2.2. INTERPOLATION METHODS

Assume that f is unimodal and continuous everywhere or in the specified interval [a,b].

2.2.1. NEWTON'S METHOD

Let f be twice continuosly differentiable. Function f is approximated by a quadratic function which is the Taylor's polynomial

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

If $f''(x_k) \neq 0$, $\hat{f}$ has a stationary point at x_{k+1} such that

$$\hat{f}'(x_{k+1}) = f'(x_k) + f''(x_k)(x_{k+1} - x_k) = 0$$

which gives the ***Newton's iteration formula***

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

2.2.2. OTHER POLYNOMIAL INTERPOLATION METHODS

Quadratic interpolation without derivatives is a combination of interpolation and bracketing. It is based on three points A < B < C such that f(A) > f(B) < f(C).

1. Find the minimum point x* of the quadratic function i.e. the second order polynomial that passes through the points (A,f(A)), (B,f(B)), (C,f(C)).
2. Carry out the elimination comparing the two values f(x*) and f(B).

The interpolation through the three new points and elimination are repeated until the convergence criteria are fulfilled.

Let the interpolating polynomial be $\hat{f}(x) = c_0 + c_1x + c_2x^2$

The coefficients can be determined by solving the linear equations $\hat{f}(x)=f(x)$, x=A,B,C:
$c_0 + c_1A + c_2A^2 = f(A)$
$c_0 + c_1B + c_2B^2 = f(B)$
$c_0 + c_1C + c_2C^2 = f(C)$.

At the minimum $\hat{f}'(x^*) = c_1 + 2c_2x^* = 0 \Rightarrow x^* = -c_1/(2c_2)$.
Solving the parameters and substituting gives

$$x^* = \frac{f(A)(B^2 - C^2) + f(B)(C^2 - A^2) + f(C)(A^2 - B^2)}{2\ [f(A)(B - C) + f(B)(C - A) + f(C)(A - B)]}$$

Qubic interpolation
A qubic function can be fitted when f and f ' values are known at two points. See the following. Alternatively: values for function or derivative must be given at four points.

Let the minimum be bracketed in the interval [a,b], such that f '(a)<0 and f '(b)>0.

The interpolating polynomial is $\hat{f}(x) = c_0 + c_1x + c_2x^2 + c_3x^3$, and $\hat{f}'(x) = c_1 + 2c_2x + 3c_3x^2$

The four coefficients can be be determined by the linear equations
$c_0 + c_1a + c_2a^2 + c_3a^3 = f(a)$
$c_0 + c_1b + c_2b^2 + c_3b^3 = f(b)$
$c_1 + 2c_2a + 3c_3a^2 = f'(a)$
$c_1 + 2c_2b + 3c_3b^2 = f'(b)$.

The two stationary points of $\hat{f}(x)$ are solved from the equation $\hat{f}'(x) = 0$. One is the minimum and one is the maximum point. The minimum point $\hat{x}^*$ belongs to the interval [a,b].

If $f'(\hat{x}^*) < 0$, set $a:=\hat{x}^*$.
If $f'(\hat{x}^*) > 0$, set $b:=\hat{x}^*$.

Repeat the interpolation until convergence attained.

TESTS OF CONVERGENCE FOR INTERPOLATION METHODS

1) $|x_k - x_{k-1}| < \varepsilon$

2) $|f'(x)| < \varepsilon$

3) $\left|\dfrac{f(x_k) - f(x_{k-1})}{f(x_{k-1})}\right| < \varepsilon$

4) $\left|\dfrac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}\right| < \varepsilon$

5) $\left|\dfrac{\hat{f}(x_k) - f(x_k)}{f(x_k)}\right| < \varepsilon$

6) $\left|\dfrac{f(x_k + \Delta) - f(x_k)}{\Delta}\right| < \varepsilon$

2.2.3. SAFEGUARDED METHODS

The best general methods are based on combining a guaranteed, reliable method (a bracketing method) with a fast-convergent method (like quadratic or cubic interpolation).

When using polynomial interpolation, safeguarding techniques may be needed for situations where the interpolated point lies outside the interval [a,b] or for preventing iterates from being too close to each other or the bounds.