This document is to remind myself of some of the numerical methods useful to the MAE 3403 class. Most of the content is a summary from "*Numerical Methods*", by *Robert W. Hornbeck*.

Ch. 2: The Taylor Series

If $f(x)$ can be represented by a convergent power series within an interval centered at b, it is said to *analytic*.

Thus for x within a convergent interval, f is given by a convergent power series: $f(x)=\sum_{n=0}^{\infty} a_n (x-b)^n$

Differentiating this power series n times and setting $x=b$ gives: $\dfrac{f^{(n)}(b)}{n!}=a_n$

Thus, the Taylor series of $f(x)$ in the region of x close to $x=a$ is given by: $f(x)=\sum_{n=0}^{\infty}\dfrac{f^{(n)}(a)}{n!}(x-a)^n$

Suppose we want to find the value of $f(x=b)$:

$$f(b)=f(a)+f'(a)(b-a)+\frac{(b-a)^2}{2}f''(a)+\frac{(b-a)^3}{3!}f'''(a)+...+\frac{(b-a)^n}{n!}f^n(a)+...$$

<u>*Example*</u>: Prove *Euler's* formula which states: $e^{jx}=\cos(x)+j\sin(x)$, where $j=(-1)^{1/2}$

If true, the Taylor's series expansions of both sides of the equation should be equal.

For LHS (e^{jx}):

$$f(x)=e^{jx}=1+jx-\frac{x^2}{2}-j\frac{x^3}{3!}+\frac{x^4}{4!}+j\frac{x^5}{5!}-\frac{x^6}{6!}-j\frac{x^7}{7!}+...=\left(1-\frac{x^2}{2}+\frac{x^4}{4!}-\frac{x^6}{6!}+...\right)+j\left(x-\frac{x^3}{3!}+\frac{x^5}{5!}-\frac{x^7}{7!}+...\right)$$

For RHS (cos(x)): recall $\dfrac{d\cos(x)}{dx}=-\sin(x)$; $\dfrac{d\sin(x)}{dx}=\cos(x)$; $\cos(0)=1$; $\sin(0)=0$

$$f(x)=\cos(x)=1-\frac{x^2}{2}+\frac{x^4}{4!}-\frac{x^6}{6!}+...$$

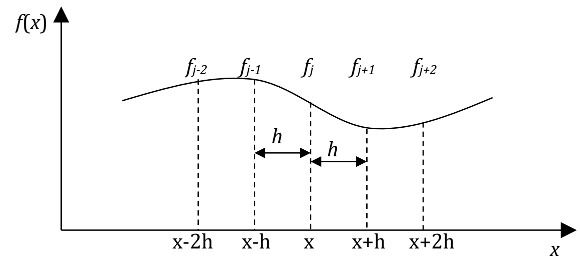
For RHS (sin(x)):

$$f(x)=\sin(x)=x-\frac{x^3}{3!}+\frac{x^5}{5!}-\frac{x^7}{7!}+...$$

Q.E.D.

Ch. 3: The Finite Difference Calculus

3.1 Forward and backward differences



Consider a function $f(x)$ which is analytic in the neighborhood of a point x. We can find $f(x+h)$ by:

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

Now, solving for $f'(x)$:

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

$$f'(x)=\frac{f(x+h)-f(x)}{h}+\mathcal{O}(h)$$

If we let $f(x+h)=f_{j+1}$ and $f(x)=f_j$ and $\Delta f_j \equiv f_{j+1}-f_j$, then:

$f'(x)=\frac{\Delta f_j}{h}+\mathcal{O}(h)$ is *the first forward difference approximation* of $f'(x)$ with error of order h.

We can do a similar process for $f(x-h)$, such that:

$f'(x)=\frac{\nabla f_j}{h}+\mathcal{O}(h)$, where $\nabla f_j = f_j - f_{j-1}$ is *the first backward difference approximation* of $f'(x)$.

3.2 Higher order derivative approximations:

Find $f(x+2h)$ by: $f(x+2h)=f(x)+2hf'(x)+\frac{2^2h^2}{2}f''(x)+\frac{2^3h^3}{3!}f'''(x)+...$

Subtracting $2f(x+h)$, I can find: $f(x+2h)-2f(x+h)=-f(x)+2h^2f''(x)+\frac{4h^3}{3}f'''(x)+...$

Solving for $f''(x)$:

$$f''(x)=\frac{f(x+2h)-2f(x+h)+f(x)}{h^2}-hf'''(x)+...\rightarrow f''(x)=\frac{f(x+2h)-2f(x+h)+f(x)}{h^2}+\mathcal{O}(h)$$

Using subscript notation: $f''(x)=\frac{f_{j+2}-2f_{j+1}+f_j}{h^2}+\mathcal{O}(h)\rightarrow f''(x)=\frac{\Delta^2 f_j}{h^2}+\mathcal{O}(h)$

In a similar way using the backward expansion: $f''(x)=\frac{f_j-2f_{j-1}+f_{j-2}}{h^2}+\mathcal{O}(h)\rightarrow f''(x)=\frac{\nabla^2 f_j}{h^2}+\mathcal{O}(h)$

These are the *second forward* & *backward difference* equations. We now note that:

$\Delta^n f_j = \Delta\left(\Delta^{n-1}f_j\right)$ and $\nabla^n f_j = \nabla\left(\nabla^{n-1}f_j\right)$

For example: $\nabla^2 f_j = \nabla\left(\nabla f_j\right)=\nabla f_j - \nabla f_{j-1} = \left(f_j - f_{j-1}\right)-\left(f_{j-1}-f_{j-2}\right)=f_j-2f_{j-1}+f_{j-2}$

Therefore: $\left.\dfrac{d^n f}{dx^n}\right|_{x_j} = \dfrac{\Delta^n f_j}{h^n} + \mathcal{O}(h)$ and $\left.\dfrac{d^n f}{dx^n}\right|_{x_j} = \dfrac{\nabla^n f_j}{h^n} + \mathcal{O}(h)$

In table form:

Forward Difference Approximation

	f_j	f_{j+1}	f_{j+2}	f_{j+3}	f_{j+4}
$hf'(x_j)=$	-1	1			
$h^2f''(x_j)=$	1	-2	1		
$h^3f'''(x_j)=$	-1	3	-3	1	
$h^4f^{iv}(x_j)=$	1	-4	6	-4	1

Backward Difference Approximation

	f_{j-4}	f_{j-3}	f_{j-2}	f_{j-1}	f_j
$hf'(x_j)=$				-1	1
$h^2f''(x_j)=$			1	-2	1
$h^3f'''(x_j)=$		-1	3	-3	1
$h^4f^{iv}(x_j)=$	1	-4	6	-4	1

To get a more accurate estimate of the *first forward* and *backward differences*, we can keep an extra term in the Taylor series expansion: $f'(x) = \dfrac{f(x+h) - f(x)}{h} - \dfrac{h}{2} f''(x) - \dfrac{h^2}{3!} f'''(x) + \ldots$ and substitute for $f''(x)$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}\left[\frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} - hf'''(x) + \ldots\right] - \frac{h^2}{3!} f'''(x) + \ldots$$

$$f'(x) = \frac{f_{j+1} - f_j}{h} - \frac{h}{2}\left[\frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} - hf'''(x) + \ldots\right] - \frac{h^2}{3!} f'''(x) + \ldots$$

$$f'(x) = \frac{4f_{j+1} - 3f_j - 2f_{j+2}}{2h} + \mathcal{O}(h^2)$$ Note: this estimate has less error

3.3 Central Differences

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots \text{ and } f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(x) + \ldots$$

So, $f(x+h) - f(x-h) = 2hf' + \dfrac{h^3}{3} f'''(x) + \ldots \rightarrow f'(x) = \dfrac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)$

$\therefore$ *first central difference*: $f'(x) = \dfrac{f_{j+1} - f_{j-1}}{2h} + \mathcal{O}(h^2)$

second central difference: $f_{j+1} + f_{j-1} = 2f_j + h^2 f''(x) + \ldots \rightarrow f''(x) = \dfrac{f_{j+1} - 2f_j + f_{j-1}}{h^2} + \mathcal{O}(h^2)$

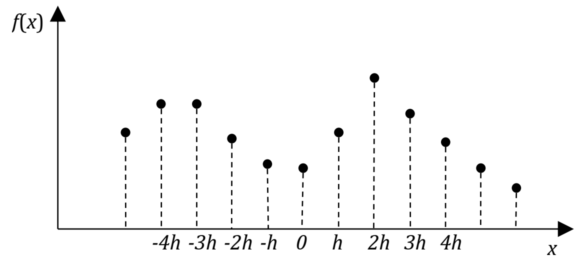
In Table form:

Central Difference

	f_{j-2}	f_{j-1}	f_j	f_{j+1}	f_{j+2}
$2hf'(x_j)=$		-1	0	1	
$h^2f''(x_j)=$		1	-2	1	
$2h^3f'''(x_j)=$	-1	2	0	-2	1
$h^4f^{iv}(x_j)=$	1	-4	6	-4	1

Ch. 4: Interpolation and Extrapolation

Consider we have some experimental data at discrete values of x, but would like to know the value of $f(x)$ at some x where no data was collected.



4.0-4.3 Evenly spaced data

Some example data might be

x	0	1	2	3	4	5
$f(x)$	-7	-3	6	25	62	129

forward difference table

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$
0	-7	4	5	5	3	1
1	-3	9	10	8	4	
2	6	19	18	12		
3	25	37	30			
4	62	67				
5	129					

$\Delta f_0 = f_1 - f_0$

$\Delta^2 f_0 = (f_2 - f_1) - (f_1 - f_0) = f_2 - 2f_1 + f_0$

$\Delta^3 f_0 = [(f_3 - f_2) - (f_2 - f_1)] - [(f_2 - f_1) - (f_1 - f_0)] = f_3 - 3f_2 + 3f_1 - f_0$

backward difference table

x	$f(x)$	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$
0	-7					
1	-3	4				
2	6	9	5			
3	25	19	10	5		
4	62	37	18	8	3	
5	129	67	30	12	4	1

central difference table

x	$f(x)$	δf	$\delta^2 f$	$\delta^3 f$	$\delta^4 f$	$\delta^5 f$
0	-7					
0.5		4				
1	-3		5			
1.5		9		5		
2	6		10		3	
2.5		19		8		1
3	25		18		4	
3.5		37		12		
4	62		30			
4.5		67				
5	129					

For Taylor series around x=0, we have: $f(x) = f(0) + xf'(0) + \frac{x^2}{2!} f''(0) + \frac{x^3}{3!} f'''(0) + \ldots$ and forward difference equation of:

$$f'(0) = \frac{f(0+h) - f(0)}{h} - \frac{h}{2!} f''(0) - \frac{h^2}{3!} f'''(0) + \ldots \rightarrow$$

$$f'(0) = \frac{f(0+h) - f(0)}{h} - \frac{1}{2!}\left[\frac{f(0+2h) - f(0+h)}{h} - \frac{f(0+h) - f(0)}{h}\right] - \frac{h^2}{3!} f'''(0) + \ldots \rightarrow$$

$$f'(0) = \frac{\Delta f_o}{h} - \frac{1}{2!}\frac{\Delta^2 f_o}{h} - \frac{h^2}{3!} f'''(0) + \ldots$$

$$f''(0) = \frac{\Delta^2 f_0}{h^2} - hf'''(x) + \ldots$$

$$f(x) = f(0) + \frac{x\Delta f_o}{h} + \frac{x(x-h)\Delta^2 f_o}{2h^2} + \ldots$$

After continuing this type of substitution…

Gregory-Newton forward interpolation formula

$$f(x) = f(0) + \frac{x}{h}\Delta f_o + \frac{x(x-h)}{2!h^2}\Delta^2 f_o + \frac{x(x-h)(x-2h)}{3!h^3}\Delta^3 f_o + \ldots$$

Gregory-Newton backward interpolation formula

$$f(x) = f(0) + \frac{x}{h}\Delta f_o + \frac{x(x+h)}{2!h^2}\Delta^2 f_o + \frac{x(x+h)(x+2h)}{3!h^3}\Delta^3 f_o + \ldots$$

If we rescale the x variable such that h=1, we have:
Gregory-Newton forward interpolation formula

$$f(x) = f(0) + x\Delta f_o + \frac{x(x-1)}{2!}\Delta^2 f_o + \frac{x(x-1)(x-2)}{3!}\Delta^3 f_o + \ldots$$

Gregory-Newton backward interpolation formula

$$f(x) = f(0) + x\Delta f_o + \frac{x(x+1)}{2!}\Delta^2 f_o + \frac{x(x+1)(x+2)}{3!}\Delta^3 f_o + \ldots$$

Note: The x axis in the difference table can be shifted so that any desired point corresponds to x=0 (i.e., where we developed the difference tables based on the Taylor expansion).

<u>*4.4 Unevenly spaced data: Lagrange Polynomials*</u>

Consider a set of data $f(x_i)$ where the x_i are not evenly spaced and there are i=n data points. We can define a polynomial of degree n associated with each point x_j as:

$$P_j(x) = A_j(x-x_0)(x-x_1)(x-x_2)\ldots(x-x_{j-1})(x-x_{j+1})(x-x_n)$$ (Note: exclude x_j term)

Where A_j is a constant. Thus, $P_j(x) = A_j \prod_{\substack{i=0 \\ i\neq j}}^{n}(x-x_i)$

So, when x is equal to any of the x_i values, P_j=0, but P_j≠0 when x=x_j.

Then, if one of the data points in the set of data is marked as x_k: $P_j(x) = \begin{cases} 0 & k \neq j \\ A_j \prod_{\substack{i=0 \\ i\neq j}}^{n}(x_j - x_i) & k = j \end{cases}$

And we define A_j as: $A_j = \dfrac{1}{\prod_{\substack{i=0 \\ i\neq j}}^{n}(x_j - x_i)}$ which means: $P_j(x) = \begin{cases} 0 & k \neq j \\ 1 & k = j \end{cases}$

The polynomials $P_j(x)$ are defined such that each one passes through zero at each data point except for the one point x_k and they are called *Lagrange polynomials.* We can form a linear combination of the $P_j(x)$:

$$p_n(x) = \sum_{j=0}^{n} f(x_j)P_j(x)$$

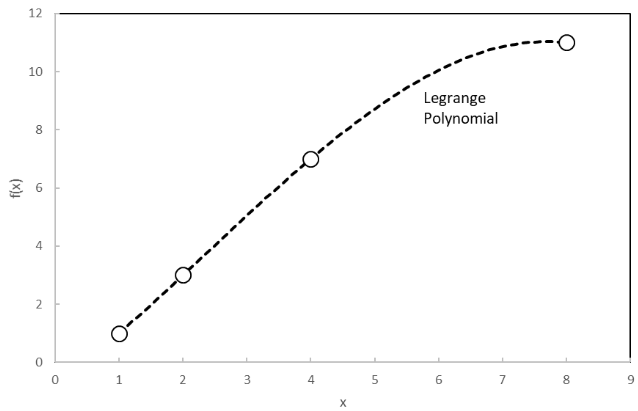
If we select one of the points (say x_2) then: $p_n(x_2) = f(x_2)$

Example: consider the following set of data
We wish to interpolate for $f(7)$, then:

i	0	1	2	3
x_i	1	2	4	8
$f(x_i)$	1	3	7	11

$$p_3(7) = f(1)P_o(7) + f(2)P_1(7) + f(4)P_2(7) + f(8)P_3(7) = 1P_o(7) + 3P_1(7) + 7P_2(7) + 11P_3(7)$$

$$P_j(x) = A_j \prod_{\substack{i=0\\ i\neq j}}^{n} (x - x_i);\ A_j = \frac{1}{\prod_{\substack{i=0\\ i\neq j}}^{n} (x_j - x_i)}$$



$$P_0(7) = \frac{(7-2)(7-4)(7-8)}{(1-2)(1-4)(1-8)} = 0.71429$$

$$P_1(7) = \frac{(7-1)(7-4)(7-8)}{(2-1)(2-4)(2-8)} = -1.5$$

$$P_2(7) = \frac{(7-1)(7-2)(7-8)}{(4-1)(4-2)(4-8)} = 1.25$$

$$P_3(7) = \frac{(7-1)(7-2)(7-4)}{(8-1)(8-2)(8-4)} = 0.53571$$

$$f(7) = 10.85710$$

4.6 Interpolation with Cubic Spline Function

Given a set of points x_i (i=0, 1, 3,…,n) which are not generally evenly spaced, and the corresponding $f(x_i)$, consider two adjacent points x_i and x_{i+1}. We wish to fit a cubic $F_i(x)$ to these two points and use it as an interpolating function between them.

$$F_i(x) = a_0 + a_1(x - x_i) + a_2(x - x_i)^2 + a_3(x - x_i)^3 \quad \text{for } (x_i \le x \le x_{i+1})$$

We have four unknowns and two end conditions: $F_i(x_i)=f(x_i)$ and $F_i(x_{i+1})=f(x_{i+1})$

The next step is to also match the first and second derivatives of $F_i(x)$ to those of the cubic $F_{i-1}(x)$ in the adjacent interval ($x_{i-1} \le x \le x_i$). Carrying out this procedure for ($x_0 \le x \le x_n$) with special treatment of the end points, an approximating function for the region will be constructed consisting of the set of cubics $F_i(x)$ (i=0,1,…n-1). This function is denoted $g(x)$ and called a cubic spline.

To construct $g(x)$, it is convenient to note that, due to the matching of second derivatives of the cubics at each point x_i, the second derivative of $g(x)$ is continuous over the entire region $x_0 \le x \le x_n$. Note that since we are dealing with a cubic, the second derivative is a straight line over each interval. At any point x in the interval $x_i \le x \le x_{i+1}$:

$$g''(x) = g''(x_i) + \frac{x - x_i}{x_{i+1} - x_i}\left[g''(x_{i+1}) - g''(x_i)\right]$$

And for interval $x_{i-1} \le x \le x_i$:

$$g''(x) = g''(x_{i-1}) + \frac{x - x_{i-1}}{x_i - x_{i-1}}\left[g''(x_i) - g''(x_{i-1})\right]$$

Integrating twice with $\Delta x_i=(x_{i+1}-x_i)$ and $\Delta x_{i-1}=(x_i-x_{i-1})$ gives :

$$g(x) = F_i(x) = \frac{g''(x_i)}{6}\left[\frac{(x_{i+1} - x)^3}{\Delta x_i} - \Delta x_i (x_{i+1} - x)\right] + \frac{g''(x_{i+1})}{6}\left[\frac{(x - x_i)^3}{\Delta x_i} - \Delta x_i (x - x_i)\right] + f(x_i)\left[\frac{x_{i+1} - x}{\Delta x_i}\right] + f(x_{i+1})\left[\frac{x - x_i}{\Delta x_i}\right]$$

$$g(x) = F_{i-1}(x) = \frac{g''(x_{i-1})}{6}\left[\frac{(x_i - x)^3}{\Delta x_{i-1}} - \Delta x_{i-1} (x_i - x)\right] + \frac{g''(x_i)}{6}\left[\frac{(x - x_{i-1})^3}{\Delta x_{i-1}} - \Delta x_{i-1} (x - x_{i-1})\right] + f(x_{i-1})\left[\frac{x_i - x}{\Delta x_{i-1}}\right] + f(x_i)\left[\frac{x - x_{i-1}}{\Delta x_{i-1}}\right]$$

The expressions above are the 3rd order polynomials we need to fit the actual function in the intervals. But, it has lost the nice form of $F_i(x) = a_0 + a_1(x - x_i) + a_2(x - x_i)^2 + a_3(x - x_i)^3$. Nevertheless, if we can find the values for $g''(x)$, we can use these expressions for interpolation. To do this, we must differentiate the above expressions and remember that $F_i'(x_i) = F_{i-1}'(x_i)$, and $F_i''(x_i) = F_{i-1}''(x_i)$. Thus:

$$F_i'(x) = \frac{g''(x_i)}{6}\left[-\frac{3(x_{i+1}-x)^2}{\Delta x_i} + \Delta x_i\right] + \frac{g''(x_{i+1})}{6}\left[\frac{3(x-x_i)^2}{\Delta x_i} - \Delta x_i\right] - \frac{f(x_i)}{\Delta x_i} + \frac{f(x_{i+1})}{\Delta x_i}$$

$$F_i''(x) = \frac{g''(x_i)}{6}\left[\frac{6(x_{i+1}-x)}{\Delta x_i}\right] + \frac{g''(x_{i+1})}{6}\left[\frac{6(x-x_i)}{\Delta x_i}\right]$$

$$F_{i-1}'(x) = \frac{g''(x_{i-1})}{6}\left[-\frac{3(x_i-x)^2}{\Delta x_{i-1}} + \Delta x_{i-1}\right] + \frac{g''(x_i)}{6}\left[\frac{3(x-x_{i-1})^2}{\Delta x_{i-1}} - \Delta x_{i-1}\right] - \frac{f(x_{i-1})}{\Delta x_{i-1}} + \frac{f(x_i)}{\Delta x_{i-1}}$$

$$F_{i-1}''(x) = \frac{g''(x_{i-1})}{6}\left[\frac{6(x_i-x)}{\Delta x_{i-1}}\right] + \frac{g''(x_i)}{6}\left[\frac{6(x-x_{i-1})}{\Delta x_{i-1}}\right]$$

At $x=x_i$:

$$F_i'(x_i) = \frac{g''(x_i)}{6}[-2\Delta x_i] + \frac{g''(x_{i+1})}{6}[-\Delta x_i] - \frac{f(x_i)}{\Delta x_i} + \frac{f(x_{i+1})}{\Delta x_i} \qquad F_i''(x_i) = g''(x_i)$$

$$F_{i-1}'(x_i) = \frac{g''(x_{i-1})}{6}[\Delta x_{i-1}] + \frac{g''(x_i)}{6}[2\Delta x_{i-1}] - \frac{f(x_{i-1})}{\Delta x_{i-1}} + \frac{f(x_i)}{\Delta x_{i-1}} \qquad F_{i-1}''(x_i) = g''(x_i)$$

Since $F_i'(x_i) = F_{i-1}'(x_i)$ & $F_i''(x_i) = F_{i-1}''(x_i)$:

$$-\Delta x_i \frac{g''(x_i)}{3} - \Delta x_i \frac{g''(x_{i+1})}{6} - \frac{f(x_i)}{\Delta x_i} + \frac{f(x_{i+1})}{\Delta x_i} = \Delta x_{i-1}\frac{g''(x_{i-1})}{6} + \Delta x_{i-1}\frac{g''(x_i)}{3} - \frac{f(x_{i-1})}{\Delta x_{i-1}} + \frac{f(x_i)}{\Delta x_{i-1}}$$

$$[\Delta x_{i-1} + \Delta x_i]\frac{g''(x_i)}{3} + \Delta x_i\frac{g''(x_{i+1})}{6} + \Delta x_{i-1}\frac{g''(x_{i-1})}{6} = \frac{f(x_{i+1})}{\Delta x_i} + \frac{f(x_{i-1})}{\Delta x_{i-1}} - f(x_i)\left[\frac{1}{\Delta x_{i-1}} + \frac{1}{\Delta x_i}\right]$$

$$2[\Delta x_{i-1} + \Delta x_i]g''(x_i) + [\Delta x_i]g''(x_{i+1}) + \Delta x_{i-1}g''(x_{i-1}) = \frac{6f(x_{i+1})}{\Delta x_i} + \frac{6f(x_{i-1})}{\Delta x_{i-1}} - 6f(x_i)\left[\frac{1}{\Delta x_{i-1}} + \frac{1}{\Delta x_i}\right]$$

$$\boxed{\frac{2[x_{i+1} - x_{i-1}]}{\Delta x_i}g''(x_i) + g''(x_{i+1}) + \frac{\Delta x_{i-1}}{\Delta x_i}g''(x_{i-1}) = 6\left[\frac{f(x_{i+1}) - f(x_i)}{\Delta x_i^2} - \frac{f(x_{i-1}) - f(x_i)}{\Delta x_{i-1}\Delta x_i}\right]}$$

We could simplify the notation to:

$$\boxed{2\lambda_i g''(x_i) + g''(x_{i+1}) + \mu_i g''(x_{i-1}) = 6f(x_{i-1}, x_i, x_{i+1})} \text{ where } \lambda_i = \frac{[x_{i+1} - x_{i-1}]}{\Delta x_i},\ \mu_i = \frac{\Delta x_{i-1}}{\Delta x_i}$$

Thus, for all intervals i=1,2,…,n-1 we have this equation.
If the x_i are evenly spaced then λ_i=2, μ_i=1 and:

$$4g''(x_i) + g''(x_{i+1}) + g''(x_{i-1}) = 6\left[\frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x_i^2}\right]$$

We can specify that $g''(x_0)$=0 and $g''(x_n)$=0 to produce a *natural cubic spline*.
Or, we can specify ghat $g'(x_0)=\alpha$ and $g'(x_n)=\beta$ to produce a *clamped cubic spline.*

<u>*Natural cubic spline*</u>:
The set of equations for n data points can be put in matrix form as follows:

$$\begin{bmatrix} 1 & 0 & & & \\ \mu_1 & 2\lambda_i & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \mu_{n-1} & 2\lambda_{n-1} & 1 \\ & & & 0 & 1 \end{bmatrix} \begin{bmatrix} g''_0 \\ g''_i \\ \vdots \\ g''_{n-1} \\ g''_n \end{bmatrix} = \begin{bmatrix} f''(x_0) \\ 6f[x_0, x_1, x_2] \\ \vdots \\ 6f[x_{n-2}, x_{n-1}, x_n] \\ f''(x_n) \end{bmatrix}$$

Now, solve this set of linear equations and use expression for $F(x)$ to find estimates of $f(x)$.

<u>*Clamped cubic spline*</u>:

For point x_0, we know that: $F'(x_0) = \alpha = \frac{g''(x_0)}{6}[-2\Delta x_0] + \frac{g''(x_1)}{6}[-\Delta x_0] - \frac{f(x_0)}{\Delta x_0} + \frac{f(x_1)}{\Delta x_0}$

and at x_n, we have: $F'_{i-1}(x_n) = \beta = \frac{g''(x_{n-1})}{6}[\Delta x_{n-1}] + \frac{g''(x_n)}{6}[2\Delta x_{n-1}] - \frac{f(x_{n-1})}{\Delta x_{n-1}} + \frac{f(x_n)}{\Delta x_{n-1}}$

The matrix equation is then:

$$\begin{bmatrix} \left(-\frac{\Delta x_0}{3}\right) & \left(-\frac{\Delta x_0}{6}\right) & & & \\ \mu_1 & 2\lambda_i & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \mu_{n-1} & 2\lambda_{n-1} & 1 \\ & & & \left(-\frac{\Delta x_{n-1}}{6}\right) & \left(-\frac{\Delta x_{n-1}}{3}\right) \end{bmatrix} \begin{bmatrix} g''_0 \\ g''_i \\ \vdots \\ g''_{n-1} \\ g''_n \end{bmatrix} = \begin{bmatrix} \alpha + \frac{f(x_0)}{\Delta x_0} - \frac{f(x_1)}{\Delta x_0} \\ 6f[x_0, x_1, x_2] \\ \vdots \\ 6f[x_{n-2}, x_{n-1}, x_n] \\ \beta + \frac{f(x_{n-1})}{\Delta x_{n-1}} - \frac{f(x_n)}{\Delta x_{n-1}} \end{bmatrix}$$

Now, solve this set of linear equations and use expression for $F(x)$ to find estimates of $f(x)$.

<u>*Natural cubic spline example*</u>:

i	0	1	2	3	4
x_i	1	4	6	9	10
$f(x_i)$	4	9	15	7	3

We want to approximate $f(5)$.
First, set $g''(1)=g''(10)=0$.

Now, for i=1: $2\frac{(6-1)}{(6-4)}g''(4) + g''(6) = 6\left[\frac{15-9}{(6-4)^2} - \frac{9-4}{(6-4)(4-1)}\right] \rightarrow 5g''(4) + g''(6) = 4$

For i=2: $0.6667g''(4) + 0.3333g''(6) + g''(9) = -11.3333$

For i=3: $3g''(6) + 8g''(9) = -8$

Solving simultaneously: $g''(4) = 1.56932;\ g''(6) = -3.84661;\ g''(9) = 0.44248$

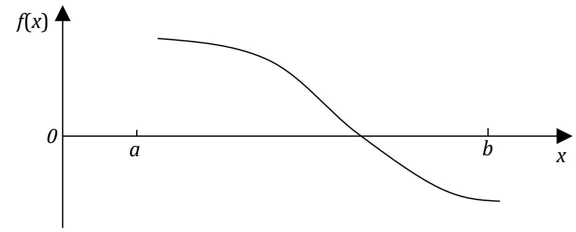
Substitution yields: $F_1(5)=12.56932$

Note: once we have all the $g''(x_i)$ values, we just pick the appropriate interval for the desired x.

Ch. 5: Roots of Equations

The usual root solving problem involves an equation such as $Ax^3 + Bx^2 = Cx + D$, which gets manipulated to $Ax^3 + Bx^2 - Cx - D = 0$ and we search for values of *x* that satisfy the equation. These values of *x* are the roots of the equation; that is, where $f(x_{root})=0$.

<ins>*5.1 Bisection*</ins>



Consider the simplest case where $f(x)$ has only one real root in the interval $a \le x \le b$. Bisect the interval $x_m=(a+b)/2$ and compute $f(x_m)*f(b)$. If the product is positive, then the root must be in the interval $a<x<x_m$ if negative $x_m<x<b$. Select the interval which contains the root, biset it and repeat the entire procedure. This works for a single root, but if multiple roots exist, bisection gets very complicated.

<ins>*5.2 Newton's Method (Newton-Raphson)*</ins>

Consider a point x_0, which is not a root of $f(x)$, but is "reasonably close" to a root. Expand $f(x)$ as a Taylor series:

$$f(x) = f(x_0) + (x-x_0) f'(x_o) + \frac{(x-x_0)^2}{2} f''(x_0) + \frac{(x-x_0)^3}{3!} f'''(x_o) + \ldots$$

If $f(x) = 0$, then *x* must be a root and the right-hand side constitutes an equation for the root *x*. Set rhs equal to zero and keep only two terms:

$$0 = f(x_0) + (x-x_0) f'(x_o) \to x = x_0 - \frac{f(x_0)}{f'(x_o)} \to x - x_0 = \delta = -\frac{f(x_0)}{f'(x_0)}$$

Now *x* represents an improved estimate of the root, and can replace x_0 to yield an even better estimate of the root on the next iteration:

$$x^{(n+1)} - x^{(n)} = \delta^{(n+1)} = -\frac{f\left(x^{(n)}\right)}{f'\left(x^{(n)}\right)}$$

Newton's method algorithm:

i) input x_0, ϵ, *ii*) $x \leftarrow x_0$, *iii*) $\delta \leftarrow f(x)/f'(x)$, *iv*) $x \leftarrow x+\delta$, *v*) $|\delta|<\epsilon$?(root←x):(step *iii-v*)

<ins>*5.3 Modified Newton's Method*</ins>

Let $u(x) = \dfrac{f(x)}{f'(x)}$. Now, $u(x)$ will have same roots as $f(x)$. Next, apply *Newton's Method* to $u(x)$:

$$x^{(n+1)} - x^{(n)} = \delta^{(n+1)} = -\frac{u\left(x^{(n)}\right)}{u'\left(x^{(n)}\right)} \text{ where } u'(x) = \frac{\left(f'(x)\right)^2 - f(x) f''(x)}{\left(f'(x)\right)^2} = 1 - \frac{f(x) f''(x)}{\left(f'(x)\right)^2}$$

Note: the *Modified Newton's Method* is useful for functions with multiple roots.

5.4 The Secant Method

The secant method is a modification to the conventional *Newton's method* with the derivative replaced by a difference expression:

$$x^{(n+1)} - x^{(n)} = \delta^{(n+1)} = -\frac{f\left(x^{(n)}\right)}{\left[f\left(x^{(n)}\right) - f\left(x^{(n-1)}\right)\right] / \delta^{(n)}}$$

Secant method algorithm to find roots of f(x)=0.

i) input values for x_0, x_{00}, and ϵ.
ii) Calculate $\delta = x_0 - x_{00}$
iii) Set $x = x_0$
iv) Compute $f_{old} = f(x_{00})$
v) Compute $f_{new} = f(x)$
vi) Compute $\delta = -f_{new}/[(f_{new} - f_{old})/\delta]$
vii) Set $x = x + \delta$
viii) If $|\delta| < \epsilon$: return x
ix) If $|\delta| > \epsilon$: $f_{old} = f_{new}$ and repeat steps ***v)*** to ***ix)***

Ch. 6 The Solution of Simultaneous Linear Algebraic Equations and Matrix Inversion

Matrix terminology:

$D=\begin{bmatrix}2\\7\\3\\5\end{bmatrix}$ is a *column matrix* (also a vector), $F=\begin{bmatrix}1 & -3 & 5 & 2\end{bmatrix}$ is a *row matrix*

$C=\begin{bmatrix}c_{11} & c_{12} & c_{13} & c_{14}\\ c_{21} & c_{22} & c_{23} & c_{24}\\ c_{31} & c_{32} & c_{33} & c_{34}\\ c_{41} & c_{42} & c_{43} & c_{44}\end{bmatrix}$ is a 4×4 square matrix with a *main diagonal* of c_{11}, c_{22}, c_{33}, c_{44}.

The square matrix is symmetric if $c_{ij}=c_{ji}$.

$C=\begin{bmatrix}c_{11} & c_{12} & c_{13} & c_{14}\\ 0 & c_{22} & c_{23} & c_{24}\\ 0 & 0 & c_{33} & c_{34}\\ 0 & 0 & 0 & c_{44}\end{bmatrix}$ is an *upper triangular* matrix, $C=\begin{bmatrix}c_{11} & c_{12} & 0 & 0\\ c_{21} & c_{22} & c_{23} & 0\\ 0 & c_{32} & c_{33} & c_{34}\\ 0 & 0 & c_{43} & c_{44}\end{bmatrix}$ is a *banded matrix*

$I=\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$ is the *identity matrix*

Basic Matix operations:

Addition: $S=A+B$; $s_{ij}=a_{ij}+b_{ij}$; A+B=B+A; A-B=-B+A

Multiplication: $P=AB$; $p_{ij}=\sum_{k=1}^{n}a_{ik}b_{ki}$ (n×m · m× w yields n×w matrix); AI=A; AB≠BA in general

Matrix Representation and Formal Solution of Simultaneous Linear Equations:

$$\begin{aligned}c_{11}x_1+c_{12}x_2+c_{13}x_3+c_{14}x_4&=r_1\\ c_{21}x_1+c_{22}x_2+c_{23}x_3+c_{24}x_4&=r_2\\ c_{31}x_1+c_{32}x_2+c_{33}x_3+c_{34}x_4&=r_3\\ c_{41}x_1+c_{42}x_2+c_{43}x_3+c_{44}x_4&=r_4\end{aligned}$$
can be expressed as:
$$\begin{bmatrix}c_{11} & c_{12} & c_{13} & c_{14}\\ c_{21} & c_{22} & c_{23} & c_{24}\\ c_{31} & c_{32} & c_{33} & c_{34}\\ c_{41} & c_{42} & c_{43} & c_{44}\end{bmatrix}\begin{bmatrix}x_1\\x_2\\x_3\\x_4\end{bmatrix}=\begin{bmatrix}r_1\\r_2\\r_3\\r_4\end{bmatrix}$$
or $CX=R$

Ways to solve $CX=R$ are:

Cramer's rule:

1.) $x_k=\dfrac{\det(C_k)}{\det(C)}$ where C_k is C with its k^{th} column replaced by R. det(C) means determinant of C

2.) $X=C^{-1}R$ where C^{-1} is the inverse of C

Gaussian elimination

Ax=b → A⁻¹Ax=A⁻¹b → x=A⁻¹b

To reduce a matrix **A** to echelon form, we perform the basic row operations of:

i) exchange rows
ii) multiply row by a scalar
iii) add scalar multiple of another row to replace a row
Goal is to get 1's along the matrix diagonal

Gauss-Jordan Method

Use Gaussian elimination the put ***A*** in echelon form and then use rule iii) to make all other values in a column 0 except for along the body diagonal.

Observation: $\mathbf{A^{-1}A = I}$
If I use Gauss-Jordan method on matrix [**A**|**I**], I will find the result to be [**I**|$\mathbf{A}^{-1}$]

Gauss-Sidel Iteration:

Consider the example of three equations solved for x_1, x_2, and x_3,:

$$\begin{aligned} c_{11}x_1 + c_{12}x_2 + c_{13}x_3 &= r_1 \qquad & x_1 &= \left(r_1 - c_{12}x_2 - c_{13}x_3\right)/c_{11} \\ c_{21}x_1 + c_{22}x_2 + c_{23}x_3 &= r_2 \rightarrow & x_2 &= \left(r_2 - c_{21}x_1 - c_{23}x_3\right)/c_{22} \\ c_{31}x_1 + c_{32}x_2 + c_{33}x_3 &= r_3 & x_3 &= \left(r_3 - c_{31}x_1 - c_{32}x_2\right)/c_{33} \end{aligned}$$

Algorithm for Gauss-Sidel for $\boldsymbol{Ax}=\boldsymbol{b}$:

i) Create an augmented matrix $\boldsymbol{M}=[\boldsymbol{A}|\boldsymbol{b}]$ such that $\boldsymbol{M}$ is $m\times n$ (generally $n=m+1$)
ii) Exchange rows of $\boldsymbol{M}$ so that the largest numbers (absolute value) occur along body diagonal.
iii) Guess initial values for $x_1, x_2, \ldots x_m$.
iv) Calculate new x_i by $x_i = \dfrac{\left(b_i - \sum_{j\neq i,\, j=1}^{n-1} c_{ij}x_j\right)}{c_{ii}}$
v) With updated x_i, calculate x_{i+1} by **iv)**. After updating x_m, one iteration is complete
vi) Repeat steps **iv)** & **v)** for desired number of iterations or until change in x_i is sufficiently small.
vii) Return $\boldsymbol{x}$.

Ch. 7 Least-Squares Curve Fitting

Consider a function $f(x)$ that is to be approximated with a function $g(x)$. The approximating function distance from the true function can be calculated as: $d(x) = \left| f(x) - g(x) \right|$

If data is available at discrete x coordinates (x_i) and there are n such coordinates, then $d(x)$ is minimized in the least-squares sense if: $E = \sum_{i=1}^{n} d^2(x_i)$ is minimized. Most commonly, we use a polynomial of degree l for the approximating function: $g(x) = a_o + a_1 x + a_2 x^2 + \dots + a_i x^l$. Now we have:

$$E = \sum_{i=1}^{n} \left[a_0 + a_1 x_i + a_2 x_i^2 + \dots + a_i x_i^l - f(x_i) \right]^2$$

Note that E is minimized by varying the (l+1) coefficients. Note, setting the partial derivative of E w.r.t. each coefficient equal to zero, accomplishes the minimization.

$$\frac{\partial E}{\partial a_0} = \frac{\partial}{\partial a_0} \sum_{i-1}^{n} \left[a_0 + a_1 x_i + a_2 x_i^2 + \dots + a_l x_i^l - f(x_i) \right]^2$$

$$= \frac{\partial}{\partial a_0} [\ \ ]^2 = \sum_{i-1}^{n} 2[\ \ ] \left\{ \frac{\partial}{\partial a_0} [\ \ ] \right\}$$

$$= \sum_{i=1}^{n} 2 \left[a_0 + a_1 x_i + a_2 x_i^2 + \dots + a_l x_i^l - f(x_i) \right] (1) = 0 \qquad \text{etc.}$$

$$= n a_0 + a_1 \left[\sum_{i=1}^{n} x_i \right] + a_2 \left[\sum_{i=1}^{n} x_i^2 \right] + a_3 \left[\sum_{i=1}^{n} x_i^3 \right] + \dots + a_l \left[\sum_{i=1}^{n} x_i^l \right] = \sum_{i=1}^{n} f(x_i)$$

$$\frac{\partial E}{\partial a_1} = a_0 \left[\sum_{i=1}^{n} x_i \right] + a_1 \left[\sum_{i=1}^{n} x_i^2 \right] + a_2 \left[\sum_{i=1}^{n} x_i^3 \right] + a_3 \left[\sum_{i=1}^{n} x_i^4 \right] + \dots + a_l \left[\sum_{i=1}^{n} x_i^{l+1} \right] = \sum_{i=1}^{n} x_i f(x_i)$$

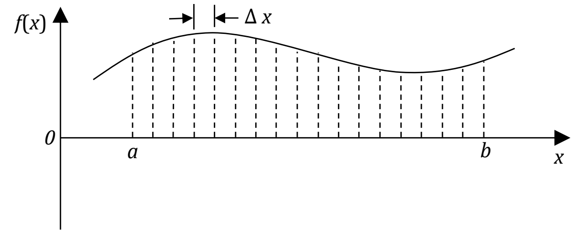
The complete set of simultaneous linear equations in the coefficients of the polynomial is:

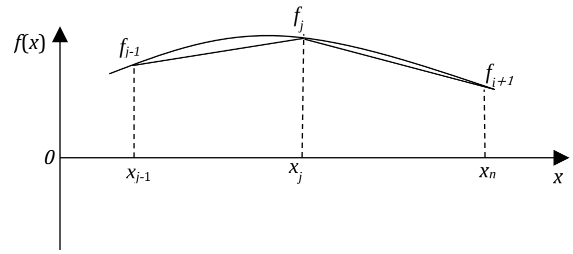
$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 & . & . & \sum x_i^l \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & . & . & \sum x_i^{l+1} \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & . & . & \sum x_i^{l+2} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \sum x_i^l & \sum x_i^{l+1} & \sum x_i^{l+2} & . & . & \sum x_i^{2l} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ . \\ . \\ a_l \end{bmatrix} = \begin{bmatrix} \sum f(x_i) \\ \sum x_i f(x_i) \\ \sum x_i^2 f(x_i) \\ . \\ . \\ \sum x_i^l f(x_i) \end{bmatrix}$$

Which, can be solved by Gauss-Jordan elimination to find the a vector and hence $g(x)$

Ch. 8: Numerical Integration

8.1 The Trapezoidal Rule





Consider an integrable function $f(x)$ on the interval $a \le x \le b$. We wish to find: $I = \int_a^b f(x)\,dx$.

We divide the interval into n equal subintervals with width of $\Delta x=(b-a)/n$ and estimate the area under each interval by:

$$\int_{x_{j-1}}^{x} f(x)\,dx \approx \frac{f_{j-1}+f_j}{2}\Delta x \text{ and } \int_{x}^{x_{j+1}} f(x)\,dx \approx \frac{f_j+f_{j+1}}{2}\Delta x$$

Thus in the interval ($x_{j-1} \le x \le x_{j+1}$):

$$\int_{x_{j-1}}^{x_{j+1}} f(x)\,dx = \int_{x_{j-1}}^{x} f(x)\,dx + \int_{x}^{x_{j+1}} f(x)\,dx \approx \frac{f_{j-1}+2f_j+f_{j+1}}{2}\Delta x$$

So for the interval $a \le x \le b$:

$$\int_a^b f(x)\,dx = \frac{\Delta x}{2}\left(f_0 + f_n + 2\sum_{j-1}^{n-1} f_j \right)$$

Note: this method implicitly uses a linear interpolation between points to estimate $f(x)$.

If the indefinite integral is defined as: $I(x)=\int_a^x f(x)\,dx$ and x_j is located at the dividing line between two panels, then $I(x_j)$ is the area under $f(x)$ from $x=a$ to this dividing line. The quantity $I(x_{j+1})$ is then composed of this area plus the area of one more panel. Assuming that $I(x)$ is analytic, then $I(x_{j+1})$ can be obtained from the Taylor series expansion about x_j:

$$I(x_j+\Delta x) = I(x_{j+1}) = I(x_j) + (\Delta x) I'(x_j) + \frac{(\Delta x)^2}{2} I''(x_j) + \frac{(\Delta x)^3}{3!} I'''(x_j) + \mathcal{O}(\Delta x)^4$$

Note: $I(x)=\int_a^x f(x)\,dx, \quad I'(x)=f(x_j), \quad I''(x)=f'(x)$, etc.

Now, $I(x_{j+1}) = I(x_j) + (\Delta x) f'(x_j) + \frac{(\Delta x)^2}{2} f'(x_j) + \frac{(\Delta x)^3}{3!} f''(x_j) + \mathcal{O}(\Delta x)^4$

We can estimate the first derivative with a simple forward difference representation:

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{\Delta x} - \frac{\Delta x}{2} f''(x_i) + \mathcal{O}(\Delta x)^2$$

And substitute this into the integral expression and collect terms:

$$I(x_{j+1}) = I(x_j) + \frac{\Delta x}{2}\left[f(x_{j+1}) + f(x_j) \right] - \frac{(\Delta x)^3}{12} f''(x_j) + \mathcal{O}(\Delta x)^4$$

The single panel integral approximation is:

$$S_{j+1} = I(x_{j+1}) - I(x_j) = \frac{\Delta x}{2}\left[f(x_{j+1}) + f(x_j) \right] - \frac{(\Delta x)^3}{12} f''(x_j) + \mathcal{O}(\Delta x)^4$$

Thus:

$$I = \sum_{j=1}^{n} S_j = \frac{\Delta x}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f(x_j) \right] - \frac{(\Delta x)^3}{12} \sum_{j=1}^{n-1} f''(x_j) + \textit{higher order terms}$$

The last term can be represented as:

$$\sum_{j=1}^{n-1} f''(x_j) = n f''(\bar{x})$$, where $a \le \bar{x} \le b$ such that $n f''(\bar{x}) = \frac{b-a}{\Delta x} f''(\bar{x})$

And the integral becomes:

$$I = \frac{\Delta x}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f(x_j) \right] - \frac{(\Delta x)^2}{12}(b-a) f''(\bar{x}) + \textit{higher order terms}$$

We can estimate $f''(\bar{x})$ as: $f''(\bar{x}) = \frac{f'(b) - f'(a)}{b-a}$

$$I \approx \frac{\Delta x}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f(x_j) \right] - \frac{(\Delta x)^2}{12}\left[f'(b) - f'(a) \right]$$

This is the *trapezoidal rule with end correction*.

8.2 Simpson's Rule

Instead of a linear interpolation, what if we use a parabolic arc interpolation function. Consider the following expansion of the integral as a function of *x*:

$$I\left(x_j+\Delta x\right)=I\left(x_{j+1}\right)=$$

$$I\left(x_j\right)+\left(\Delta x\right)f'(x_j)+\frac{\left(\Delta x\right)^2}{2}f'(x_j)+\frac{\left(\Delta x\right)^3}{3!}f''(x_j)+\frac{\left(\Delta x\right)^4}{4!}f'''(x_j)+\frac{\left(\Delta x\right)^5}{5!}f^{iv}(x_j)+\frac{\left(\Delta x\right)^6}{6!}f^{v}(x_j)+\mathcal{O}\left(\Delta x\right)^7$$

and

$$I\left(x_j-\Delta x\right)=I\left(x_{j-1}\right)=$$

$$I\left(x_j\right)-\left(\Delta x\right)f'(x_j)+\frac{\left(\Delta x\right)^2}{2}f'(x_j)-\frac{\left(\Delta x\right)^3}{3!}f''(x_j)+\frac{\left(\Delta x\right)^4}{4!}f'''(x_j)-\frac{\left(\Delta x\right)^5}{5!}f^{iv}(x_j)+\frac{\left(\Delta x\right)^6}{6!}f^{v}(x_j)+\mathcal{O}\left(\Delta x\right)^7$$

Subtracting:

$$I\left(x_{j-1}\right)-I\left(x_{j+1}\right)=2\left(\Delta x\right)f(x_j)+\frac{\left(\Delta x\right)^3}{3}f''(x_j)+\frac{\left(\Delta x\right)^5}{60}f^{iv}(x_j)+\mathcal{O}\left(\Delta x\right)^7$$

Using a central difference for $f''(x_j)$:

$$f''\left(x_j\right)=\frac{f\left(x_{j+1}\right)-2f\left(x_j\right)+f\left(x_{j-1}\right)}{\left(\Delta x\right)^2}-\frac{\left(\Delta x\right)^2}{12}f^{iv}\left(x_j\right)+\mathcal{O}\left(\Delta x\right)^4$$

Substituting into the previous equation to get area between two panels x_{j-1} and x_{j+1}:

$$I\left(x_{j-1}\right)-I\left(x_{j+1}\right)=\frac{\left(\Delta x\right)}{3}\left[f\left(x_{j+1}\right)+4f\left(x_j\right)+f\left(x_{j-1}\right)\right]-\frac{\left(\Delta x\right)^5}{90}f^{iv}\left(x_j\right)+\mathcal{O}\left(\Delta x\right)^7$$

For the integral over the interval $a\le x\le b$ if $D_j=I(x_{x+1})-I(x_{j-1})$:

$I=\sum_{\substack{j=1\\ j\,odd}}^{n-1}D_j$ Note: just odd so we don't double count and this requires number of panels to be even.

If we sum for all pairs of panels then:

$$I=\frac{\Delta x}{3}\left[f_2+4f_1+f_0+f_4+4f_3+f_2+f_6+4f_5+f_4+\ldots\right]+\mathcal{O}\left(\Delta x\right)^4$$

$$I=\frac{\left(\Delta x\right)}{3}\left[f_0+f_n+4\sum_{\substack{j=1\\ j\,odd}}^{n-1}f_j+2\sum_{\substack{j=2\\ j\,even}}^{n-2}f_j\right]-\frac{\left(\Delta x\right)^4}{180}\left(b-a\right)f^{iv}\left(\bar{x}\right)+\mathcal{O}\left(\Delta x\right)^6$$

Or

$$I=\frac{\left(\Delta x\right)}{3}\left[f_0+f_n+4\sum_{\substack{j=1\\ j\,odd}}^{n-1}f_j+2\sum_{\substack{j=2\\ j\,even}}^{n-2}f_j\right]+\mathcal{O}\left(\Delta x\right)^4$$