Lecture 3

Interpolation and Numerical Differentiation

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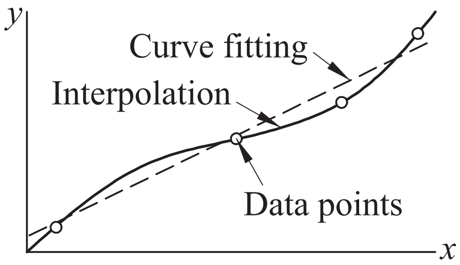
Outline

Introduction

- Interpolation is a method to estimate the value of a function between two known values.
- Curve fitting is a method to estimate the value of a function outside the range of known values.



Interpolation

- Discrete data sets of the form

x	x_0	x_1	x_2	$\cdots$	x_n
y	y_0	y_1	y_2	$\cdots$	y_n

  are commonly involved in technical calculations.
- Is it possible to find a simple and convenient formula that reproduces the given points exactly?
- If the data set contains errors, is it possible to find a formula to represent the data approximately and, filters out the errors?
- If the computation of a function f is very expensive to evaluate, is it possible to find another function g which is simpler to evaluate and gives a reasonable approximation of f?

Polynomial Interpolation

- Given discrete data sets of the form

x	x_0	x_1	x_2	$\cdots$	x_n
y	y_0	y_1	y_2	$\cdots$	y_n

  where x_i's form a set of $n+1$ distinct points.
- Find a polynomial that is defined for all x, and takes on the corresponding values of y_i for each of the $n+1$ distinct x_i's.
- A polynomial p for which $p(x_i) = y_i$ when $0 \leq i \leq n$ is said to interpolate the table. The points x_i are called nodes.

Lagrange's Method

- It is always possible to construct a unique polynomial of degree n that passes through $n+1$ distinct data points.
- The polynomial can be written as

$$P_n(x) = \sum_{i=0}^{n} l_i(x) y_i$$

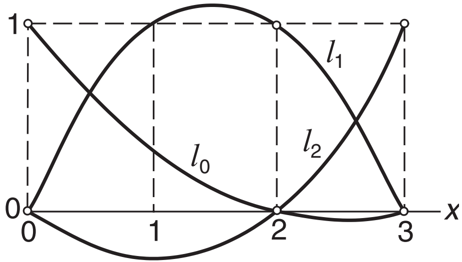
where the cardinal functions $l_i(x)$ are

$$\begin{aligned} l_i(x) &= \frac{x - x_0}{x_i - x_0} \cdot \frac{x - x_1}{x_i - x_1} \cdots \frac{x - x_{i-1}}{x_i - x_{i-1}} \cdot \frac{x - x_{i+1}}{x_i - x_{i+1}} \cdots \cdot \frac{x - x_n}{x_i - x_n} \\ &= \prod_{j=0; j\neq i}^{n} \frac{x - x_j}{x_i - x_j} \end{aligned}$$

- The cardinal functions are n degree polynomials and have the property $l_i(x_j) = \delta_{ij}$.

Example: Cardinal Functions

- Cardinal functions for a three point interpolation $(n = 2)$ with $x_0 = 0, x_1 = 2$ and $x_2 = 3$.



Newton's Method

- Lagrange's method is conceptually simple, but it can not be computed efficiently.
- A better computational method is the Newton's method, and the resulting polynomial is said to have the Newton form.

$$\begin{aligned} P_n(x) = a_0 + (x - x_0)a_1 + (x - x_0)(x - x_1)a_2 + \cdots \\ + (x - x_0)(x - x_1)(x - x_2)\cdots(x - x_{n-1})a_n. \end{aligned}$$

- The Newton and Lagrange forms are just two different derivations for precisely the same polynomial.
- The Newton form has the advantage of easy extensibility to accommodate additional data points.

Newton's Method

- Consider there are four data points ($n = 3$), and the interpolating polynomial is

$$\begin{aligned} P_n(x) &= a_0 + (x - x_0)a_1 + (x - x_0)(x - x_1)a_2 \\ &+ (x - x_0)(x - x_1)(x - x_2)a_3 \\ &= a_0 + (x - x_0)\{a_1 + (x - x_1)[a_2 + (x - x_2)a_3]\} \end{aligned}$$

- The polynomial can be evaluated backwards with the recurrence relation:

$$\begin{aligned} P_0(x) &= a_3 \\ P_1(x) &= a_2 + (x - x_2)P_0(x) \\ P_2(x) &= a_1 + (x - x_1)P_1(x) \\ P_3(x) &= a_0 + (x - x_0)P_2(x) \end{aligned}$$

Newton's Method

- For arbitrary n,

$$P_0(x) = a_n \; P_k(x) = a_{n-k} + (x - x_{n-k})P_{k-1}(x), \quad k = 1, 2, \ldots, n$$

- The coefficients of P_n are determined by the condition $y_i = P_n(x_i), i = 0, 1, \ldots, n$. This yields the coupled equations

$$\begin{aligned}
y_0 &= a_0 \\
y_1 &= a_0 + (x_1 - x_0)a_1 \\
y_2 &= a_0 + (x_2 - x_0)a_1 + (x_2 - x_0)(x_2 - x_1)a_2 \\
&\vdots \\
y_n &= a_0 + (x_n - x_0)a_1 + \cdots + (x_n - x_0)(x_n - x_1)\cdots(x_n - x_{n-1})a_n
\end{aligned}$$

Divided Differences

- Define the divided-difference notation

$$
\begin{aligned}
\nabla y_i &= \frac{y_i - y_0}{x_i - x_0}, \ i = 1, 2, \ldots, n \\
\nabla^2 y_i &= \frac{\nabla y_i - \nabla y_1}{x_i - x_1}, \ i = 2, 3, \ldots, n \\
\nabla^3 y_i &= \frac{\nabla^2 y_i - \nabla^2 y_2}{x_i - x_2}, \ i = 3, 4, \ldots, n \\
&\vdots \\
\nabla^n y_n &= \frac{\nabla^{n-1} y_i - \nabla^{n-1} y_{n-1}}{x_n - x_{n-1}}.
\end{aligned}
$$

- The solution for the coefficients is

$$
a_0 = y_0, \ a_1 = \nabla y_1, \ a_2 = \nabla^2 y_2, \ \cdots \ a_n = \nabla^n y_n
$$

Dvivided Difference Table

- It is convenient to organize the divided differences in a table.

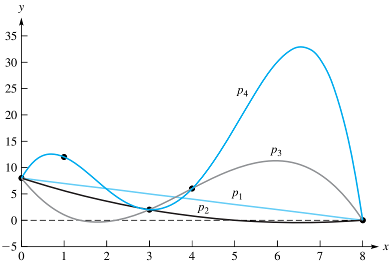
x_0	y_0				
x_1	y_1	∇y_1			
x_2	y_2	∇y_2	$\nabla^2 y_2$		
x_3	y_3	∇y_3	$\nabla^2 y_3$	$\nabla^3 y_3$	
x_4	y_4	∇y_4	$\nabla^2 y_4$	$\nabla^3 y_4$	$\nabla^4 y_4$

Errors in Polynomial Interpolation

- When a function f is approximated on an interval $[a, b]$ by an interpolating polynomial p, the discrepancy between f and p will (theoretically) be zero at each node of interpolation.
- A natural expectation is that the function f will be well approximated at all intermediate points and that as the number of nodes increases, this agreement will become better and better.
- If the function f is well-behaved, it is dangerous to assume that the differences $|f(x) - p(x)|$ will be small when the number of interpolating nodes is large, even for functions that possess continuous derivatives of all orders on the interval.

Errors in Polynomial Interpolation

- Five data points: (0, 8), (1, 12), (3, 2), (4, 6), (8, 0).



- With more points added, the situation became worse instead of better!
- The reason is that a polynomial of degree n has n zeros. If all of these zero points are real, then the curve crosses the x-axis n times, resulting in wild oscillations.

Errors in Polynomial Interpolation

- It can be shown that the error in polynomial interpolation is

$$f(x) - P_n(x) = \frac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi),$$

where ξ lies in the interval (x_0, x_n).

Warning

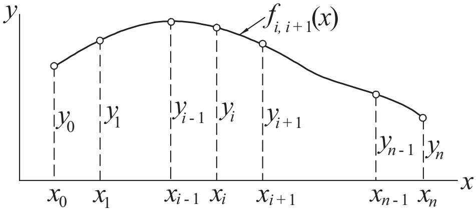
- An interpolating polynomial intersecting more than six points must be viewed with suspicion.
- The data points that are far from the point of interest do not contribute to the accuracy of the interpolating polynomial.
- If extrapolation using the interpolating polynomial is necessary, one should be careful.
- Plot the data and visually verify that the extrapolated value makes sense.
- Use a low-order polynomial based on nearest-neighbor data points.
- Work with a plot of $\log x$ vs. $\log y$, which is usually much smoother than the $x - y$ curve, and thus safer to extrapolate.

- Some data are better interpolated by rational functions rather than polynomials.
- A rational function $R(x)$ is a ratio of two polynomials:

$$R(x) = \frac{P_m(x)}{Q_n(x)} = \frac{a_1 x^m + a_2 x^{m-1} + \cdots + a_m x + a_{m+1}}{b_1 x^n + b_2 x^{n-1} + \cdots + b_n x + b_{n+1}}$$

Cubic Spline Interpolation

- A spline function is a function that consists of polynomial pieces joined together with certain smoothness conditions.
- A cubic spline is a piecewise cubic polynomial that is continuous in the first and second derivatives.



Numerical Differentiation: Introduction

- Numerical differentiation deals with the following problem: given the function $y = f(x)$, obtain its derivatives at the point $x = x_k$.
- The function is usually given as a set of discrete data points $(x_i, y_i), i = 0, 1, \dots, n$, which can be the output of some computation or measurement.
- One method to obtain numerical differentiation is through interpolation. Approximate the function locally by a polynomial and then differentiate it.
- Another method is using finite difference method based on the Taylor series.

Warning

- Numerical differentiation is not a particularly accurate process.
- It suffers from a conflict between roundoff errors (due to limited machine precision) and errors inherent in interpolation.
- A derivative of a function can never be computed with the same precision as the function itself.

Finite Difference Approximation

- Finite difference approximation is based on Taylor series expansion. It has the advantage of providing us with information about the error involved in the approximation.
- The derivation of the finite difference approximations for the derivatives of $f(x)$ is based on forward and backward Taylor series expansions of $f(x)$ about x.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \cdots$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f'''(x) + \frac{(2h)^4}{4!}f^{(4)}(x) + \cdots$$

$$f(x-2h) = f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x) - \frac{(2h)^3}{3!}f'''(x) + \frac{(2h)^4}{4!}f^{(4)}(x) - \cdots$$

Taylor Series

- The sums and differences of the series are given by

$$
\begin{aligned}
f(x+h) + f(x-h) &= 2f(x) + h^2 f''(x) + \frac{h^4}{12} f^{(4)}(x) + \cdots \\
f(x+h) - f(x-h) &= 2hf'(x) + \frac{h^3}{3} f'''(x) + \cdots \\
f(x+2h) + f(x-2h) &= 2f(x) + 4h^2 f''(x) + \frac{4h^4}{3} f^{(4)}(x) + \cdots \\
f(x+2h) - f(x-2h) &= 4hf'(x) + \frac{8h^3}{3} f'''(x) + \cdots
\end{aligned}
$$

- The sums contain only even derivatives, whereas the differences retain just the odd derivatives.
- These can be viewed as simultaneous equations that can be solved for various derivatives of $f(x)$.

First-Derivative Formulas

- The derivative for the function f at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

- The obvious method to approximate $f'(x_0)$ is

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of h.

Error

- To estimate the error in the finite difference approximation, we keep the order h^2 term in the Taylor expansion,

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{1}{2}f''(\xi)h^2,$$

where ξ is in the interval between x_0 and x_0+h.

- Rearranging, we have

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{1}{2}f''(\xi)h$$

- The truncation error of our approximation is $-\frac{1}{2}f''(\xi)h \sim O(h)$. This error will be present even if the calculations are performed with infinite precision.
- Additional round-off errors will be present when performing the calculation on a finite-precision machine.

First Non-Central Difference Formulas

- For positive h, we have the forward-difference formula

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

  and the backward-difference formula

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

- The truncation error is of order $O(h)$.

Higher Derivatives

- Approximations for higher derivatives can be derived in the same manner.
- The second derivative of $f(x)$ in the forward difference approximation is

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

- The truncation error is of order $O(h)$.
- Higher order derivatives can be obtained in the same way.

Higher Derivatives: $O(h)$

- Forward finite difference approximations of $O(h)$

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$
$hf'(x)$	-1	1			
$h^2f''(x)$	1	-2	1		
$h^3f'''(x)$	-1	3	-3	1	
$h^4f^{(4)}(x)$	1	-4	6	-4	1

- Backward finite difference approximations of $O(h)$

	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$hf'(x)$				-1	1
$h^2f''(x)$			1	-2	1
$h^3f'''(x)$		-1	3	-3	1
$h^4f^{(4)}(x)$	1	-4	6	-4	1

First Central Difference Formulas

- To improve the accuracy, one could combine the following two Taylor series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots$$
$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots$$

- Subtracting them, we obtain the first central difference approximation for $f'(x)$:

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

- The truncation error is of order $O(h^2)$.
- This formula for numerical differentiation is very useful in the numerical solution of certain differential equations.

Higher Derivatives: $O(h^2)$

- Second derivative is

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

- The truncation error is of order $O(h^2)$.
- Central finite difference approximations of $O(h^2)$:

	$f(x-2h)$	$f(x-h)$	$f(x)$	$f(x+h)$	$f(x+2h)$
$2hf'(x)$		-1	0	1	
$h^2f''(x)$		1	-2	1	
$2h^3f'''(x)$	-1	2	0	-2	1
$h^4f^{(4)}(x)$	1	-4	6	-4	1

Second Non-Central Difference Formulas

- For the forward or backward difference approximations, it is also preferable to use formulas with error of order $O(h^2)$.
- For example, to obtain $f'(x)$, we use

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots$$

$$f(x+2h) = f(x) + 2hf'(x) + 2h^2f''(x) + \frac{4h^3}{3}f'''(x) + \frac{2h^4}{3}f^{(4)}(x) + \cdots$$

- Eliminate $f''(x)$, we obtain the second forward difference formula,

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + O(h^2)$$

- The truncation error is of order $O(h^2)$.

Higher Derivatives: $O(h^2)$

- Forward finite difference approximations of $O(h^2)$

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$	$f(x+5h)$
$2hf'(x)$	-3	4	-1			
$h^2f''(x)$	2	-5	4	-1		
$2h^3f'''(x)$	-5	18	-24	14	-3	
$h^4f^{(4)}(x)$	3	-14	26	-24	11	-2

- Backward finite difference approximations of $O(h^2)$

	$f(x-5h)$	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$2hf'(x)$				1	-4	3
$h^2f''(x)$			-1	4	-5	2
$2h^3f'''(x)$		3	-14	24	-18	5
$h^4f^{(4)}(x)$	-2	11	-24	26	-14	3

Errors in Finite Difference Approximations

- The effect on since in all finite difference expressions the sum of the coefficients is zero.
- If h is very small, the values of $f(x), f(x \pm h), f(x \pm 2h)$, etc. will be approximately equal. The roundoff error can be dominant and significant figures will be lost.
- If h is too big, the truncation errors can dominate.
- To minimize this problem, use double- or higher-precision arithmetics, and employ finite difference formulas of $O(h^2)$.

Derivatives by Interpolation

- If $f(x)$ is given as a set of discrete data points, interpolation can be a very effective means of computing its derivatives.
- The derivative of $f(x)$ is approximated by the derivative of the interpolant.
- This method is particularly useful if the data points are located at uneven intervals of x, when the finite difference approximations discussed previously are not applicable.

Polynomial Interpolant

- We want to fit the data to the polynomial of degree n

$$P_{n-1}(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_n x^n$$

  through $n+1$ data points and evaluate its derivative.
- The degree of the polynomial is limited to less than 6 in order to avoid spurious oscillations of the interpolant.
- These oscillations are magnified with each differentiation.
- The interpolation should be a local one, involving no more than a few nearest-neighbor data points.
- When the data is noisy, it is advisable to use the least-squares fit to find the best fitting polynomial.

First-Derivative Formulas via Interpolation Polynomial

- If p is the polynomial of degree ≤ 1 that interpolate f at two nodes x_1, x_2,

$$p_1(x) = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_1) = f(x_1) + f[x_1, x_2](x - x_1)$$

- The first derivative

$$f'(x) \approx p_1'(x) = f[x_1, x_2] = \frac{f(x_2) - f(x_1)}{x_2 - x_1}.$$

- Interpolation through 3 nodes x_1, x_2, x_3,

$$p_2(x) = f(x_1) + f[x_1, x_2](x - x_1) + f[x_1, x_2, x_3](x - x_1)(x - x_2)$$

where $f[x_1, x_2, x_3] = (f[x_2, x_3] - f[x_1, x_2])/(x_3 - x_1)$.

- The first derivative

$$f'(x) \approx p_2'(x) = f[x_1, x_2] + f[x_1, x_2, x_3](2x - x_1 - x_2).$$

Richardson's Extrapolation

- Richardson's extrapolation is a method to generate high-accuracy results using low-order formulas.
- For a given quantity G, if we can approximate it by $g(h)$, which depends on h, with an error $E(h) = ch^p$, where c and p are constants, such that,

$$G = g(h) + E(h).$$

- For a given $h = h_1$, $G = g(h_1) + ch_1^p$, and for $h = h_2$, $G = g(h_2) + ch_2^2$.
- Eliminating c and solving for G, we obtain the Richardson extrapolation formula,

$$G = \frac{\left(\frac{h_1}{h_2}\right)^p g(h_2) - g(h_1)}{\left(\frac{h_1}{h_2}\right)^p - 1}.$$

Application to Differentiation

- It is common practice to choose $h_2 = h_1/2$, and

$$G = \frac{2^p g(h_1/2) - g(h_1)}{2^p - 1}.$$

- Consider the central difference formula

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x-h)}{2h} + a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots \\ &= \phi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots \end{aligned}$$

- $\phi(h) = \frac{f(x+h) - f(x-h)}{2h}$ is an approximation to $f'(x)$ with an error of order $O(h^2)$.

Central Difference Approximation

- Evaluate ϕ at h and $h/2$,

$$\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \dots$$
$$\phi\left(\frac{h}{2}\right) = f'(x) - a_2\left(\frac{h}{2}\right)^2 - a_4\left(\frac{h}{2}\right)^4 - a_6\left(\frac{h}{2}\right)^6 - \dots$$

- Eliminate the dominant error term $O(h^2)$,

$$\phi\left(\frac{h}{2}\right) + \frac{1}{3}\left[\phi\left(\frac{h}{2}\right) - \phi(h)\right] = f'(x) + \frac{1}{4}a_4 h^4 + \frac{5}{16}a_6 h^6 + \cdots$$

- The precision is improved to $O(h^4)$ because the error series of the new combination begins with $\frac{1}{4}a_4 h^4$.

Improved Precision

- Define
$$\Phi(h) = \phi\left(\frac{h}{2}\right) + \frac{1}{3}\left[\phi\left(\frac{h}{2}\right) - \phi(h)\right]$$
- Repeat the process, we obtain
$$\Phi\left(\frac{h}{2}\right) + \frac{1}{15}\left[\Phi\left(\frac{h}{2}\right) - \Phi(h)\right] = f'(x) - \frac{1}{20}b_6 h^6 + \cdots$$
- The precision is improved to $O(h^6)$.
- The same procedure can be repeated over and over again to kill higher and higher terms in the error.

General Form

- Let $N(h)$ be a function which approximates an unknown M, such that

$$M = N(h) + \sum_{k=1}^{\infty} a_k h^k.$$

- Assumed that $N(h)$ can be computed for any $h > 0$, so

$$M = N\left(\frac{h}{2}\right) + \sum_{k=1}^{\infty} a_k \left(\frac{h}{2}\right)^k.$$

- Eliminate the term involving a_1,

$$M = \left[2N_1\left(\frac{h}{2}\right) - N_1(h)\right] + a_2\left(\frac{h^2}{2} - h^2\right) + a_3\left(\frac{h^3}{4} - h^3\right) + \cdots,$$

where $N_1(h) \equiv N(h)$.

General Form

- Define

$$N_2(h) = \left[2N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

  and we obtain the $O(h^2)$ approximation formula ,

$$M = N_2(h) - \frac{a_2}{2}h^2 - \frac{3a_3}{4}h^3 - \cdots .$$

- Repeat the process again, we obtain the $O(h^3)$ formula,

$$\begin{aligned} M &= \left[N_2\left(\frac{h}{2}\right) - \frac{N_2\left(\frac{h}{2}\right) - N_2(h)}{3}\right] + \frac{a_3}{8}h^3 + \cdots \\ &= N_3(h) + \frac{a_3}{8}h^3 + \cdots . \end{aligned}$$

General Form

- The process can be repeated to construct an $O(h^4)$ approximation,

$$N_4(h) = N_3\left(\frac{h}{2}\right) + \frac{N_3\left(\frac{h}{2}\right) - N_3(h)}{7},$$

and $O(h^5)$ approximation ,

$$N_5(h) = N_4\left(\frac{h}{2}\right) + \frac{N_4\left(\frac{h}{2}\right) - N_4(h)}{15}.$$

General Form

- In general, if M can be written as

$$M = N(h) + \sum_{j=1}^{m-1} a_j h^j + O(h^m)$$

then for each $j = 2, 3, \cdots m$, we have an $O(h^j)$ approximation of the form

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}\left(\frac{h}{2}\right) - N_{j-1}(h)}{2^{j-1} - 1}.$$

General Form

- The approximations are generated by rows in the order indicated in the following table ($N_1(h) \equiv N(h)$):

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
1: $N_1(h)$			
2: $N_1\left(\frac{h}{2}\right)$	3: $N_2(h)$		
4: $N_1\left(\frac{h}{4}\right)$	5: $N_2\left(\frac{h}{2}\right)$	6: $N_3(h)$	
7: $N_1\left(\frac{h}{8}\right)$	8: $N_2\left(\frac{h}{4}\right)$	9: $N_3\left(\frac{h}{2}\right)$	10:$N_4(h)$