Numerical methods and optimization

Week 2.

The Fibonacci search

As seen in the case of the golden section method the length of the uncertainty intervals decreases in the same proportion in every step, that is, $L_{k+1} = \alpha L_k$. In the Fibonacci method, the rate of reduction varies stepwise, but the advantageous property of the golden section method consisting of evaluating two functions in the first interval and only one in the remaining intervals, is preserved.

The Fibonacci method is based on the Fibonacci numbers which are defined recursively as follows:

$$\begin{aligned} F_0 &= F_1 = 1, \\ F_k &= F_{k-1} + F_{k-2} \qquad k = 2, 3, \ldots \end{aligned}$$

Some few elements at the beginning of the sequence are: $1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, \ldots$

To begin the method we select a counting number n, which will be used later to determine the number of steps. In the Fibonacci method the number n and the Fibonacci numbers will be used to compute the interior points c_k, d_k of the interval $[a_k, b_k]$:

$$\begin{aligned} c_k &= a_k + \frac{F_{n-k-1}}{F_{n-k+1}} L_k, \\ d_k &= a_k + \frac{F_{n-k}}{F_{n-k+1}} L_k. \end{aligned}$$

When $k = 1$, i.e. in the first interval the denominators of the two intermediate points are both equal to F_n, their numerators consist of the first two Fibonacci numbers that immediately precede F_n. In the remaining steps the indexes of the Fibonacci numbers always decrease by one unit.

Remark

Whether the resulting uncertainty interval is a left-interval or a right-interval, in both cases we have

$$L_{k+1} = \frac{F_{n-k}}{F_{n-k+1}} L_k,$$

and for the lengths of the intervals formally similar relationship can be observed as in the case of Fibonacci numbers

$$L_k = L_{k+1} + L_{k+2}, \qquad k = 1, 2, \ldots, n-3.$$

Whether the resulting uncertainty interval is a left-interval or a right-interval, in both cases one of the point in the new uncertainty interval coincides with one of the interior points in the preceding uncertainty interval, i.e., if the new uncertainty interval is given by

$$[a_{k+1}, b_{k+1}] = [c_k, b_k]\,, \text{ then } d_{k+1} = c_k,$$

if otherwise the new uncertainty interval is given by

$$[a_{k+1}, b_{k+1}] = [a_k, d_k]\,, \text{ then } c_{k+1} = d_k.$$

In the case when $k = n - 1$,

$$c_{n-1} = d_{n-1}.$$

This statement expresses that the algorithm will stop after some step, it is so because the two internal points coincide. In summary, in the Fibonacci method the new uncertainty interval and its interior points can be computed as follows:
If $f(c_k) > f(d_k)$, then the new uncertainty interval

$$\begin{aligned} [a_{k+1}, b_{k+1}] &= [c_k, b_k] \\ c_{k+1} &= d_k \\ d_{k+1} &= a_{k+1} + \frac{F_{n-k}}{F_{n-k+1}} L_{k+1}, \end{aligned}$$

If $f(c_k) \leq f(d_k)$, the new uncertainty interval

$$\begin{aligned} [a_{k+1}, b_{k+1}] &= [a_k, d_k] \\ c_{k+1} &= a_{k+1} + \frac{F_{n-k-1}}{F_{n-k+1}} L_{k+1} \\ d_{k+1} &= c_k, \end{aligned}$$

The Fibonacci search algorithm

INPUT $[a_1, b_1]$ and n

$L_1 = b_1 - a_1$

$c_1 = a_1 + \frac{F_{n-2}}{F_n} L_1$

$d_1 = a_1 + \frac{F_{n-1}}{F_n} L_1$

FOR $k = 1$ TO $n - 1$ DO

  IF $f(c_k) > f(d_k)$

    THEN $a_{k+1} = c_k, b_{k+1} = b_k, L_{k+1} = b_{k+1} - a_{k+1}$

      $c_{k+1} = d_k, d_{k+1} = a_{k+1} + \frac{F_{n-k}}{F_{n-k+1}} L_{k+1}$

    ELSE $a_{k+1} = a_k, b_{k+1} = d_k, L_{k+1} = b_{k+1} - a_{k+1}$

      $c_{k+1} = a_{k+1} + \frac{F_{n-k-1}}{F_{n-k+1}} L_{k+1}, d_{k+1} = c_k$

The procedure makes $k = n - 1$ steps and the minimum point is the common $c_{n-1} = d_{n-1}$ value. In this case the error is at most $L_{n-1}/2$.
It is easy to see the common point is the midpoint of the interval $[a_{n-1}, b_{n-1}]$. The value of n is chosen as follows: In the first step we need two, in the further step we need only one function evaluation. If we require that the error of an approximation of the minimum point at most $\varepsilon > 0$, that is

$$L_{n-1} < 2\varepsilon,$$

then we get n with the following formula: The length of the $k+1$th interval is

$$L_{k+1} = \frac{F_{n-k}}{F_{n-k+1}} L_k = \frac{F_{n-k}}{F_{n-k+1}} \frac{F_{n-k+1}}{F_{n-k+2}} L_{k-1} = \ldots = \frac{F_{n-k}}{F_n} L_1 .$$

Use this with the choice $k = n - 2$ we obtain

$$L_{n-1} = \frac{F_2}{F_n} L_1 = \frac{2}{F_n} L_1,$$

which means that

$$\frac{L_1}{F_n} < \varepsilon.$$

So we can determine the number of steps (using the length of the first interval (L_1) and a tolerance ε) in the following way

$$F_n > \frac{L_1}{\varepsilon}.$$

Example

Determine the minimum point of the function $f(x) = x^2 - 7x + 12$ with Fibonacci search method, if the first uncertainty interval is $[a, b] = [2, 4]$.

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Solution

Let $n = 4$. Then the elements of the Fibonacci sequence what we needed is: $F_0 = F_1 = 1, F_2 = 2, F_3 = 3, F_4 = 5$.
Step 1: The first uncertainty interval is $[a_1, b_1] = [2, 4]$; its length is $L_1 = 2$. The interior points in this step

$$\begin{aligned} c_1 &= a_1 + \frac{F_2}{F_4} L_1 = 2 + \frac{2}{5} \cdot 2 = 2.8, & f(c_1) = 0.24, \\ d_1 &= a_1 + \frac{F_3}{F_4} L_1 = 2 + \frac{3}{5} \cdot 2 = 3.2, & f(d_1) = -0.16. \end{aligned}$$

Solution

Step 2: Since $f(c_1) > f(d_1)$, the uncertainty interval is $[a_2, b_2] = [2.8, 4]$, with length $L_2 = 1.2$. The two interior points and their corresponding function values are as follows. Point c_2 and point d_1 of previous interval are identical.

$$\begin{aligned} c_2 &= d_1 = 3.2 & f(c_2) = -0.16, \\ d_2 &= a_2 + \frac{F_2}{F_3} L_2 = 2.8 + \frac{2}{3} \cdot 1.2 = 3.6, & f(d_2) = -0.24. \end{aligned}$$

Step 3: Since $f(c_2) > f(d_2)$, the new uncertainty interval $[a_3, b_3] = [3.2, 4]$ is of length $L_3 = 0.8$. The two interior points and their corresponding function values are as follows. In this case point c_3 is identical with point d_2 from the previous interval.

$$\begin{aligned} c_3 &= d_2 = 3.6 & f(c_3) = -0.24, \\ d_3 &= a_3 + \frac{F_1}{F_2} L_3 = 3.2 + \frac{1}{2} \cdot 0.8 = 3.6, & f(d_3) = -0.24. \end{aligned}$$

Solution

Step 4: Since $c_3 = d_3$, stop the algorithm. The approximated value of the minimum point can is $x_{\text{min}} \approx 3.6$.

Remark

One can see that the lengths of the uncertainty intervals decrease proportionally with the ratios of the Fibonacci numbers. For example $L_3 = \frac{F_2}{F_3} L_2$.
If the n value arbitrarily chosen, then - as seen - we cannot influence the accuracy. If we want to use the precision tolerances such as $\varepsilon = 0.05$, the value of n should be chosen so to maintain consistency with the relation

$$F_n > \frac{L_1}{\varepsilon}$$

which means in our example that $F_n > \frac{2}{0.05} = 40$. Since $F_9 = 55$ from the Fibonacci we get $n = 9$.

The necessary condition for $f(x)$ to have a minimum of x^* is that $f'(x) = 0$.
The direct root methods seek to find the root (or solution) of the equation, $f'(x) = 0$.
Three root-finding methods:

- the Newton method,
- the quasi-Newton method,
- the secant method

Newton Method

Consider the quadratic approximation of the function $f(x)$ at $x = x_k$ using the Taylor's series expansion:

$$f(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2$$

By setting the derivative of this equation equal to zero for the minimum of $f(x)$, we obtain

$$f'(x) = f'(x_k) + f''(x_k)(x - x_k) = 0$$

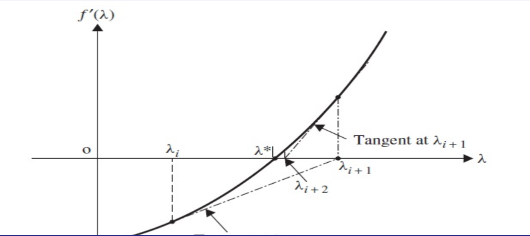
If x_k denotes an approximation to the minimum of $f(x)$, then we get the following approximation:

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

Thus the Newton method is equivalent to using a quadratic approximation for the function $f(x)$ and applying the necessary conditions. The iterative process given by the equation can be assumed to have converged when the derivative, $f'(x_{k+1})$, is close to zero:

$$|f'(x_{k+1})| \leq \varepsilon$$

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

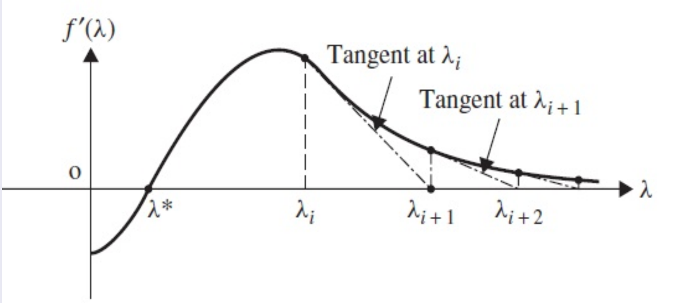


Remarks

- 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.
- The method requires both the first- and second-order derivatives of $f(x)$.
- If $f''(x_k) = 0$ (in the formula), the Newton iterative method has a powerful (fastest) convergence property, known as quadratic convergence.

Remarks

- If the starting point for the iterative process is not close to the true solution x^*, the Newton iterative process might diverge as illustrated in



Example

Find the minimum of the function

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

using the Newton - Raphson method with the starting point $x_1 = 0.1$. Use $\varepsilon = 0.01$ (checking the convergence).

Solution

The first and second derivatives of the function $f(x)$ are given by

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

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

Iteration 1 $x_1 = 0.1, f(x_1) = -0.188197, f'(x_1) = -0.744832, f''(x_1) = 2.68659,$

$$x_2 = x_1 - \frac{f'(x1)}{f''(x_1)} = 0.377241$$

Convergence check: $|f'(x_2)| = |-0.138230| > \varepsilon$.

Solution

Iteration 2:

$f(x_2) = -0.303279, f'(x_2) = -0.138230, f''(x_2) = 1.57296,$

$$x_3 = x_2 - \frac{f'(x_2)}{f''(x_2)} = 0.465119.$$

Convergence check: $|f'(x_3)| = |-0.0179078| > \varepsilon$.

Iteration 3:

$f(x_3) = -0.309881, f'(x_3) = -0.0179078, f''(x_3) = 1.17126$ and

$$x_4 = x_3 - \frac{f'(x_3)}{f''(x_3)} = 0.480409.$$

Convergence check: $|f'(x_4)| = |-0.0005033| < \varepsilon$.
Since the process has converged, the optimum solution is taken as $x^* \approx x_4 = 0.480409$