it makes sense to look for poly of degree ≤ 3 since this forms a 4 dimensional supspace spanned by the monomials $\{1, x, x^2, x^3\}$. However it simplifies life to consider another basis:

$$p(x) = a + b(x-x_0) + c(x-x_0)^2 + d(x-x_0)^2(x-x_1)$$

$$p'(x) = b + 2c(x-x_0) + 2d(x-x_0)(x-x_1) + d(x-x_0)^2$$

Writing interpolation conditions we get:

$$f(x_0) = a$$
$$f'(x_0) = b$$
$$f(x_1) = a + b(x_1-x_0) + c(x_1-x_0)^2$$
$$f'(x_1) = b + 2c(x_1-x_0) + d(x_1-x_0)^2$$

a, b easy to get. Then c follows and then d
→ problem is solvable for any prescribe values of $f(x_i), f'(x_i)$.

However the general problem where some derivatives are missing doesn't need to be solvable and is called Birkhoff interp.
Here is an example of the possible subtleties one can encounter.

Example: Find a polyn s.t. $p(0)=0,\ p'(\frac{1}{2})=2,\ p(1)=1$.

Three conditions ⇒ natural choice is:

$$p(x) = a + bx + cx^2,\quad p'(x) = b + 2cx$$

$p(0)=0 \Rightarrow a=0$ other conditions become: $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} b \\ c \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$

singular matrix

Try cubic:

$p(x) = a + bx + cx^2 + dx^3$ we get $a = 0$

$p'(x) = b + 2cx + 3dx^2$

and equations become:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & \frac{3}{4} \end{bmatrix} \begin{bmatrix} b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

which has infinitely many sol:

$$\begin{pmatrix} b \\ c \\ d \end{pmatrix} = \begin{bmatrix} -4 \\ 5 \\ 0 \end{bmatrix} + \underset{\text{some const.}}{k} \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}$$

Hermite interpolation conditions (which give uniquely solvable problems)

$$\boxed{(HiC) \quad p^{(j)}(x_i) = c_{ij} \quad \text{for } 0 \le j \le k_i - 1, \quad 0 \le i \le m}$$

how many conditions do we have in total?

$$k_1 + k_2 + k_3 + \dots + k_m = m+1$$

↓ degree of poly we will use to interpolate.

note: # of derivatives can vary from node to node. However if a derivative is known at a node all previous (lower order) derivatives need to be known as well.

Theorem (on Hermite interp) There is a unique poly of degree $\le m = k_1 + k_2 + \dots + k_m - 1$ satisfying (HiC).

<u>proof</u>: Assume there are two polynomials p, q of degree $\leq m$ satisfying (HiC). We will show that $p \equiv q$, i.e. that (HiC) uniquely determines a poly of degree $\leq m$.

Let $r(x) = p(x) - q(x)$, by (HiC):

$$r^{(j)}(x_i) = 0 \qquad \text{for } i = 0, \ldots, n \text{ and } j = 0, \ldots, k_i - 1$$

This means x_i is a zero of multiplicity k_i of r; which gives us a total of $k_1 + k_2 + \cdots + k_n = m+1$ zeros.

Since $r(x)$ is poly of degree $\leq m$ with $m+1$ zeros:

$r \equiv 0$ and $p \equiv q$. QED.

<u>Example</u>: what if we did Hermite interp at only one node?

$$p^{(j)}(x_0) = c_{0j} \quad , \; j = 0, 1, \ldots, k$$

$$p(x) = \underline{\text{Taylor poly of degree } k}$$

$$= c_{00} + c_{01}(x - x_0) + \frac{c_{02}}{2!}(x - x_0)^2 + \cdots + \frac{c_{0k}}{k!}(x - x_0)^k$$

Hermite interpolation using Newton divided differences

First a simple example:

(HIC): $p(x_0) = c_{00}$, $p'(x_0) = c_{01}$, $p(x_1) = c_{10}$

(Hermite interp poly will be a quadratic)

x_0	c_{00}	c_{01}	?
x_0	c_{01}	?	
x_1	c_{10}		

why do we say $f[x_0, x_0] \overset{?}{\equiv} f'(x_0)$

well recall:

$$f[x_0, x] = \frac{f(x) - f(x_0)}{x - x_0}$$

Thus. $\lim_{x \to x_0} f[x_0, x] = f'(x_0)$

$\leadsto$ Hermite conditions give entries in divided difference Table.
a node is repeated as many times as there are deriv. specified.

Back to example we started with:

$p(x_0) = f(x_0)$ and $p(x_1) = f(x_1)$
$p'(x_0) = f'(x_0)$ $\qquad$ $p'(x_1) = f'(x_1)$

we can write table:

x_0	$f(x_0)$	$f'(x_0)$	$f[x_0\, x_0\, x_1]$	$f[x_0\, x_0\, x_1\, x_1]$
x_0	$f(x_0)$	$f[x_0, x_1]$	$f[x_0\, x_1\, x_1]$	
x_1	$f(x_1)$	$f'(x_1)$		
x_1	$f(x_1)$			

and

$$p(x) = f(x_0) + f'(x_0)(x - x_0) + f[x_0\, x_0\, x_1](x - x_0)^2$$
$$+ f[x_0\, x_0\, x_1\, x_1](x - x_0)^2 (x - x_1)$$

(by reading first row)

How to interpret divided differences with more than 2 repetitions?

Recall last theorem of interp section:

$$f[x_0, x_1, x_2, \dots x_n] = \frac{f^{(n)}(\xi)}{n!}$$

where the ξ lies in same interval containing $x_0, \dots x_n$.

Now shrink interval to a single point (x_0):

$$\boxed{f[\underbrace{x_0, x_0, \dots, x_0}_{n+1 \text{ times}}] = \frac{f^{(n)}}{n!}(x_0).}$$

Example:

x	1	2
$P(x)$	2	6
$P'(x)$	3	7
$P''(x)$		8

$$\begin{array}{cc|cccc} 1 & 2 & 3 & ? & ? & ? \\ 1 & 2 & ? & ? & ? & \\ 2 & 6 & 7 & 4 & & \\ 2 & 6 & 7 & & & \\ 2 & 6 & & & & \end{array} \longrightarrow \text{why?}$$

Calculating missing entries gives:

$$\begin{array}{cc|cccc} 1 & 2 & 3 & 1 & 2 & -1 \\ 1 & 2 & 4 & 3 & 1 & \\ 2 & 6 & 7 & 4 & & \\ 2 & 6 & 7 & & & \\ 2 & 6 & & & & \end{array}$$

Thus the interp poly is:

$$p(x) = 2 + 3(x-1) + 1\cdot(x-1)^2 + 2(x-1)^2(x-2)$$
$$- 1\cdot(x-1)^2(x-2)^2$$

Divided differences with repetitions:

Def interpolation with repeated nodes

We say f interpolates 0 at $x_0, x_1, \dots, x_n$ if $f^{(k-1)}(\xi) = 0$ for each point that occurs k or more times in the list $x_0, x_1, \dots x_n$.

Example: f interpolates 0 at the points $1, 3, 4, 1, 3, 1, 10$ if:

$$f(1) = f'(1) = f''(1) = 0$$
$$f(3) = f'(3) = 0$$
$$f(4) = 0$$
$$f(10) = 0$$

Note: p interpolates 0 at $x_0, x_1, \dots, x_n$ iff

$$p(x) = \prod_{j=0}^{n} (x - x_j) \underbrace{r(x)}_{\text{poly}}.$$

Def: f interp. g at $x_0, \dots x_n$ if $f - g$ interp. 0 at $x_0 \dots x_n$.

We can rephrase the theorem on uniqueness of interpolation to nodes with repetition as follows:

Theorem: Let $x_0, x_1, \dots, x_m$ be a list of points with no element repeated more than k times, and let f be a $C^{k-1}[a,b]$ function ($[a,b]$ contains points). Then there is a unique polynomial of degree $\le m$ interpolating f at $x_0, x_1 \dots x_m$.

Note: $f[x_0, x_1, \dots, x_n] \equiv$ coeff of x^n in poly of degree $\le n$ interp f at $x_0, x_1, \dots, x_n$.
if ξ appears k times in list then $f^{(k-1)}(\xi)$ must exist. if not then divided difference does not exist.

Theorem (General Newton interp poly)

If f is sufficiently diff'ble so that divided differences below exist then the unique poly of degree $\le n$ interp. f at $x_0, x_1, \dots, x_n$ (allowing repetitions) is given by:

$$p(x) = \sum_{j=0}^{n} f[x_0, x_1, \dots, x_j] \prod_{i=0}^{j-1} (x - x_i)$$

(by convention: $\prod_{i=0}^{-1} (x - x_i) = 1$.)

proof: by induction

$n=0$: $f[x_0]$ is constant poly interp f at x_0

Induction hypothesis: assume

$$q(x) = \sum_{j=0}^{n-1} f[x_0\, x_1 \dots x_j] \prod_{i=0}^{j-1} (x - x_i)$$

interpolates f at node $x_0, x_1, \dots x_{n-1}$ (i.e. theorem is true for $n-1$ nodes)

Let $p(x)$ be poly interp f at $x_0, \dots, x_n$. We know such poly exists and is unique. By def of div. diff:

$$f[x_0\, x_1 \dots x_n] = \text{coeff in front of } x^n \text{ in } p$$

Therefore:

$$r(x) = p(x) - f[x_0, \dots, x_n] \prod_{i=0}^{n-1} (x - x_i)$$

is of degree $\le n-1$

and it interpolates f at the nodes $x_0, x_1, \dots x_{n-1}$. (why?)

$$\Rightarrow \quad q(x) = p(x) - f[x_0, \dots, x_n] \prod_{i=0}^{n-1} (x - x_i)$$

$$\Rightarrow \quad p(x) = \sum_{i=0}^{n} f[x_0, \dots, x_i] \prod_{j=0}^{i-1} (x - x_j) \qquad \text{QED.}$$

<u>Question</u>: Assume wlog that $x_0 \le x_1 \le \dots \le x_n$. Do we have a formula like:

$$f[x_0, x_1, \dots x_n] = \frac{f[x_1, \dots, x_n] - f[x_0, x_1 \dots x_{n-1}]}{x_n - x_0} \,?$$

when repetitions are allowed?

obviously there is a problem with $x_n = x_0$ but then:

$$f[\underbrace{x_0, x_0, \dots x_0}_{n+1 \text{ times}}] = \frac{1}{n!} f^{(n)}(x_0)$$

Thus we get the theorem (stated w/o proof here)

<u>Thm (recursive formula for divided differences)</u>

Let $x_0 \le x_1 \le \dots \le x_n$. Then

$$f[x_0\, x_1 \dots x_n] = \begin{cases} \dfrac{f[x_1\, x_2 \dots x_n] - f[x_0, \dots, x_{n-1}]}{x_n - x_0} & \text{if } x_n \ne x_0 \\[2ex] \dfrac{1}{n!} f^{(n)}(x_0) & \text{if } x_n = x_0 \end{cases}$$

<u>note</u>: ordering of nodes is here only to simplify test "all nodes are the same".

§3.4 Cubic Spline interpolation

Big problems with polynomial interpolation: can come when we increase the number of points or the degree of the interpolating polynomial:

- the higher the degree of a polynomial, the more oscillatory it is (in general)
- the interpolation error depends on $n+1$-th derivative of function. so in order for poly interp to work well we need a very smooth underlying function, which is not always the case

Splines $\equiv$ piecewise polynomial interp: i.e. we subdivide interval in many subintervals and interpolate w/ polynomial inside each subinterval, enforcing some continuity conditions.

A spline of degree k having $n+1$ distinct knots (=nodes) $x_0, x_1, \dots, x_n$ is a function $S(x)$ s.t.

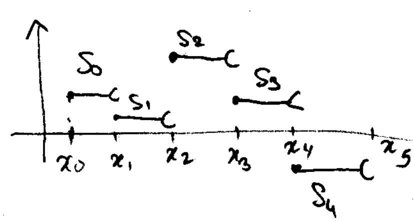
i) On $[x_{i-1}, x_i)$, S is a polynomial of degree $< k$.

ii) S has continuous $k-1$ derivatives on $[x_0, x_n]$.

Examples:

Spline of degree 0: piecewise constant

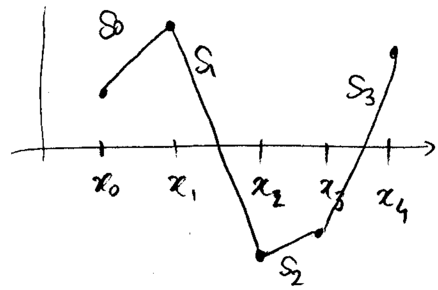
$$S(x) = \begin{cases} S_0(x) = c_0 & x \in [x_0, x_1) \\ S_1(x) = c_1 & x \in [x_1, x_2) \\ \vdots & \\ S_{n-1}(x) = c_{n-1} & x \in [x_{n-1}, x_n) \end{cases}$$



Spline of degree 1:

$$S(x) = \begin{cases} S_0(x) = a_0 x + b_0 & [x_0, x_1] \\ S_1(x) = a_1 x + b_1 & [x_1, x_2] \\ \vdots & \vdots \\ S_{n-1}(x) = a_{n-1}x + b_{n-1} & [x_{n-1}, x_n] \end{cases}$$

piecewise linear interp



Spline of degree 2? Can construct quadratics on each subinterval s.t. values match, however there are not enough degrees of freedom to enforce continuity of S' at the knots.

cubic splines: are the most commonly used spline and are "optimal" in a sense we shall see later. Assume we are given a table:

x	x_0 x_1 $x_2 \cdots x_n$	← knots
y	y_0 y_1 $y_2 \cdots y_n$	← values at knots.

On each subinterval $[x_i, x_{i+1}]$, $S(x) \equiv$ cubic function $S_i(x)$:

$$S(x) = \begin{cases} S_0(x) & x \in [t_0, t_1] \\ S_1(x) & x \in [t_1, t_2] \\ \vdots & \\ S_{n-1}(x) & x \in [t_{n-1}, t_n] \end{cases}$$

with the conditions:

i) $S_j(x_j) = y_j$ and $S_j(x_{j+1}) = y_{j+1}$, $j = 0, \ldots, n-1$

ii) $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$, $j = 0 \ldots n-2$

iii) $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$, $j = 0 \ldots n-2$

or in words:

i) ≡ continuity at the knots = $2n$ conditions
(2 per subinterval)

ii) ≡ continuity of derivatives at all internal knots ≡ $n-1$ conditions

iii) ≡ ——— second deriv. ——— ≡ $n-1$ conditions

TOTAL = $4n-2$ equations

unknowns = $4 \times n$ (since a cubic per interval can be def using four parameters).

→ we need 2 more conditions, which are usually specified by:

a) $S''(x_0) = S''(x_n) = 0$ ≡ free or natural boundary

b) $S'(x_0) = f'(x_0)$, $S'(x_n) = f'(x_n)$ ≡ clamped boundary.

"Spline" is actually a term used in shipyards for thin wood strips that were used to draw the shape of the hull.

- Condition a) gives the shape of a strip of wood constrained to passing through certain points and left free at the ends.
- condition b) means the spline is clamped at its end points. (but requires knowledge of derivative of function, i.e. strip direction is known at end points).

Spline construction

$$S_j(x) = a_j + b_j(x-x_j) + c_j(x-x_j)^2 + d_j(x-x_j)^3$$

$j=0 \dots n-1$.

function values (condi)

$$\boxed{S_j(x_j) = a_j = y_j} \quad j=0 \dots n-1$$

We also need $S_j(x_{j+1}) = y_{j+1}$, $j = 0..n-1$ ie.

$$\boxed{a_j + b_j h_j + c_j h_j^2 + d_j h_j^3 = y_{j+1}} \quad j = 0..n-1 \quad (*)$$

where $h_j \equiv x_{j+1} - x_j$ to simplify notation.

derivatives (cond ii)

$$S_j'(x) = b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2$$

$$S_j'(x_{j+1}) = S_{j+1}'(x_{j+1}), \quad j = 0, .. n-2.$$

$$\Leftrightarrow \boxed{b_{j+1} = b_j + 2c_j h_j + 3d_j h_j^2} \quad j = 0.. n-2 \quad (**)$$

second derivatives (cond iii)

$$S_j''(x) = 2c_j + 6d_j(x - x_j)$$

$$S_j''(x_{j+1}) = S_{j+1}''(x_{j+1}), \quad j = 0, .., n-2$$

$$\Leftrightarrow \boxed{2c_{j+1} = 2c_j + 6d_j h_j} \quad (**')$$

Solving for d_j we get: $\boxed{d_j = \frac{1}{3h_j}(c_{j+1} - c_j)}$ replacing in $(*)$ and $(**)$

$$\Rightarrow \begin{cases} a_j + b_j h_j + \frac{h_j^2}{3}(2c_j + c_{j+1}) = a_{j+1} & (1) \\ b_j + h_j(c_j + c_{j+1}) = b_{j+1} & (2) \end{cases}$$

Solving for b_j in (1):

$$b_j = \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}) \qquad (3)$$

for $j = 0, \dots, n-1$

replacing in (2):

$$\frac{1}{h_{j+1}}(a_{j+2} - a_{j+1}) - \frac{h_{j+1}}{3}(2c_{j+1} + c_{j+2}) = \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1})$$
$$- h_j(c_j + c_{j+1})$$

$$h_j c_j + 2(h_j + h_{j+1})c_{j+1} + h_{j+1} c_{j+2} = \frac{3}{h_{j+1}}(a_{j+2} - a_{j+1}) - \frac{3}{h_j}(a_{j+1} - a_j)$$

$j = 0, \dots, n-2$

These are $n-1$ equations for $n+1$ unknowns $c_0, c_1, \dots c_n$.
If we use for simplicity natural boundary conditions:

$$S''(x_0) = 2c_0 = 0 \; ; \; S''(x_n) = 2c_n = 0$$

$\rightsquigarrow$ get additional eq: $\boxed{c_0 = c_n = 0}$.

Algorithm:

- Input $x_0, \dots x_n$; $y_0, \dots, y_n$.
- Build matrix A (see below) and rhs.
- Solve linear system $Ax = b$, $x = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix}$
- a_j are given by y_j
- b_j ——— (3)
- d_j ——— (**')

Here: $x = \begin{bmatrix} c_0 \\ \vdots \\ c_n \end{bmatrix}$ $\quad b = \begin{bmatrix} 0 \\ \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}) \\ 0 \end{bmatrix}$

$$A = \begin{bmatrix} 1 & 0 & 0 & & & & \\ h_0 & 2(h_0+h_1) & h_1 & & & & \\ & h_1 & 2(h_1+h_2) & h_2 & & & \\ & & h_2 & 2(h_2+h_3) & h_3 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & h_{n-2} & 2(h_{n-2}+h_{n-1}) & h_{n-1} \\ & & & & 0 & 0 & 1 \end{bmatrix}$$

first and last line force $c_0 = c_n = 0$. Book: uses special purpose linear system solving algorithm for tridiagonal matrices. Also system can be shown to be solvable.

Moreover cubic splines are the smoothest possible as is shown by:

Theorem (optimality of natural cubic splines)

Let f'' be continuous on $[a, b]$ and let $a = x_0 < x_1 < \dots < x_n = b$.

If S is the natural spline interp f at the nodes $x_0, x_1 \dots x_n$ then

$$\int_a^b (S''(t))^2 dt \leq \int_a^b (f''(x))^2 dx$$

This theorem means cubic splines are the curves passing through knots that have the smallest second derivatives.

Physical interpretation: "spline" or thin strip of wood is at equilibrium when its elastic energy is minimum.

Mathematical interpretation:

recall curvature $= \dfrac{|f''(x)|}{(1+(f'(x))^2)^{3/2}} \sim |f''(x)|$

spline = curve with minimal curvature passing through knots.

We can now prove theorem:

proof: Let $g = f - S$ then $g(x_i) = 0$, $i = 0, 1, \dots, n$.

$$\int_a^b (f'')^2 dx = \int_a^b (g'')^2 dx + \int_a^b (S'')^2 dx + 2\int_a^b g'' S'' \, dx.$$

all we need to show is that $\int_a^b g'' S'' \geq 0$.

$$\int_a^b g'' S'' = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} S'' g'' \, dx \qquad \text{(chopping integral)}$$

$$\stackrel{IBP}{=} \sum_{i=1}^{n} \left\{ S'' g' \Big|_{x_{i-1}}^{x_i} - \int_{x_{i-1}}^{x_i} S''' g' \, dx \right\}$$

telescoping sum

$$\stackrel{?}{=} S''(\underset{b}{\underset{\parallel}{x_n}}) g'(\underset{b}{\underset{\parallel}{x_n}}) - S''(\underset{a}{\underset{\parallel}{x_0}}) g'(\underset{a}{\underset{\parallel}{x_0}})$$

$$- \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} \boxed{S'''} g' \, dx$$

constant since S = cubic

because of natural bdry conditions

$$= 0 - \sum_{i=1}^{n} c_i \int_{x_{i-1}}^{x_i} g' \, dx$$

$$= - \sum_{i=1}^{n} c_i \big(\underbrace{g(x_i) - g(x_{i-1})}_{=0}\big)$$

$$= 0.$$

QED

CHAPTER 4 NUMERICAL DIFFERENTIATION AND INTEGRATION

Idea: if we only have pointwise values of a function, we can approximate its derivative (and integral) by using the derivative (or integral) of its polynomial interpolant. Of course if polynomial interpolant is not a good approx between nodes, then our approx derivative (or integral) will not be very good.

§4.1 NUMERICAL DIFFERENTIATION

Recall Taylor's theorem:

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(\xi).$$

where ξ is between x and $x+h$.

This gives us a way of approximating derivative since.

$$(*) \quad \boxed{f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi).}$$

- Forward difference: if $h > 0$
- Backward ——— : if $h < 0$

error should decay as $h \to 0$

the function better be differentiable two times!

Formula $(*)$ was obtained by truncating Taylor's expansion; the truncation error is the term $-\frac{h}{2} f''(\xi)$

A better formula is given by looking at Taylor's theorem:

(1) $$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f^{(3)}(\xi_1)$$

(2) $$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f^{(3)}(\xi_2)$$

(1) - (2):

(* *) $$\boxed{f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \frac{h^2}{12}\left[f^{(3)}(\xi_1) + f^{(3)}(\xi_2)\right]}$$

Better behaved error term but requires more smoothness of f.

To simplify the error term assume $f^{(3)}$ is continuous over $[x-h, x+h]$

$$\min_{t\in[x-h,x+h]} f^{(3)}(t) \leq C = \frac{f^{(3)}(\xi_1) + f^{(3)}(\xi_2)}{2} \leq \max_{t\in[x-h,x+h]} f^{(3)}(t)$$

Therefore by intermediate value theorem, there is some $\xi \in [x-h, x+h]$ s.t.

$$f^{(3)}(\xi) = C.$$

Thus (**) becomes:

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \frac{h^2}{6} f^{(3)}(\xi).$$

Another useful formula can be obtained by (1) + (2) and adding $\frac{h^4}{4!}$ term. In this case:

(***) $$\boxed{f''(x) = \frac{1}{h^2}\left[f(x+h) - 2f(x) + f(x-h)\right] - \frac{h^2}{12} f^{(4)}(\xi)}$$

where $\xi \in (x-h, x+h)$.

we have used same trick as before to simplify error term

(*) (**) and (***) are probably the most used differentiation formulas, and we will use them repeatedly when dealing with ODEs.