\tilde{x}^*$  lies between  $x_2$  and  $x_3$ :

(a)  $f^* < f_2$  Pick  $x_2, \tilde{x}^*, x_3$   
 $f^* < f_3$

(b)  $f^* > f_2$  Pick  $x_1, x_2, \tilde{x}^*$   
 $f^* < f_3$

(a)  $f^* > f_2$  Numerical error  
 $f^* > f_3$



II. If  $\tilde{x}^*$  lies between  $x_1$  and  $x_2$ :

(a)  $f^* < f_2$  Pick  $x_1, \tilde{x}^*, x_2$   
 $f^* < f_1$

(b)  $f^* > f_2$  Pick  $\tilde{x}^*, x_2, x_3$   
 $f^* < f_1$

(a)  $f^* > f_2$  Numerical error  
 $f^* > f_1$

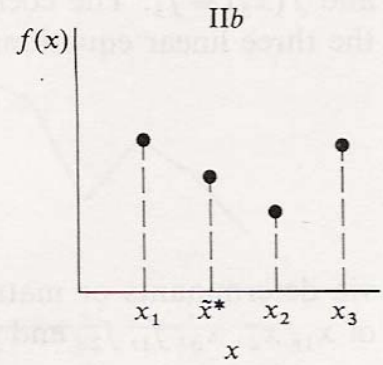
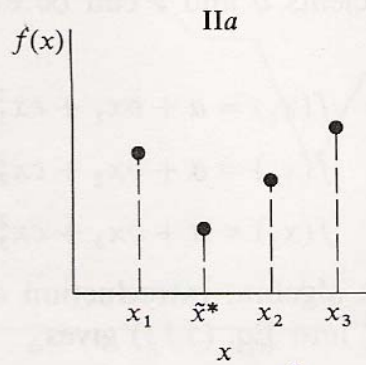


Figure 5.8 How to maintain a bracket on the minimum in quadratic interpolation.

# Interpolación cúbica

$$f(x) = a_1x^3 + a_2x^2 + a_3x + a_4$$

$$\mathbf{X} = \begin{bmatrix} x_1^3 & x_1^2 & x_1 & 1 \\ x_2^3 & x_2^2 & x_2 & 1 \\ x_3^3 & x_3^2 & x_3 & 1 \\ x_4^3 & x_4^2 & x_4 & 1 \end{bmatrix}$$

$$\mathbf{F}^T = [f(x_1) \quad f(x_2) \quad f(x_3) \quad f(x_4)]$$

$$\mathbf{A}^T = [a_1 \quad a_2 \quad a_3 \quad a_4]$$

$$\mathbf{F} = \mathbf{X}\mathbf{A}$$

$$\mathbf{A} = \mathbf{X}^{-1}\mathbf{F}$$

$$\tilde{x}^* = \frac{-2a_2 \pm \sqrt{4a_2^2 - 12a_1a_3}}{6a_1}$$

$$\tilde{x}^* = x_2 - \left[ \frac{f'_2 + w - z}{f'_2 - f'_1 + 2w} \right] (x_2 - x_1)$$

where  $z = 3[f'_1 - f'_2]/[x_2 - x_1] + f'_1 + f'_2$

$$w = [z^2 - f'_1 \cdot f'_2]^{1/2}$$

Para minimización

$$x_1 < x_2, f'_1 < 0, \text{ and } f'_2 > 0$$

## Bibliografía:

- \* Edgar T.F. and Himmelblau D.M.,1988, “Optimization of Chemical Processes”, Mc.Graw Hill.
- \* Beveridge and Schechter, "Optimization: Theory and Practice“, Mac Graw Hill