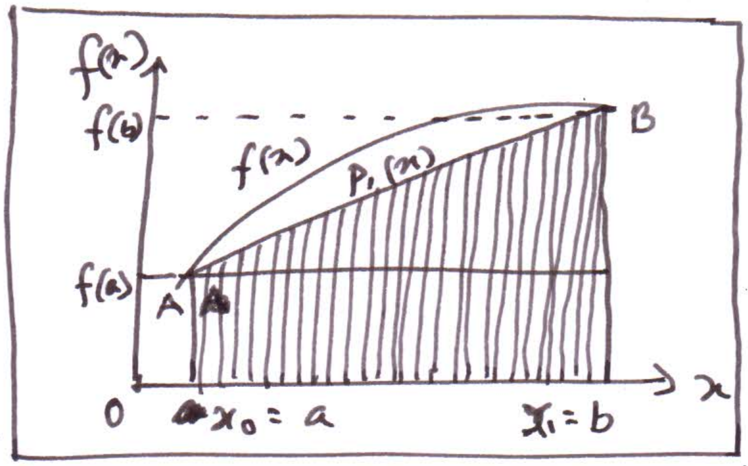
NUMERICAL INTEGRATION AND DIFFERENTIATION

Numerical Integration: Trapezoidal Rule

$$\boxed{\mathcal{I} = \int_a^b f(x)\,dx}$$



Replace $f(x)$ by an approximating function.

A linear interpolating approximation gives,

$$\boxed{P_1(x) = \frac{y_0(x-x_1)}{(x_0-x_1)} + \frac{y_1(x-x_0)}{(x_1-x_0)} = \frac{y_0(x_1-x)+y_1(x-x_0)}{x_1-x_0}}$$

Now $x_0 = a$, $x_1 = b$, $y_0 = f(a)$, $y_1 = f(b)$.

$$\therefore \boxed{P_1(x) = \frac{f(a)(b-x) + f(b)(x-a)}{b-a}}$$

Now replace $f(x)$ with $P_1(x)$.

$$\therefore \boxed{\mathcal{I} = \int_a^b f(x)\,dx \simeq \int_a^b P_1(x)\,dx = T_1(f).}$$

$$\Rightarrow T_1(f) = \frac{f(a)}{b-a}\int_a^b (b-x)\,dx + \frac{f(b)}{b-a}\int_a^b (x-a)\,dx$$

$$\Rightarrow T_1(f) = \frac{f(a)}{b-a}\cdot -\frac{(b-x)^2}{2}\Big|_a^b + \frac{f(b)}{b-a}\frac{(x-a)^2}{2}\Big|_a^b$$

$$\Rightarrow T_1(f) = \frac{f(a)}{(b-a)}\frac{(b-a)^2}{2} + \frac{f(b)}{(b-a)}\frac{(b-a)^2}{2}.$$

$$\Rightarrow \boxed{T_1(f) = \frac{(b-a)}{2}\left[f(a)+f(b)\right]}$$. This result can also be

obtained by measuring the area of the TRAPEZIUM below $f(x)$ in the figure.

The area of the rectangle is $\boxed{(b-a)f(a)}$ and the area of the triangle is $\boxed{\frac{1}{2}(b-a)\left[f(b)-f(a)\right]}$.

Total area, $T_1(f) = (b-a)\left[f(a)+\frac{f(b)}{2}-\frac{f(a)}{2}\right]$

$$\Rightarrow \boxed{T_1(f) = \frac{1}{2}(b-a)\left[f(a)+f(b)\right]}$$ (same as the integral)

Example: $\boxed{I = \int_0^1 \frac{dx}{1+x}}$ Here $\boxed{f(x) = \frac{1}{1+x}}$

$\therefore I = \ln(1+x)\Big|_0^1 = \ln 2 \simeq 0.69$ (By exact integration).

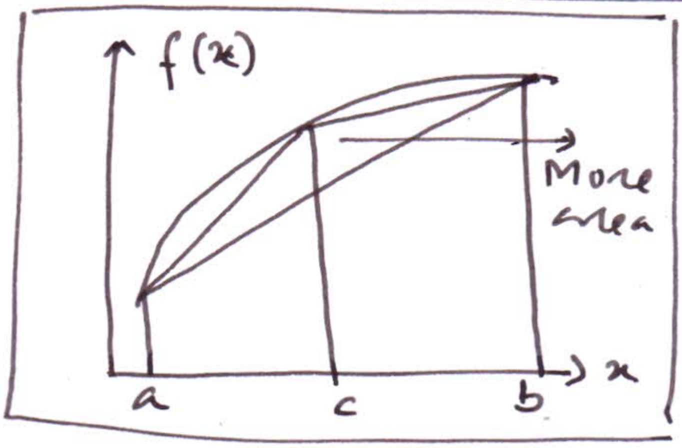
By trapezoidal rule, $T_1(f) = \frac{1}{2}\left[\frac{1}{1+0}+\frac{1}{1+1}\right]$

$$\Rightarrow T_1(f) = \frac{1}{2}\left[1+\frac{1}{2}\right] = \frac{3}{4} = 0.75 \quad (8.7\% \text{ error})$$

By subdividing the interval and then by applying the trapezoidal rule we get more area under the function.

$$I = \int_0^{1/2}\frac{dx}{1+x} + \int_{1/2}^1 \frac{dx}{1+x}$$

$$\Rightarrow T_2(f) = \frac{1}{2}\cdot\frac{1}{2}\left[\frac{1}{1+0}+\frac{1}{1+1/2}\right] + \frac{1}{2}\left(1-\frac{1}{2}\right)\left[\frac{1}{1+1/2}+\frac{1}{1+1}\right]$$



$$\therefore T_2(f) = \frac{1}{4}\left[1 + \frac{2}{3}\right] + \frac{1}{4}\left[\frac{2}{3} + \frac{1}{2}\right]$$

$$\Rightarrow T_2(f) = \frac{1}{4}\left[1 + \frac{4}{3} + \frac{1}{2}\right] \simeq 0.708 \quad (2.6\% \text{ error})$$

Hence, subdividing the interval gives more accuracy.

Let there be n subintervals between a and b, with each interval of length h. $\therefore \boxed{h = (b-a)/n}$

Define $\boxed{x_j = a + jh}$ $(j = 0, 1, 2, \dots, n)$

$\Rightarrow \boxed{x_0 = a}$ and $\boxed{x_n = a + nh = b}$

$$\Rightarrow I = \int_a^b f(x)\,dx = \int_{x_0}^{x_n} f(x)\,dx$$

We break this integral into its n subintervals.

$$\Rightarrow I = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots \int_{x_{n-1}}^{x_n} f(x)\,dx$$

$x_{j+1} - x_j = h$.

Each of the integrals above is approximated by the trapezoidal rule over a length h.

$$\therefore I \simeq T_n(f) = h\left[\frac{f(x_0) + f(x_1)}{2}\right] + h\left[\frac{f(x_1) + f(x_2)}{2}\right] + h\left[\frac{f(x_2) + f(x_3)}{2}\right] + \cdots + h\left[\frac{f(x_{n-1}) + f(x_n)}{2}\right]$$

$$\Rightarrow \boxed{T_n(f) = h\left[\frac{f(x_0)}{2} + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{f(x_n)}{2}\right]}$$

The above numerical integration can be applied to any number of nodes $\{x_j\}$ $(j = 0, 1, \dots, n)$.

Simpson's Rule | Quadratic Interpolation

By this rule a quadratic Lagrange interpolation is carried out on $f(x)$ in the interval $[a, b]$. This improves on the linear interpolation of the trapezoidal rule.

$$\boxed{I = \int_a^b f(x)\,dx \simeq \int_a^b P_2(x)\,dx}$$

$P_2(x) \rightarrow$ Quadratic Lagrange Polynomial.

For three data points $(x_0, y_0), (x_1, y_1), (x_2, y_2)$,

$$\boxed{P_2(x) = \frac{y_0(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + \frac{y_1(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + \frac{y_2(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}}.$$

$x_0 = a$, $x_2 = b$, $x_1 = c = \frac{a+b}{2}$. $y_0 = f(a)$, $y_2 = f(b)$, $y_1 = f(c)$.

$$\therefore \boxed{P_2(x) = f(a)\frac{(x-c)(x-b)}{(a-c)(a-b)} + f(c)\frac{(x-a)(x-b)}{(c-a)(c-b)} + f(b)\frac{(x-a)(x-c)}{(b-a)(b-c)}}$$

Define $\boxed{b-a = 2h} \Rightarrow \boxed{a-b = -2h} \Rightarrow \boxed{b-c = h}$

$\Rightarrow \boxed{a-c = -h}$ $\therefore$ $\boxed{c-a = h}$ and $\boxed{c-b = -h}$

Further define $\boxed{x = u+a} \Rightarrow \boxed{dx = du}$.

$$\int_a^b P_2(x)\,dx = \int_a^b \left[f(a)\frac{(x-c)(x-b)}{(a-c)(a-b)} + f(c)\frac{(x-a)(x-b)}{(c-a)(c-b)} + f(b)\frac{(x-a)(x-c)}{(b-a)(b-c)} \right] dx$$

We substitute $\boxed{x = u + a}$ in every term.

<u>First term</u>: $f(a)\dfrac{(u+a-c)(u+a-b)}{(a-c)(a-b)} = \dfrac{f(a)(u-h)(u-2h)}{(-h)(-2h)}$

$$= \frac{f(a)}{2h^2}\left(u^2 - uh - 2uh + 2h^2\right) = \frac{f(a)}{2h^2}\left(u^2 - 3uh + 2h^2\right)$$

The limits of the integral are transformed as $\boxed{a \longrightarrow 0}$ and $\boxed{b = a + 2h \longrightarrow 2h}$ in the variable u.

<u>Integral</u>: $\dfrac{f(a)}{2h^2}\displaystyle\int_0^{2h}\left(u^2 - 3uh + 2h^2\right)du = \dfrac{f(a)}{2h^2}\left[\dfrac{u^3}{3} - \dfrac{3hu^2}{2} + 2h^2u\right]_0^{2h}$

$$= \frac{f(a)}{2h^2}\left[\frac{u^3}{3} - \frac{3hu^2}{2} + 2h^2u\right]_0^{2h} = \frac{f(a)}{2h^2}h^3\left[\frac{8}{3} - \frac{3\cdot 4}{2} + 2\cdot 2\right]$$

<u>Integral of the first term is</u>: $\dfrac{hf(a)}{2}\left[\dfrac{16-36+24}{6}\right] = \dfrac{hf(a)}{2}\cdot\dfrac{4}{6} = \dfrac{hf(a)}{3}$

<u>Second term</u>: $f(c)\dfrac{u(u-2h)}{-h^2} = \dfrac{-f(c)}{h^2}\left(u^2 - 2hu\right)$

<u>Integral</u>: $\displaystyle\int_0^{2h}\frac{-f(c)}{h^2}\left(u^2 - 2hu\right)du = \frac{-f(c)}{h^2}\left[\frac{u^3}{3} - \frac{\cancel{2}hu^2}{\cancel{2}}\right]_0^{2h}$

$$= \frac{-f(c)}{h^2}h^3\left[\frac{8}{3} - 4\right]$$

(P.T.O.)

Integral of the second term: $\frac{f(c)}{h^2} h^3 \left[4 - \frac{8}{3}\right] = h f\left(\frac{a+b}{2}\right) \cdot \frac{4}{3}$

Third Term: $f(b) \frac{u(u+a-c)}{2h \cdot h} = \frac{f(b)\, u(u-h)}{2h^2}$

Integral: $\frac{f(b)}{2h^2} \int_0^{2h} (u^2 - uh)\, du = \frac{f(b)}{2h^2} \left[\frac{u^3}{3} - h\frac{u^2}{2}\right]_0^{2h}$

Integral of the third term: $\frac{f(b)}{2h^2} h^3 \left[\frac{8}{3} - \frac{4}{2}\right] = f(b)\, h \cdot \frac{1}{3}$

Gathering all the terms together,

$$\boxed{S_2(f) = \frac{h}{3}\left[f(a) + 4 f\left(\frac{a+b}{2}\right) + f(b)\right]}$$

Simpson's Rule for Numerical Integration.

Example: $\boxed{I = \int_0^1 \frac{dx}{1+x}}$ $\boxed{f(x) = \frac{1}{1+x}}$

$h = \frac{b-a}{2} = \frac{1-0}{2} = 1/2$. $S_2(f) = \frac{1/2}{3}\left[f(0) + 4 f(1/2) + f(1)\right]$.

$\Rightarrow S_2(f) = \frac{1}{6}\left[\frac{1}{1+0} + 4\frac{1}{1+1/2} + \frac{1}{1+1}\right]$

$\Rightarrow S_2(f) = \frac{1}{6}\left[1 + 4 \cdot \frac{2}{3} + \frac{1}{2}\right] = \frac{1}{6} \cdot \left[\frac{3}{2} + \frac{8}{3}\right]$

$\Rightarrow S_2(f) = \frac{1}{6} \cdot \frac{25}{6} = \frac{25}{36} = \underline{0.694}$.

Actual value of $I = \ln 2 = \underline{0.693}$ ($\underline{\%\ \text{error} = 0.14\%}$)

Significantly less error compared to trapezoidal rule.

Simpson's Rule over Large Subintervals

$$\boxed{I = \int_a^b f(x)\,dx}$$

Divide $b-a$ into n sub-intervals, each of length h, where n is an even integer.

$\therefore \boxed{b-a = nh}$

$\boxed{x_j = a + jh}$ $\quad j = 0, 1, \ldots, n. \Rightarrow x_0 = a$, $x_n = a + nh = b$

$$\therefore \boxed{I = \int_a^b f(x)\,dx = \int_{x_0}^{x_n} f(x)\,dx}$$

Each subinterval will have three nodes.

$$\Rightarrow I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx .$$

Now approximate each integral by the Simpson rule.

$$\therefore S_n(f) = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right] + \cdots + \frac{h}{3}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right].$$

$$\Rightarrow \boxed{S_n(f) = \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]}$$

$\boxed{I \simeq S_n(f)}$. If j is odd then $f(x_j)$ carries a factor of 4 in the series.

With a large number (even number) of sub-intervals high accuracy is obtained.

Numerical Differentiation: Numerical Derivative

A derivative ~~fn~~ of a function $f(x)$ is

$$\boxed{f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \frac{df}{dx}}$$

For small (but not infinitesimal) values of h

$$\boxed{f'(x) \simeq \frac{f(x+h) - f(x)}{h} \equiv D_h f(x)},$$

with $D_h f(x)$ being the numerical derivative of $f(x)$.

The Error Due to $D_h f(x)$: (because of a finite step size of h)

$$\boxed{f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \cdots}$$

by a Taylor expansion up to the second order.

$$\therefore \frac{f(x+h) - f(x)}{h} = f'(x) + \frac{f''(x)}{2}h + \cdots$$

$$\Rightarrow D_h f(x) - f'(x) = \frac{f''(x)}{2}h + \cdots$$

$$\Rightarrow \boxed{\text{Error}(f) = D_h f(x) - f'(x) \simeq \frac{f''(x)}{2}h}$$

The error is proportional to the step size.

Forward Difference Formula is given by

$$\boxed{D_h f(x) = \frac{f(x+h) - f(x)}{h}}$$

. If $h \to -h$ then

$$\boxed{D_{-h} f(x) = \frac{-f(x) + f(x-h)}{-h} = \frac{f(x) - f(x-h)}{h}},$$

which is known as the backward difference formula, in which now $\boxed{h > 0}$. The error formula can be estimated as before by a Taylor expansion,

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

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

$$\Rightarrow \frac{f(x) - f(x-h)}{h} = f'(x) - \frac{f''(x)}{2}h + \dots$$

$$\Rightarrow \boxed{D_{-h} f(x) - f'(x) = \text{Error}(f) \simeq -\frac{f''(x)h}{2}}$$

As before the error is proportional to h.

In all numerical exercises h will have a finite non-zero value (h can <u>never</u> be infinitesimal) and there will remain an error.

Differentiation using Interpolation

$f(x)$ can be replaced by an n-degree polynomial $P_n(x)$ that interpolates $f(x)$ at $n+1$ nodes $x_0, x_1, \ldots, x_n$. At a point $x = t$, $\boxed{f'(t) \simeq P_n'(t)}$. We consider $\boxed{n=2}$, $\boxed{t = x_1}$, $\boxed{x_0 = x_1 - h}$ and $\boxed{x_2 = x_1 + h}$.

$\therefore$ $x_1 - x_0 = h$, $x_0 - x_1 = -h$, $x_2 - x_0 = 2h$, $x_0 - x_2 = -2h$, $x_2 - x_1 = h$ and $x_1 - x_2 = -h$. We use these in

$$\boxed{\begin{aligned} P_2(x) = {} & f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\ & + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \end{aligned}},$$

and after that get,

$$P_2(x) = f(x_0)\frac{(x-x_1)(x-x_2)}{2h^2} + f(x_1)\frac{(x-x_0)(x-x_2)}{-h^2} + f(x_2)\frac{(x-x_0)(x-x_1)}{2h^2}$$

$$\Rightarrow \boxed{\begin{aligned} P_2'(x) = {} & f(x_0)\frac{(2x-x_1-x_2)}{2h^2} + f(x_1)\frac{(2x-x_0-x_2)}{-h^2} \\ & + f(x_2)\frac{(2x-x_0-x_1)}{2h^2} \end{aligned}}$$

At $x = x_1$, the term containing $f(x_1)$ will vanish because $2x_1 - x_0 - x_2 = \cancel{h} - \cancel{h} = 0$

$$\Rightarrow P_2'(x_1) = f(x_0)\frac{x_1 - x_2}{2h^2} + f(x_2)\frac{x_1 - x_0}{2h^2}$$

$$\Rightarrow P_2'(x_1) = f(x_0)\cdot\frac{-h}{2h^2} + f(x_2)\cdot\frac{h}{2h^2}$$

$$\Rightarrow \boxed{P_2'(x_1) = \frac{f(x_2) - f(x_0)}{2h} = \frac{f(x_1+h) - f(x_1-h)}{2h}}.$$

This gives the Central Difference formula, going as $\boxed{P_2'(x_1) = \frac{f(x_1+h) - f(x_1-h)}{2h} \equiv D_h f(x_1) \simeq f'(x_1)}$.

To estimate the error in this formula, we expand

$$f(x_1+h) = f(x_1) + f'(x_1)h + \frac{f''(x_1)h^2}{2!} + \frac{f'''(x_1)h^3}{3!} + \cdots$$

and

$$f(x_1-h) = f(x_1) - f'(x_1)h + \frac{f''(x_1)}{2!}h^2 - \frac{f'''(x_1)}{3!}h^3 + \cdots$$

$$\therefore D_h f(x_1) \simeq \frac{\cancel{f(x_1)} + f'(x_1)h + \cancel{\frac{f''(x_1)h^2}{2}} + \frac{f'''(x_1)h^3}{6} - \left[\cancel{f(x_1)} - f'(x_1)h + \cancel{\frac{f''(x_1)}{2}h^2} - \frac{f'''(x_1)}{6}h^3\right]}{2h}$$

$$\Rightarrow D_h f(x_1) \simeq \frac{\cancel{2} f'(x_1)\cancel{h} + 2\frac{f'''(x_1)}{6}\cancel{h^3}\,h^2}{\cancel{2h}}$$

$$\Rightarrow D_h f(x_1) \simeq f'(x_1) + f'''(x_1)h^2/6$$

$$\therefore \boxed{\text{Error}(f) = D_h f(x_1) - f'(x_1) \simeq \frac{f'''(x_1)}{6} h^2}$$

Since h is usually very small, errors of the order of h^2 are smaller than errors that are proportional to h.

Examples: $\boxed{f(x) = \cos x}$ $\boxed{x = \pi/6}$ $\boxed{f'(x) = -\sin x}$

$\therefore$ for $x = \pi/6$, $\boxed{f'(x) = -\sin x = -1/2 = -0.5}$ $\cos \pi/6 = \sqrt{3}/2$

i.) By the forward difference formula for $h = 0.1$

$$D_h f(x) = \frac{\cos(\pi/6 + 0.1) - \cos(\pi/6)}{0.1} = -0.54243$$

$\text{Error}(f) = D_h f(x) - f'(x) = -0.04253$ (for $h = 0.1$)

ii.) For $h = 0.05$, $D_h f(x) = \dfrac{\cos(\pi/6 + 0.05) - \cos(\pi/6)}{0.05}$

$\Rightarrow D_h f(x) = -0.52144$. $\text{Error}(f) = -0.02144$.

The error margin has reduced by approximately 1/2

iii.) By the Central difference formula for $h = 0.1$

$$D_h f(x) = \frac{\cos(\pi/6 + 0.1) - \cos(\pi/6 - 0.1)}{2 \times 0.1} = -0.499167$$

$\text{Error}(f) = D_h f(x) - f'(x) \simeq -8 \times 10^{-4}$ much less than for forward difference

iv.) For $h = 0.05$, $D_h f(x) = \dfrac{\cos(\pi/6 + 0.05) - \cos(\pi/6 - 0.05)}{2 \times 0.05}$

$\Rightarrow D_h f(x) = -0.499792$. $\text{Error}(f) \simeq -2 \times 10^{-4}$. The error has reduced by a factor of $(1/2)^2 = 1/4$.

The Method of Undetermined Coefficients

First Derivative: $\boxed{f'(t) \simeq D_h f(t)}$

Write $\boxed{D_h f(t) \equiv A f(t+h) + B f(t)}$ in which A and B are two undetermined coefficients.

Now $\boxed{f(t+h) \simeq f(t) + f'(t)h + \dfrac{f''(t)h^2}{2}}$ by a Taylor expansion.

$$\Rightarrow \quad f'(t) \simeq A f(t) + A f'(t)h + A f''\frac{(t)h^2}{2} + B f(t).$$

Comparing coefficients on both sides of,

$$\boxed{f'(t) = (A+B) f(t) + A h f'(t)}$$ (The two most significant terms)

we get $\boxed{A+B=0}$ and $\boxed{Ah=1}$ $\Rightarrow$ $\boxed{A = 1/h}$
and $\boxed{B = -A = -1/h}$. Using these we get,

$$\boxed{D_h f(t) = \frac{f(t+h) - f(t)}{h}}$$, which is the forward difference formula

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Second Derivative: $\boxed{f''(t) \simeq D_h^{(2)} f(t)}$

Write $\boxed{D_h f(t) = A f(t+h) + B f(t) + C f(t-h)}$ with A, B and C being three undetermined coefficients.

Again by Taylor expansion we get

$$\boxed{f(t+h) \simeq f(t) + f'(t)h + \frac{f''(t)}{2!}h^2 + \frac{f'''(t)h^3}{3!} + \frac{f^{(4)}(t)h^4}{4!}}$$

and

$$\boxed{f(t-h) \simeq f(t) - f'(t)h + \frac{f''(t)h^2}{2!} - \frac{f'''(t)h^3}{3!} + \frac{f^{(4)}(t)h^4}{4!}}$$

Combining the two expansions in $D_h f(t)$,

$$\boxed{\begin{aligned} f''(t) \simeq (A+B+C)f(t) + h(A-C)f'(t) + (A+C)\frac{h^2}{2}f''(t) \\ + (A-C)\frac{f'''(t)h^3}{6} + \frac{(A+C)h^4}{4!}f^{(4)}(t) \end{aligned}}$$

Comparing coefficients on both sides,

$\boxed{(A+B+C) = 0}$, $\boxed{h(A-C) = 0}$ and $\boxed{(A+C)\frac{h^2}{2} = 1}$,

from the first three significant terms.

$\Rightarrow \boxed{A = C} \Rightarrow 2A\frac{h^2}{2} = 1 \Rightarrow \boxed{A = \frac{1}{h^2}}$ and $B = -A-C = -2A$
$\Rightarrow \boxed{B = -2/h^2}$

Using these values we get.

$$\boxed{\mathcal{D}_h^2 f(t) = \frac{f(t+h) - 2f(t) + f(t-h)}{h^2} = \frac{1}{h}\left[\frac{f(t+h)-f(t)}{h} - \frac{f(t)-f(t-h)}{h}\right]}$$

which is the difference of the forward and backward differences (the second derivative). Also with all the determined values of A, B and C, we get,

$$\boxed{\mathcal{D}_h f(t) \simeq f''(t) + \frac{h^2}{12}f^{(4)}(t)} \Rightarrow \boxed{\mathcal{D}_h f(t) - f''(t) \simeq \frac{h^2}{12}f^{(4)}t}$$

$\therefore$ $\boxed{\mathcal{E}rror(f) \simeq h^2 f^{(4)}t/12}$ Of the order of h^2