The one dimensional forms of some constitutive laws commonly used

Law	Equation	Physical Area	Gradient	Flux	Proportional constat
Fourier's law	$q = -k \frac{dT}{dx}$	Heat conduction	Temperature	Heat	Thermal conductivity
Fick's law	$J = -D \frac{dc}{dx}$	Mass diffusion	Concentration	Mass	Diffusivity
D'Arcy' law	$q = -k \frac{dh}{dx}$	Flow through porous media	Head	Flow	Hydraulic conductivity
Ohm's law	$J = -\sigma \frac{dV}{dx}$	Current flow	Voltage	Current	Electrical conductivity
Newton's viscosity law	$\tau = -\mu \frac{du}{dx}$	Fluids	Velocity	Shear Stress	Dynamic Viscosity
Hooke's law	$\sigma = E \frac{\Delta L}{L}$	Elasticity	Deformation	Stress	Young's modulus

$y = f(x)$	Position (Displacement)
$\frac{dy}{dx} = y' = f'(x)$	Velocity
$\frac{d^2y}{dx^2} = y'' = f''(x)$	Acceleration
$\frac{d^3y}{dx^3} = y''' = f'''(x)$	Jerk
$\frac{d^4y}{dx^4} = y^{(4)} = f^{(4)}(x)$	Snap (Jounce)
$\frac{d^5y}{dx^5} = y^{(5)} = f^{(5)}(x)$	Crackle (Flounce)
$\frac{d^6y}{dx^6} = y^{(6)} = f^{(6)}(x)$	Pop (Pounce)

Numerical Differentiation

Given a complicated f(x) or a set of tabulated values, x_i's and corresponding $f(x_i)$'s:

Question: For a given x, in the table or not in the table

$$\frac{df}{dx} = ? \quad , \quad \frac{d^2f}{dx^2} = ? \quad , \quad \text{etc.}$$

Answer: Replace f(x), or the tabulated data, with a **simple** function g(x).

Then, operate on g(x) instead

$$f(x) \cong g(x) \quad , \quad \frac{df}{dx} \cong \frac{dg}{dx} \quad , \quad \frac{d^2f}{dx^2} \cong \frac{d^2g}{dx^2} \quad , \quad \text{etc.}$$

What is this simple fuction, g(x)?

Truncated Taylor series	$g(x) = f(x_0) + (x - x_0) f'(x_0) + \ldots$ passes throught x_0 only
Least Squares	Data should have random statistical errors
Newton-Gregory Polynomials	Forward, Backward, Central ... Divided difference table
Cubic Splines	$g_k(x) = a_k (x - x_i)^3 + b_k (x - x_i)^2 + c_k (x - x_i) + d_k$ passes through all the points with equal first and second derivatives at the junctions
Something else	Ratio of polynomials (Padé approximation), sine and cosine functions (Fourier series), Hermite, Chebyshev, others

Newton-Gregory forward polynomial $s = \dfrac{x - x_0}{h}$ where h is constant

$$f(s) \cong P_n(s) = f_0 + s\,\Delta f_0 + \frac{s\,(s-1)}{2\,!}\,\Delta^2 f_0 + \frac{s\,(s-1)\,(s-2)}{3\,!}\,\Delta^3 f_0 + \ldots$$

$$f\,'(s) \cong \frac{dP_n(x)}{dx} = \frac{1}{h}\left[\Delta f_0 + \frac{1}{2}\,(2\,s-1)\,\Delta^2 f_0 + .\frac{1}{6}\,(\ldots.)\,\Delta^3 f_0 + \ldots\right]$$

If $x = x_0$, $f\,'(x_0) = ?$

Use one term: $f\,'(x_0) \cong \dfrac{1}{h}\,\Delta f_0 = \dfrac{f_1 - f_0}{h}$

Use two terms: $f\,'(x) \cong \dfrac{1}{h}\left[\Delta f_0 + \dfrac{1}{2}\,(2\,s-1)\,\Delta^2 f_0\right] = \dfrac{1}{2\,h}\left(-\,f_2 + 4\,f_1 - 3\,f_0\right)$

$f'(x_0) \cong \frac{1}{h}(f_1 - f_0)$	$E'(x_0) = \frac{-h}{2} f''(\xi)$	One-term forward
$f'(x_0) \cong \frac{1}{2h}(f_1 - f_{-1})$	$E'(x_0) = \frac{-h^2}{6} f'''(\xi)$	One-term central
$f'(x_0) \cong \frac{1}{2h}(-f_2 + 4f_1 - 3f_0)$	$E'(x_0) = \frac{h^2}{3} f'''(\xi)$	Two-term forward
$f'(x_0) \cong \frac{1}{12h}(-f_2 + 8f_1 - 8f_{-1} + f_{-2})$	$E'(x_0) = \frac{-h^4}{30} f^{(5)}(\xi)$	Two-term central
$f'(x_0) \cong \frac{1}{6h}(2f_3 - 9f_2 + 18f_1 - 11f_0)$	$O(h^3)$	Three-term forward

Note that, using central differences, we get better accuracy with two-terms than we do with four terms using forward differences.

$$f''(x_0) \cong \frac{1}{h^2}\left(f_2 - 2\,f_1 + f_0\right) \qquad E''(x_0) = h\ f'''(\xi)$$

Two-term forward

$$f''(x_0) \cong \frac{1}{h^2}\left(f_1 - 2f_0 + f_{-1}\right) \qquad E''(x_0) = \frac{-h^2}{12}\ f^{(4)}(\xi)$$

Two-term central

$$f''(x_0) \cong \frac{1}{h^2}\left(-f_3 + 4\,f_2 - 5\,f_1 + 2\,f_0\right) \qquad O(h^2)$$

Three-term forward

$$f''(x_0) \cong \frac{1}{12\,h^2}\left(-f_2 + 16\,f_1 - 30\,f_0 + 16\,f_{-1} - f_{*2}\right) \qquad O(h^4)$$

Three-term central

Error estimates for
Newton-Gregory forward polynomial

$$s = \frac{x - x_0}{h} \quad \text{where } h \text{ is constant}$$

$$f(x) = P_n(x) + \prod_{i=0}^{n}(x - x_i)\ \frac{f^{(n+1)}(\xi)}{(n+1)!}$$

$$E(x) = f(x) - P_n(x) = \prod_{i=0}^{n}(x - x_i)\ \frac{f^{(n+1)}(\xi)}{(n+1)!}$$

$$E'(x) = f\,'(x) - P_n(x) = \frac{d}{dx}\left(\prod_{i=0}^{n}(x - x_i)\ \frac{f^{(n+1)}(\xi)}{(n+1)!}\right)$$

$$= \frac{d}{dx}\left(\prod_{i=0}^{n}(x - x_i)\right)\frac{f^{(n+1)}(\xi)}{(n+1)!} + \frac{d}{dx}\left(\frac{f^{(n+1)}(\xi)}{(n+1)!}\right)\prod_{i=0}^{n}(x - x_i)$$

$$E'(x) = \frac{d}{dx}\left(\prod_{i=0}^{n}(x - x_i)\right)\frac{f^{(n+1)}(\xi)}{(n+1)!} + \frac{f^{(n+2)}(\eta)}{(n+2)!}\prod_{i=0}^{n}(x - x_i)$$

$$E'(x) = \frac{d}{dx}\left(\prod_{i=0}^{n}(x - x_i)\right)\frac{f^{(n+1)}(\xi)}{(n+1)!} + \frac{f^{(n+2)}(\eta)}{(n+2)!}\prod_{i=0}^{n}(x - x_i)$$

If $x = x_j$, one of the tabulated values, the second term becomes zero, and the first term is reduced to one product of $(x_j – x_i)$'s:

$$E'(x_j) = \prod_{\substack{i=0 \\ i \neq j}}^{n}(x_j - x_i)\frac{f^{(n+1)}(\xi)}{(n+1)!}$$

For example, for the one-term forward formula, when $x_j = x_0$ is

$$E'(x_0) = (x_0 - x_1)\frac{f''(\xi)}{2!} = \frac{-h}{2}f''(\xi)$$

Difference Table for f(x) = e^{-x}

x	f (x)	Δ f	Δ^2 f	Δ^3 f	Δ^4 f
0	1				
		- 0.632120559			
1	0.367879441		0.399576401		
		- 0.232544158		- 0.252580458	
2	0.135335283		0.146995943		0.1596613
		- 0.085548215		- 0.092919158	
3	0.049787068		0.054076785		0.05873611
		- 0.031471429		- 0.034183048	
4	0.018315639		0.019893738		0.021607807
		- 0.011577692		- 0.012575241	
5	0.006737947		0.007318497		
		- 0.004259195			
6	0.002478752				

Example: Using Newton-Gregory forward interpolating polynomial, calculate $f'(x_0)$ at $x_0 = 2.0$ for the function given in the difference table and estimate the error.

Exact solution: $f'(2) = -e^{-2} = -0.1353353$

$$f'(x) \cong \frac{dP}{dx} = \frac{1}{h}\left(\Delta f_0 - \frac{\Delta^2 f_0}{2} + \frac{\Delta^3 f_0}{3} - \frac{\Delta^4 f_0}{4} + \ldots\right)$$

N-G Forward Polynomial	1 term	2 terms	3 terms	4 terms
P'(2)	- 0.085	- 0.112	- 0.123	- 0.127
True % Error	37 %	17 %	9 %	6 %

Error estimation

One-term forward: $$E^{'}(x_0) = -\frac{h}{2} f^{''}(\xi) \cong -\frac{h}{2}\left(\frac{\Delta^2 f_0}{h^2}\right) = -\frac{\Delta^2 f_0}{2h}$$

$$E^{'}_{est}(2) = -\frac{\Delta^2 f_0}{2h} = -\frac{0.054}{2} = -0.027$$

True error: $$E^{'}_{true}(2) = f^{'}(2) - P^{'}(2) = -0.135 - (-0.085) = -0.05$$

Note that, with our definition of differences:

$$\boxed{f^{(n)}(\xi) \cong \Delta^n f_0 \left(\frac{1}{h^n}\right)} \qquad \boxed{f^{(n)}(\xi) \cong D^n f_0 \,(n!)}$$

Example: Consider the data points

i	1	2	3	4	5
x_i	- 2	- 1	0	1	2
y_i	4	- 1	2	1	8

a) Fit a fourth-degree polynomial, $P_4(x)$, in Lagrange form, passing through all the given data points;

b) Interpolate y(x) at x = 0.5 and estimate the error;

c) Find the first derivative y’(x) at x = 1 and estimate the error;

d) Compare answers in (b) and (c) with those of the previous example where a set of cubic splines is fitted to the same data points;

Solution: (a) Fourth-degree polynomial in **Lagrange form**:

$$P_4(x) = \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)}\, y(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)(x_1-x_4)}\, y(x_1) +$$

$$\frac{(x-x_0)(x-x_1)(x-x_3)(x-x_4)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)}\, y(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_4)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)(x_3-x_4)}\, y(x_3) +$$

$$\frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)}\, y(x_4)$$

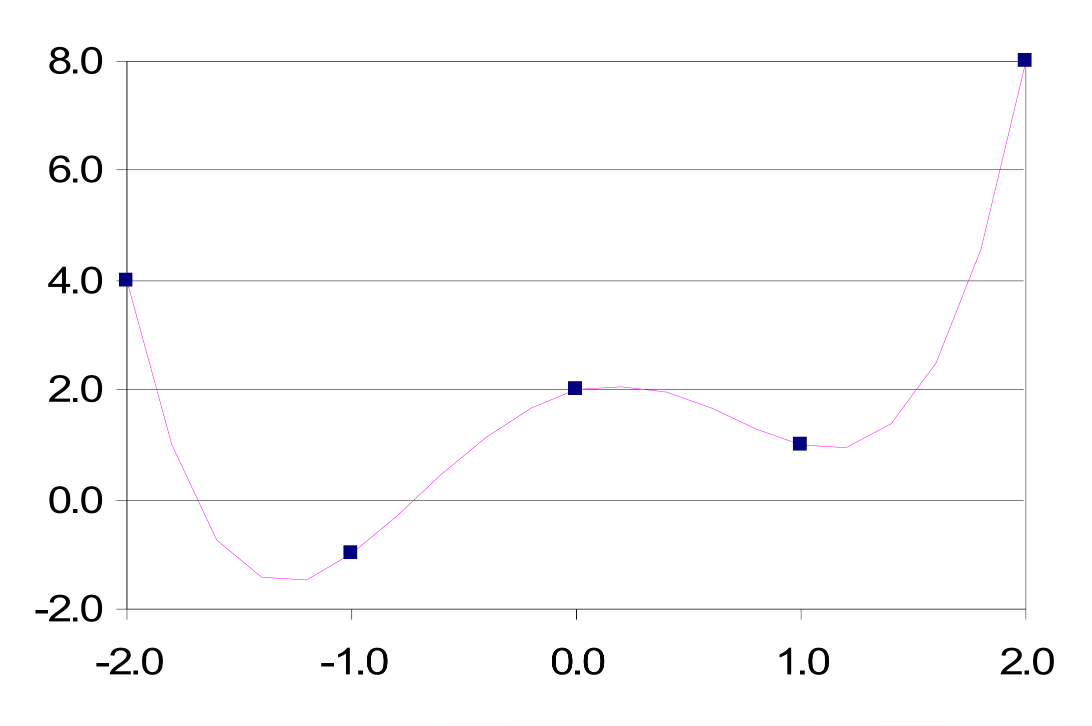
$$P_4(x) = 0.16666667\,(x+1)\,(x)\,(x-1)\,(x-2) + 0.16666667\,(x+2)\,(x)\,(x-1)\,(x-2) +$$

$$0.5\,(x+2)\,(x+1)\,(x-1)\,(x-2) - 0.16666667\,(x+2)\,(x+1)\,(x)\,(x-2) +$$

$$0.33333333\,(x+2)\,(x+1)\,(x)\,(x-1)$$

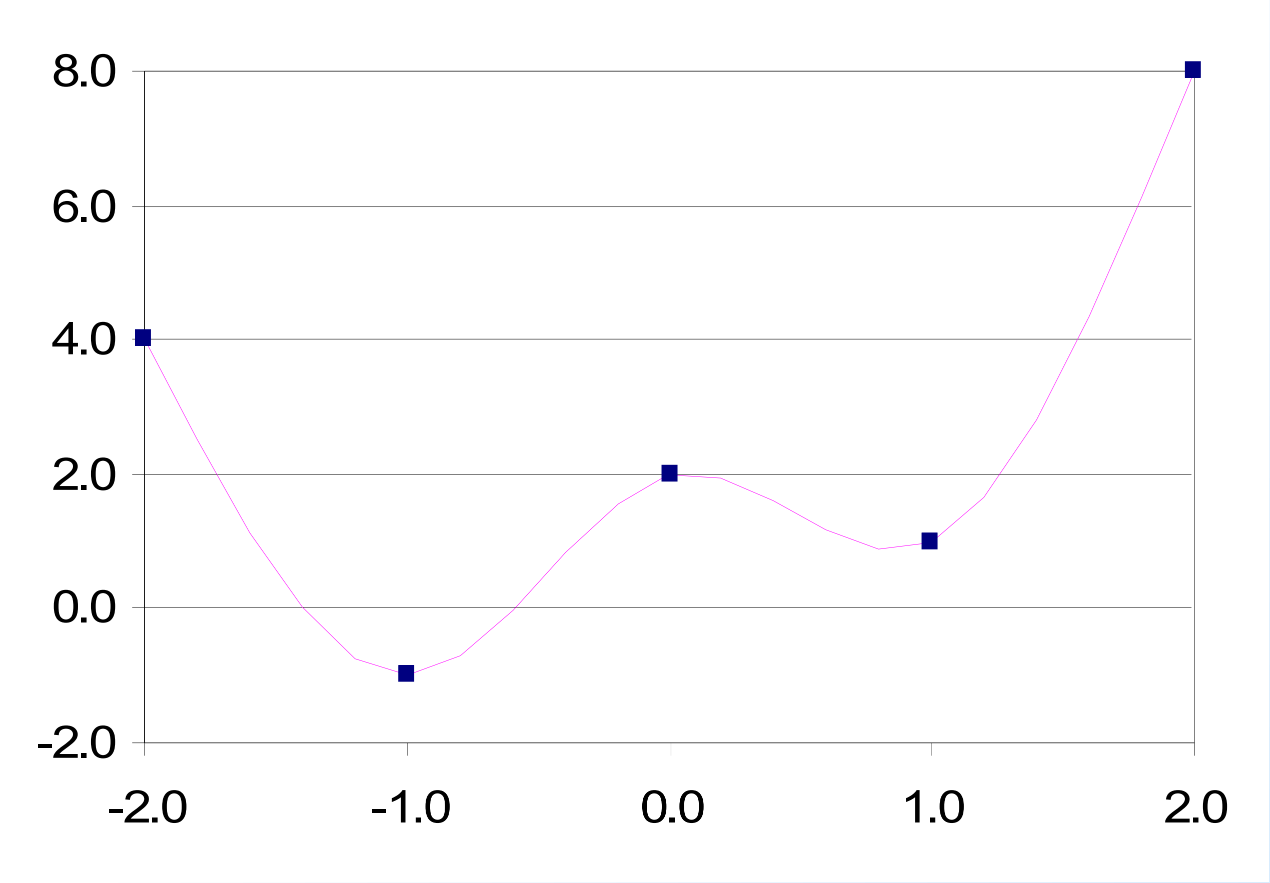
This is the fourth-degree polynomial passing through all the given data points.

The plot is given below.



Compare this with the plot of the cubic splines.

Plots of the data and cubic splines



The divided difference table for the given data is:

x_i	y_i	Dy_i	D^2y_i	D^3y_i	D^4y_i
-2.00	4.00				
		-5.00			
-1.00	-1.00		4.00		
		3.00		-2.00	
0.00	2.00		-2.00		1.00
		-1.00		2.00	
1.00	1.00		4.00		
		7.00			
2.00	8.00				

Note that the same fourth-degree interpolating polynomial can be found using the divided difference table and the formula

$$P_n(x) = f(x_i) + (x - x_i)\, Df_i + (x - x_i)(x - x_{i+1})\, D^2f_i + \ldots + (x - x_i)(x - x_{i+1}) \ldots (x - x_{i+n-1})\, D^nf_i$$

$$P_4(x) = 4 - 5(x + 2) + 4(x + 2)(x + 1)\, D^2f_i - 2(x + 2)(x + 1)\, x + (x + 2)(x + 1)\, x\, (x - 1)$$

The error estimator for the Newton-Gregory interpolating polynomial is

$$E(x) = f(x) - P_n(x) = \prod_{i=0}^{n} (x - x_i)\, \frac{f^{(n+1)}(\xi)}{(n + 1)!}$$

The error estimator for the first derivative at a tabulated data point x_j is:

$$E'(x_j) = f'(x_j) - P_n'(x_j) = \prod_{\substack{i=0 \\ i \neq j}}^{n} (x_j - x_i)\, \frac{f^{(n+1)}(\xi)}{(n + 1)!}$$

Lagrange form:

$$
\begin{aligned}
P_4(0.5) = {} & 0.16666667\,(0.5 + 1)\,(0.5)\,(0.5 - 1)\,(0.5 - 2) + \\
& 0.16666667\,(0.5 + 2)\,(0.5)\,(0.5 - 1)\,(0.5 - 2) + \\
& 0.5\,(0.5 + 2)\,(0.5 + 1)\,(0.5 - 1)\,(0.5 - 2) - \\
& 0.16666667\,(0.5 + 2)\,(0.5 + 1)\,(0.5)\,(0.5 - 2) + \\
& 0.33333333\,(0.5 + 2)\,(0.5 + 1)\,(0.5)\,(0.5 - 1)
\end{aligned}
$$

$$P_4(0.5) = 1.812500$$

Using divided differences:

$$
\begin{aligned}
P_4(x) = {} & f(x_0) + (x - x_0)\,Df_0 + (x - x_0)(x - x_1)\,D^2 f_0 + (x - x_0)(x - x_1)(x - x_2)\,D^3 f_0 \\
& + (x - x_0)(x - x_1)(x - x_2)(x - x_3)\,D^4 f_0
\end{aligned}
$$

$$P_4(x) = 4.0 - 5.0\,(x - x_0) + 4.0\,(x - x_0)(x - x_1) - 2.0\,(x - x_0)(x - x_1)(x - x_2) + (x - x_0)(x - x_1)(x - x_2)(x - x_3)$$

$$P_4(0.5) = 4.0 - 5.0\,(0.5 + 2) + 4.0\,(0.5 + 2)(x + 1) - 2.0\,(x + 2)(x + 1)(x) + (0.5 + 2)(0.5 + 1)(0.5)(0.5 - 1)$$

$P_4(0.5) = 1.812500$

The same answer is obtained because they are the same polynomial.

The cubic spline answer was 1.392857.

Error Calculation:

$$E(x) = f(x) - P_4(x) = \prod_{i=0}^{4}(x - x_i)\,\frac{f^{(5)}(\xi)}{5\,!}$$

$$= (x - x_0)(x - x_1)(x - x_2)(x - x_3)(x - x_4)\,\frac{f^{(5)}(\xi)}{5\,!}$$

The fifth derivative is to be replaced by the fifth divided difference: $\dfrac{f^{(5)}(\xi)}{5\,!} \cong D^5 f$

$$E(x) \approx (x - x_0)(x - x_1)(x - x_2)(x - x_3)(x - x_4)\, D^5 f$$

But, the fifth divided difference does not exist. From the trend in the divided difference table, assume that $D^5 f = 0.5$. Then:

$$E(0.5) \approx (0.5 + 2)(0.5 + 1)(0.5)(0.5 - 1)(0.5 - 2)(0.5) = 0.703125$$

The error estimate is almost 40 %. It was about 20% with cubic splines.

(c) One may use either the polynomial in Lagrange form or the polynomial obtained from the divided difference table. It seems that it is easier to take the first derivative of the later polynomial. Let's do that:

$$P_4(x) = 4.0 - 5.0\,(x - x_0) + 4.0\,(x - x_0)\,(x - x_1) - 2.0\,(x - x_0)\,(x - x_1)\,(x - x_2) + (x - x_0)\,(x - x_1)\,(x - x_2)\,(x - x_3)$$

$$\begin{aligned} P_4'(x) = {} & -5.0 + 4.0\left[(x - x_0) + (x - x_1)\right] \\ & - 2.0\left[(x - x_1)\,(x - x_2) + (x - x_0)\,(x - x_2) + (x - x_0)\,(x - x_1)\right] \\ & + (x - x_1)\,(x - x_2)\,(x - x_3) + (x - x_0)\,(x - x_2)\,(x - x_3) \\ & + (x - x_0)\,(x - x_1)\,(x - x_3) + (x - x_0)\,(x - x_1)\,(x - x_2) \end{aligned}$$