Chapter 11. Numerical Differentiation.

Let a function be given in table

$$y_0\,,\ y_1\,,\ y_2\,,\ \ldots,\ y_n$$

$$x_0\,,\ x_1\,,\ x_2\,,\ \ldots,\ x_n$$

Assume $h = x_{i+1} - x_i = \text{const}$.

$$y'_i = \ ?$$ approximately

It is well known from Mathematical Analysis that

$$f(x_{i+1}) = f(x_i) + f'(x_i)\, h + f''(c)\, h^2/2\,.$$

The same formula using notation y_i **looks :**

$$y_{i+1} = y_i + y'_i\, h + f''(c)\, h^2/2\,,$$

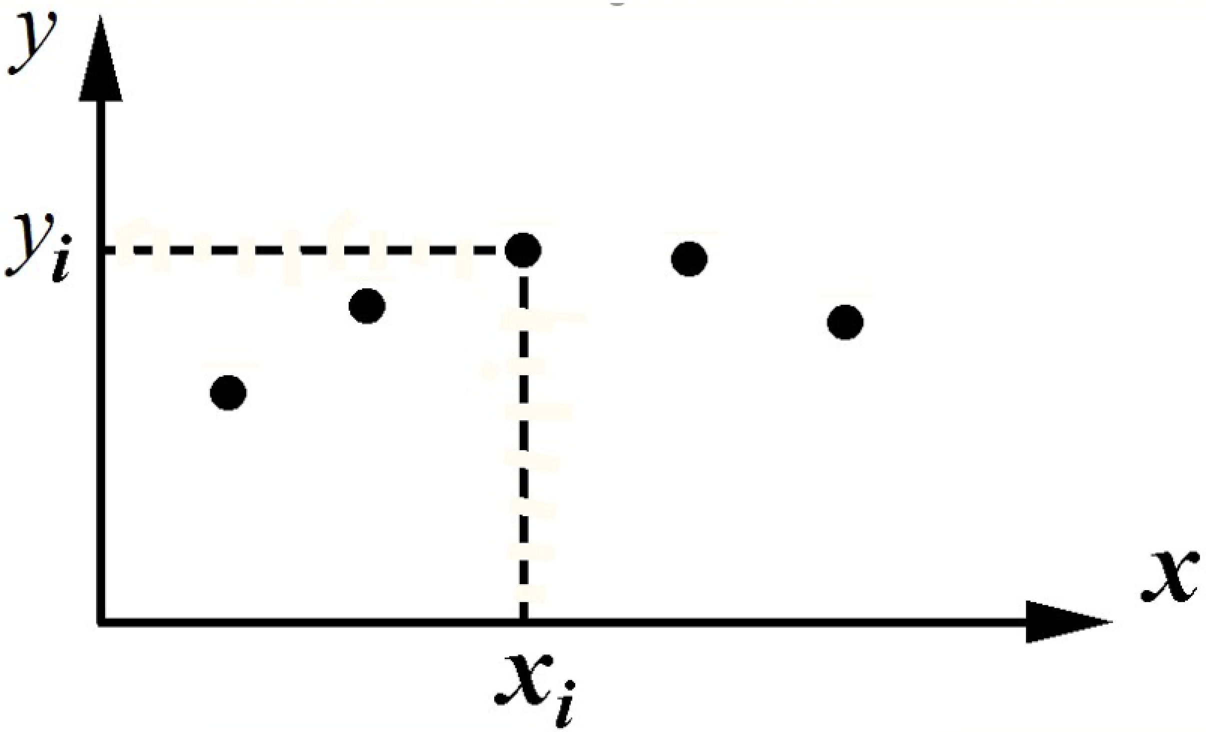
therefore,

$$y'_i = (y_{i+1} - y_i)/\,h - f''(c)\cdot h/2$$

Similarly, for node i and previous node i-1 :

$$y_{i-1} = y_i - y'_i\, h + f''(c)\, h^2/2$$

$$y'_i = (y_i - y_{i-1})/\,h + f''(c)\cdot h/2$$



$y'_i \approx (y_{i+1} - y_i)/h$

forward difference

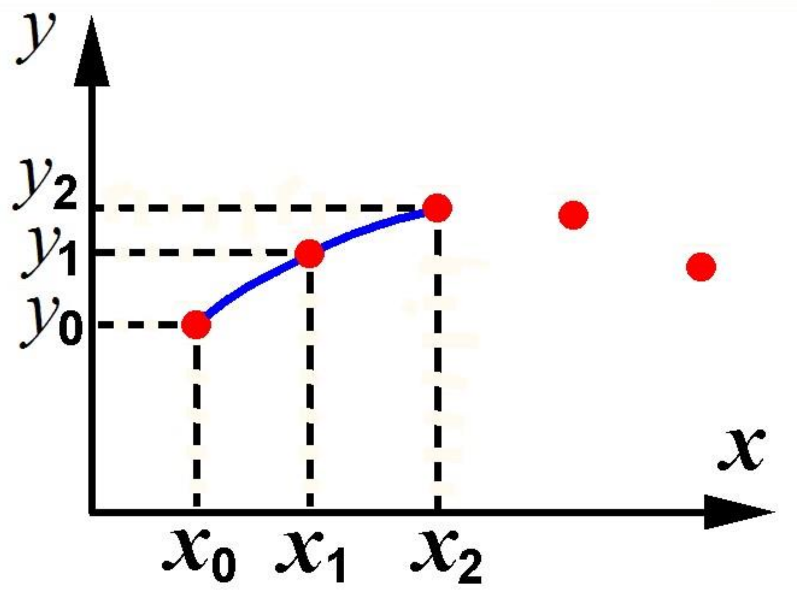
$y'_i \approx (y_i - y_{i-1})/h$

backward difference

These expressions are of first-order accuracy, as the error involves the first degree of h (see previous page).

There exist formulae of higher accuracy for y'_i

Let us derive a formula of second-order accuracy for y'_0 at the left end x_0 of interval $[x_0, x_n]$



To do this, we write Lagrangian's polynomial, that passes through 3 points

$(x_0, y_0) \quad (x_1, y_1) \quad (x_2, y_2)$

$$P(x) = y_0 \, (x - x_1)\,(x - x_2)/\,(2h^2\,) \; -$$

$$- \, y_1 \, (x - x_0)\,(x - x_2)/\,h^2 \; +$$

$$+ \, y_2 \, (x - x_0)\,(x - x_1)/\,(2h^2\,)$$

$$x_{i+1} - x_i = h$$

The derivative of $P(x)$**:**

$$P'(x) = y_0 \, (x - x_1 + x - x_2)/\,(2h^2\,) \; -$$

$$- \, y_1 \, (x - x_0 + x - x_2)/\,h^2 \; +$$

$$+ \, y_2 \, (x - x_0 + x - x_1)/\,(2h^2\,)$$

Now we set $x = x_0$:

$$P'(x_0) = y_0\,(x_0 - x_1 + x_0 - x_2)/\,(2h^2) -$$
$$- y_1\,(\;x_0 - x_2)/\,h^2 +$$
$$+ y_2\,(\;x_0 - x_1)/\,(2h^2)$$

$$= y_0\,(-h\;-2h)/\,(2h^2\,) -$$
$$- y_1\,(\;-2h)/\,h^2 +$$
$$+ y_2\,(\;-h)/\,(2h^2\,)$$

$$= y_0\,(-3)\,/(2h\,) - y_1\,(-2)/\,h + y_2\,(-1)/\,(2h\,)$$

$$= (-3y_0 + 4y_1 - y_2)\,/\,(2h)$$

Thus,

$$y'_0 = f'(x_0) \approx P'(x_0) = (-3y_0 + 4y_1 - y_2)\,/\,(2h)$$

This is formula of the second-order accuracy, as error involves the second degree of h:

$$\boxed{y'_0 = (-3y_0 + 4y_1 - y_2) / (2h) + O(h^2)}$$

Proof. **Theorem of Chapter 5, page 6, says:**

$$f(x) - P(x) = f^{(n+1)}(c) \cdot (x-x_0)(x-x_1) \ldots (x-x_n)/(n+1)!$$

For n=2:

$$f(x) - P(x) = f'''(c) \cdot (x-x_0)(x-x_1)(x-x_2)/3!$$

$$[f(x)-P(x)]'\big|_{x=x0} = f'''(c)\cdot[(x-x_0)(x-x_1)(x-x_2)]'/6\big|_{x=x0}$$

$$= f'''(c)\cdot(x_0-x_1)(x_0-x_2)/6$$

$$= f'''(c)\cdot(-h)(-2h)/6 = f'''(c)\cdot h^2/3$$

For the last node x_n of given segment, in a similar way we obtain:

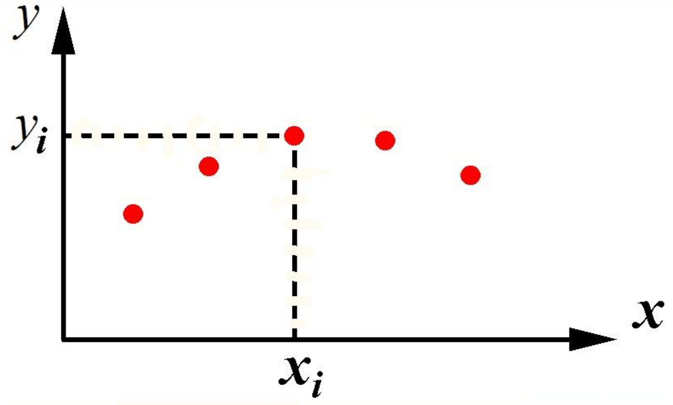
$$\boxed{y'_n = (3y_n - 4y_{n-1} + y_{n-2}) / (2h) + O(h^2)}$$

Second-order accuracy is much better than first-order,

as the error $O(h^2) \rightarrow 0$ much faster than $h \rightarrow 0$

Now let us derive the formula of second-order accuracy for y'_i at inner nodes i=1, 2, . . . , n-1.

Write Lagrange's polynomial that passes 3 points



(x_{i-1}, y_{i-1}) (x_i , y_i) (x_{i+1}, y_{i+1})

$$P(x)= y_{i-1} (x - x_i)(x - x_{i+1})/ (2h^2) +$$
$$+ y_i (x - x_{i-1})(x - x_{i+1})/(-h^2) +$$
$$+ y_{i+1}(x - x_{i-1})(x - x_i)/(2h^2)$$

$$P'(x)= y_{i-1} (x - x_i + x - x_{i+1})/ (2h^2) +$$
$$+ y_i (x - x_{i-1} + x - x_{i+1})/(-h^2) +$$
$$+ y_{i+1}(x - x_{i-1} + x - x_i)/(2h^2) \qquad (*)$$

Setting $x = x_i$, we obtain

$$P'(x_i) = y_{i-1}(-h)/(2h^2) +$$
$$+ y_i(h - h)/(-h^2) +$$
$$+ y_{i+1}(h)/(2h^2)$$

$$P'(x_i) = (y_{i+1} - y_{i-1})/(2h)$$

$$y'_i = f'(x_i) \approx P'(x_i) = (y_{i+1} - y_{i-1})/(2h)$$

Regarding the error:

$$y'_i = f'(x_i) = (y_{i+1} - y_{i-1})/(2h) - f'''(c)\, h^2/6$$

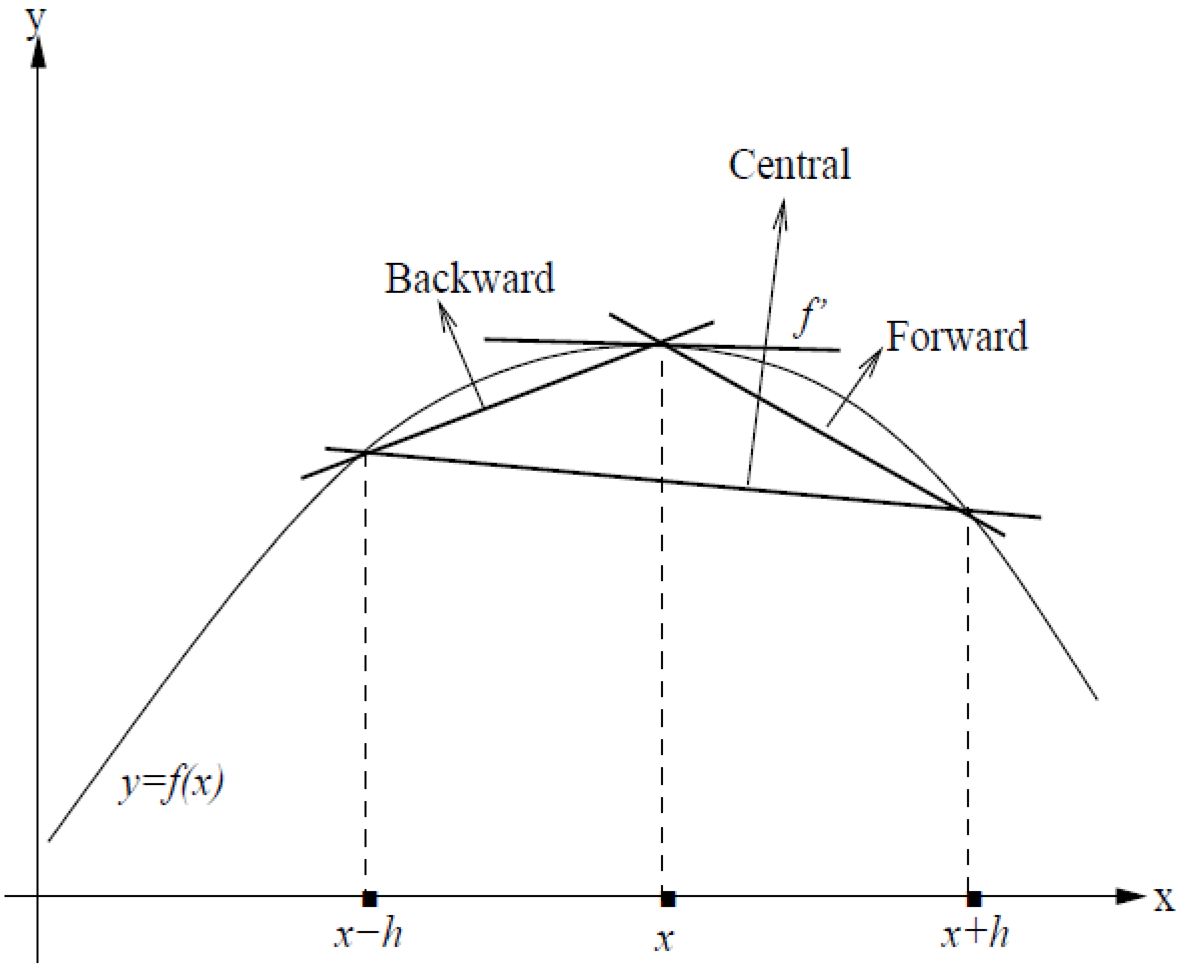
$$\boxed{y'_i = (y_{i+1} - y_{i-1})/(2h) + O(h^2)}$$

Proof:

$$[f(x)-P(x)]'\Big|_{x=x1} = f'''(c)\cdot[(x-x_0)(x-x_1)(x-x_2)]'/6\Big|_{x=x1}$$

$$= f'''(c)\cdot(x_1-x_0)(x_1-x_2)/6$$

$$= f'''(c)\cdot(h)(-h)]/6 = -f'''(c)\cdot h^2/6$$



Geometrical interpretation of difference formulae.

Illustration:

To find the value of derivative of *f(x)=sin x* at *x*=1

we use the three primitive difference formulas

$$f(x-h) = f(0.996094) = 0.839354, \qquad f(x) = f(1) = 0.841471,$$

$$f(x+h) = f(1.003906) = 0.843575.$$

$$h = 0.003906$$

I. Backward difference: $f'(x) = \frac{f(x)-f(x-h)}{h} = 0.541935.$

II. Central Difference: $f'(x) = \frac{f(x+h)-f(x-h)}{2h} = 0.540303.$

III. Forward Difference: $f'(x) = \frac{f(x+h)-f(x)}{h} = 0.538670.$

Note that the exact value is $f'(1) = \cos 1 = 0.540302.$

Formula of 4th-order accuracy for y'_i at inner nodes:

$$y'_i = (y_{i-2} - 8y_{i-1} + 8y_{i+1} - y_{i+2})/(12h) - f^{(5)}(c)h^4/30$$

It can be derived using polynomial of the degree n=4

For <u>second-order derivative</u> y''_i, differentiation of (*) gives at $i=1, 2, \ldots, n-1$:

$$P''(x) = y_{i-1}\,(2)/(2h^2) + $$
$$+\, y_i\,(2)/(-h^2) + $$
$$+\, y_{i+1}(2)/(2h^2) = (y_{i-1} - 2y_i + y_{i+1})/h^2$$

$$y''_i = (y_{i-1} - 2y_i + y_{i+1})/h^2 + f^{(4)}(c)h^2/12$$

(formula of 2nd order accuracy). This will be of use for solving differential equations.

Formula of higher-order accuracy:

$$y''(x_i) = \frac{-y_{i+2} + 16\,y_{i+1} - 30\,y_i + 16\,y_{i-1} - y_{i-2}}{12h^2}$$

Calculation of derivatives with splines

Quadratic splines

$$S(x) = a_i + b_i \cdot (x - x_i) + c_i \cdot (x - x_i)^2$$

at $x_i \le x \le x_{i+1}$, $i = 0, 1, \ldots, n-1$

coefficients a_i , b_i , c_i **are calculated using 3 conditions:**

1) The condition that $S(x)$ equals to given y_i at the left endpoint x_i :

$$S(x_i) = y_i \quad \Rightarrow \quad a_i = y_i \qquad i = 0, 1, \ldots, n-1$$

2)The condition that $S(x)$ equals to given value y_{i+1} at x_{i+1} :

$$S(x_{i+1}) = y_{i+1} \Rightarrow$$

$$\Rightarrow a_i + b_i \cdot (x_{i+1} - x_i) + c_i \cdot (x_{i+1} - x_i)^2 = y_{i+1} \qquad (1)$$

3) The condition that dS/dx is continuous at inner nodes x_{i+1}:

$$dS/dx = b_i + 2c_i \cdot (x - x_i) \qquad at \; x_i \le x \le x_{i+1}$$

$$\downarrow$$

$$b_i + 2c_i \cdot (x_{i+1} - x_i) = b_{i+1} + 2c_{i+1} \cdot (x_{i+1} - x_{i+1})$$

$$\begin{cases} b_i + 2c_i \cdot (x_{i+1} - x_i) = b_{i+1} & (2) \quad i=0, 1, \ldots, n-2 \\ b_i \cdot (x_{i+1} - x_i) + c_i \cdot (x_{i+1} - x_i)^2 = y_{i+1} - y_i & (1) \quad i=0, 1, \ldots, n-1 \end{cases}$$

In fact, coefficients *b_i, c_i* can be calculated <u>sequentially</u> for $i=1,2,\dots,n$:

b_1, c_1,

then b_2 from (1),

then c_2 from (2),

then b_3 from (1), . . .

Therefore $$y'_i \approx dS/dx\big|_{x_i} = b_i$$

Cubic spline

$$S_{cub}(x) = a_i + b_i \cdot (x - x_i) + c_i \cdot (x - x_i)^2 + d_i \cdot (x - x_i)^3$$

$$x_i \le x \le x_{i+1}\ , \qquad i = 0, 1, \ldots, n-1,$$

provides the continuity of both dS_{cub}/dx *and* d^2S_{cub}/dx^2

Coefficients of the spline are calculated using 4 conditions:

1) $S_{cub}(x)$ **is equal to** y_i **at left end of segment**

$$x_i \le x \le x_{i+1} : \qquad y_i = a_i$$

2) $S_{cub}(x)$ **is equal to** y_{i+1} **at right end of the segment**

$$y_{i+1} = a_i + b_i \cdot (x_{i+1} - x_i) + c_i \cdot (x_{i+1} - x_i)^2 + d_i \cdot (x_{i+1} - x_i)^3$$

3) First-order derivative:

$$dS_{cub}/dx = b_i + 2c_i \cdot (x - x_i) + 3d_i \cdot (x - x_i)^2$$

the condition of equal derivatives at the right endpoint:

$$b_i + 2c_i \cdot (x_{i+1} - x_i) + 3d_i \cdot (x_{i+1} - x_i)^2 = b_{i+1}$$

$$i = 1, 2, \ldots, n-1$$

4) Second-order derivative :

$$d^2S_{cub}/dx^2 = 2c_i + 6d_i \cdot (x - x_i)$$

the condition of equal second derivatives at the right endpoint:

$$2c_i + 6d_i \cdot (x_{i+1} - x_i) = 2c_{i+1} \qquad i = 1, 2, \ldots, n-1$$

We have got 2n+2(n-1) equations with respect to 4n coefficients of spline S_{cub} .

We add two conditions $d^2S_{cub}/dx^2 = 0$ at the first and last segments :

$$c_0 = 0, \qquad 2c_{n-1} + 6d_{n-1} \cdot (x_n - x_{n-1}) = 0$$

Therefore, we finally have system of 4n equations for finding 4n coefficients.

After calculation of the coefficients, we can find

$$dS_{cub}/dx = b_i + 2c_i \cdot (x - x_i) + 3d_i \cdot (x - x_i)^2$$

$$y'_i \approx dS_{cub}/dx \Big|_{xi} = b_i$$

$$d^2S_{cub}/dx^2 = 2\,c_i + 6d_i \cdot (x-x_i)$$

$$y''_i \approx d^2S_{cub}/dx^2 \Big|_{xi} = 2\,c_i$$