Grid Point Notation and Taylor Series

Grid point notation:
Assume you have grid points that are equally-spaced apart. Each distance D from its closest neighbors:

grid pts	*	*	*	*	*
x grid locations	x-2D	x-D	x	x+D	x+2D
variable f values	f_{m-2}	f_{m-1}	f_m	f_{m+1}	f_{m+2}

Relationships implied above:

continuum mathematics	subscript notation	fortran array subscripts
f(x)	f_m	f(m)
f(x+D)	f_{m+1}	f(m+1)
f(x-D)	f_{m-1}	f(m-1)
x is the space variable	m is grid point marker	m is DO loop index

Taylor series expansions:
Notation: i,ii,iii,iv,v, etc. superscripts here denote differentiation. i.e. $f^{ii} = d^2f / dx^2$

Usage in calculus: to obtain an estimate at one location based on information (including derivatives) at another location. Generic form is:

$$f(x+D) = f(x) + f^{i}(x)\{D/1!\} + f^{ii}(x)\{D^2/2!\} + f^{iii}(x)\{D^3/3!\} + f^{iv}(x)\{D^4/4!\} + f^{v}(x)\{D^5/5!\} + \ldots$$

In numerical analysis, one uses the Taylor series to do the opposite. You estimate the derivative(s) at a location from the known values at nearby locations.

Expressing the Taylor series for grid points above:

(1) $f_{m+2} = f_m + f^{i}_m\{2D/1!\} + f^{ii}_m\{4D^2/2!\} + f^{iii}_m\{8D^3/3!\} + f^{iv}_m\{16D^4/4!\} + f^{v}_m\{32D^5/5!\} + \ldots$

(2) $f_{m+1} = f_m + f^{i}_m\{D/1!\} + f^{ii}_m\{D^2/2!\} + f^{iii}_m\{D^3/3!\} + f^{iv}_m\{D^4/4!\} + f^{v}_m\{D^5/5!\} + \ldots$

(3) $f_{m-1} = f_m - f^{i}_m\{D/1!\} + f^{ii}_m\{D^2/2!\} - f^{iii}_m\{D^3/3!\} + f^{iv}_m\{D^4/4!\} - f^{v}_m\{D^5/5!\} + \ldots$

(4) $f_{m-2} = f_m - f^{i}_m\{2D/1!\} + f^{ii}_m\{4D^2/2!\} - f^{iii}_m\{8D^3/3!\} + f^{iv}_m\{16D^4/4!\} - f^{v}_m\{32D^5/5!\} + \ldots$

An obvious relation is (D=0):

(\$) $f_m = f_m$

Now add equations as follows: (2) + (3) – 2* (\$)

The result is:

$f_{m+1} = f_m \quad +f^{i}_{m}\{D/1! \ \ +f^{ii}_{m}\{D^2/2!\} \quad +f^{iii}_{m}\{D^3/3!\} +f^{iv}_{m}\{D^4/4!\} +f^{v}_{m}\{D^5/5!\} \quad + \ldots$

$f_{m-1} = f_m \quad -f^{i}_{m}\{D/1!\} +f^{ii}_{m}\{D^2/2!\} \quad -f^{iii}_{m}\{D^3/3!\} \ +f^{iv}_{m}\{D^4/4!\} -f^{v}_{m}\{D^5/5!\} \quad + \ldots$

$-2 f_m = -2 f_m$

$f_{m+1} + f_{m-1} \ \ -2 f_m =$

$$0 + \quad 0 + \quad f^{ii}_{m}\{D^2\} \quad + \quad 0 \quad + 2 f^{iv}_{m}\{D^4/4!\} \quad + \ 0 + \ 2 f^{vi}_{m}\{D^6/6!\} + \ \ldots$$

The formula is easily rearranged as a definition for the second derivative at grid point location ‘m’

$f^{ii}_{m} = \{ f_{m+1} + f_{m-1} \ \ -2 f_m \}/\{D^2\}$ plus residual ‘R’ where R is an infinite series:

$R = 2 f^{iv}_{m}\{D^2/4!\} \quad + \ 2 f^{vi}_{m}\{D^4/6!\} + \ \ldots$

Note: This formula assumes data at equal intervals ‘D’ apart, as indicated by the subscripts m. The ‘accuracy’ of the scheme depends on the shape of the quantity being represented. For a polynomial function of order x^3 or higher the formula is ‘exact’ because that quantity has all derivatives above third order being zero. A rough, relative estimate is that the scheme is ‘second order’ because the leading term in R is the interval raised to the second power.

Other formulas are possible, including one-sided formulas, and formulas at higher or order by similar combining of the Taylor series expansions.