Numerical Methods in Engineering - LW5

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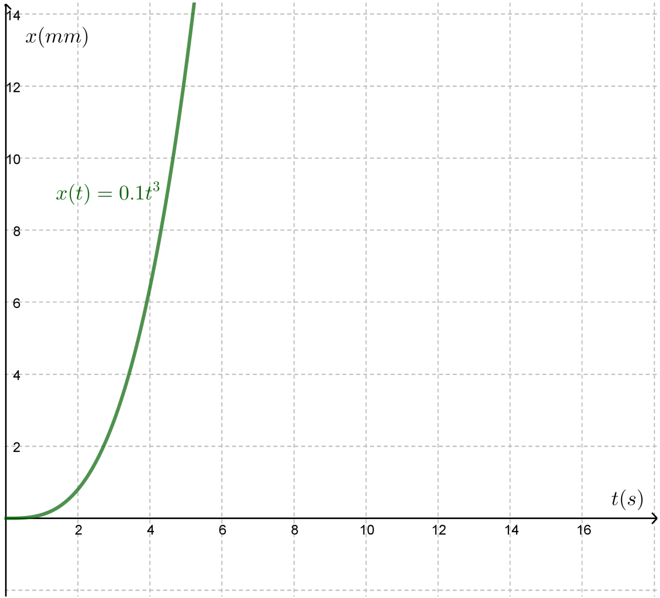
Numerical Differentiation

Introduction

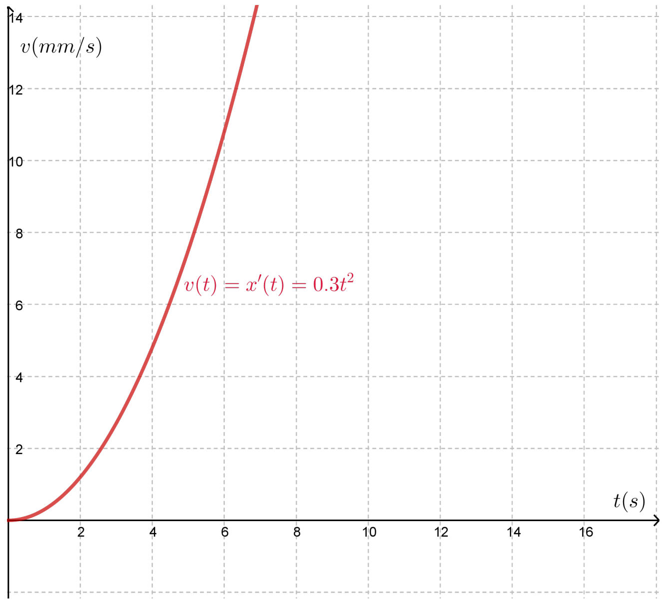
Introduction

- Differentiation provides a measure of the rate of which a certain quantity changes, [1].
- Rates of changes appear in many disciplines in science and engineering.
- The most fundamental quantities that are related with rates of change are:
  1. Position
  2. Velocity
  3. Acceleration

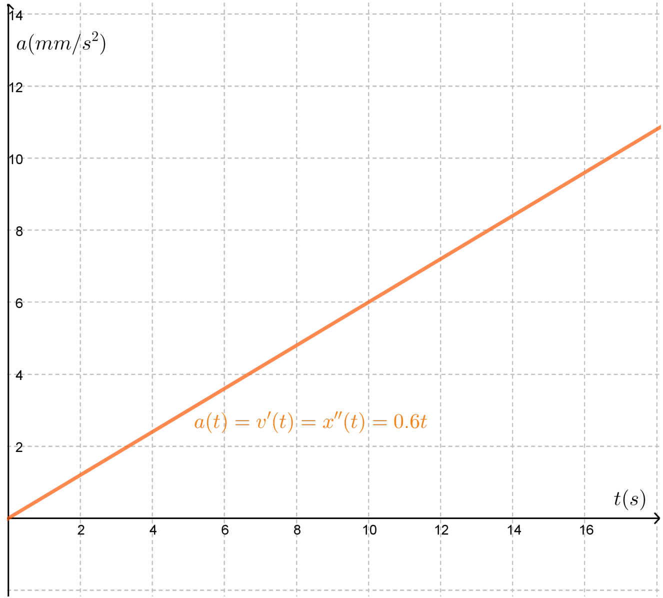
Introduction - Position



Introduction - Velocity



Introduction - Acceleration



Numerical Differentiation

- The function to be differentiated can be given as:
  1. analytical form
  2. discrete points
- In simple cases of analytical form, the derivative can be calculated analytically.
- In most cases, analytical differentiation is not possible.
- A numerical differentiation in needed.
- In addition, numerical differentiation plays important role in numerical methods used for solving differential equations.

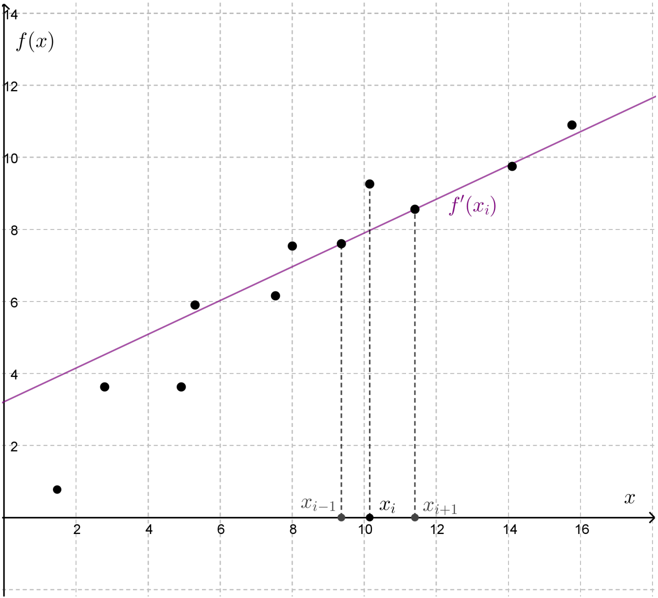
Numerical Differentiation - Approaches

There are two approaches to derive numerical differentiation for a given set of points:

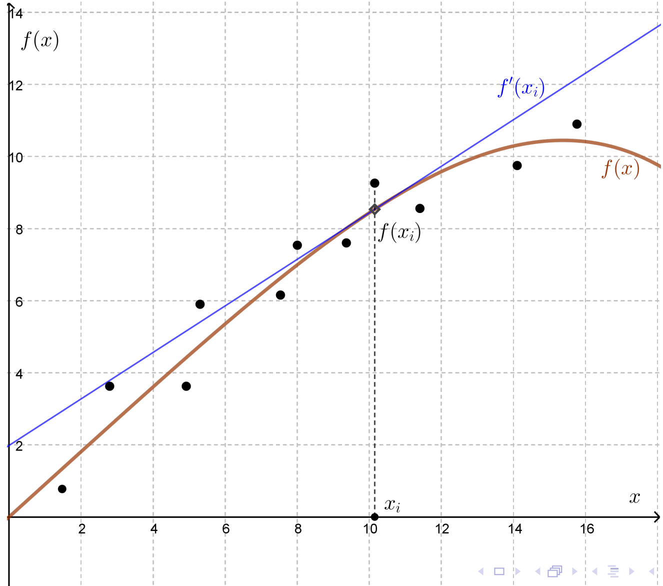
1. Finite difference approximation
2. Approximate analytical expression

- Finite difference approximation is based on the neighborhood of the points by connecting two adjacent points.
- Approximate analytical expression is based on deriving an analytical expression by using curve fitting.

Numerical Differentiation - Finite difference approximation



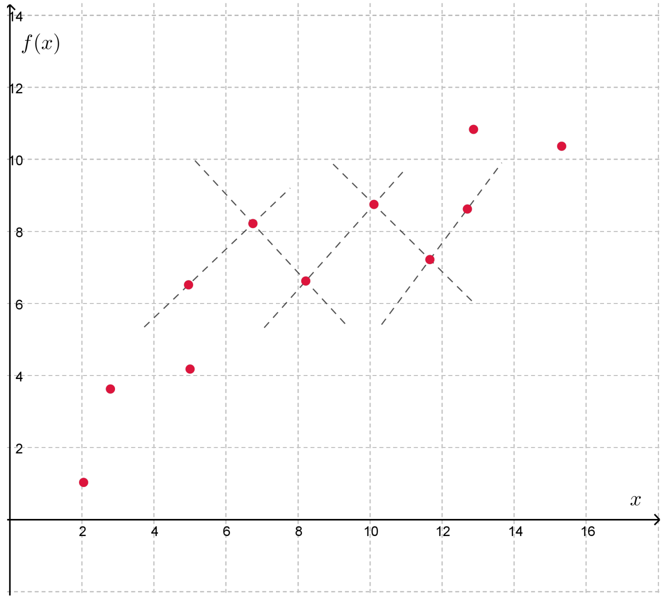
Numerical Differentiation - Approximate analytical expression



Numerical Differentiation - Approaches

- The accuracy of a finite difference approximation depends on the accuracy of the data points, the spacing between the points, and the specific formula used for the approximation.

Numerical Differentiation - Scatter Data



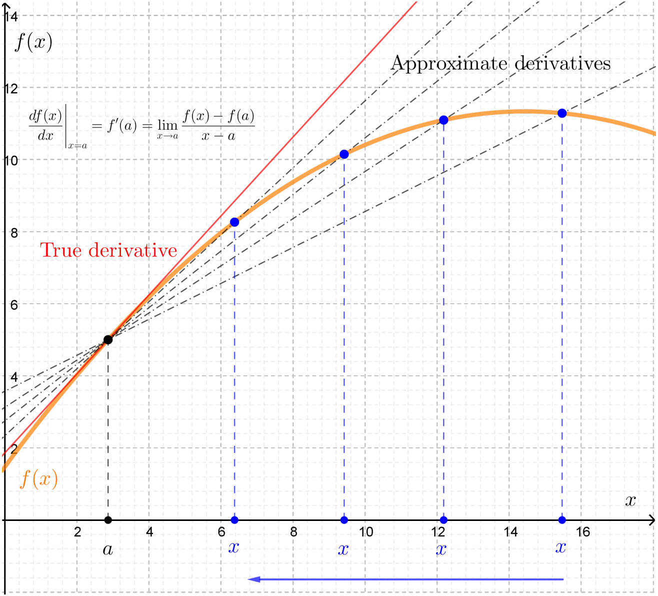
Numerical Differentiation - Scatter Data

- When data are collected through experimental measurements, there is scatter in the data due to errors or uncertainties.
- When using finite difference approximation the derivatives will vary a lot
- Higher order formulas of finite difference approximations needed that involve more than two points to derive the derivative.
- The differentiation can also be done with curve fitting, which will give reasonable results.

Numerical Differentiation - Finite Difference

Finite Difference Approximation

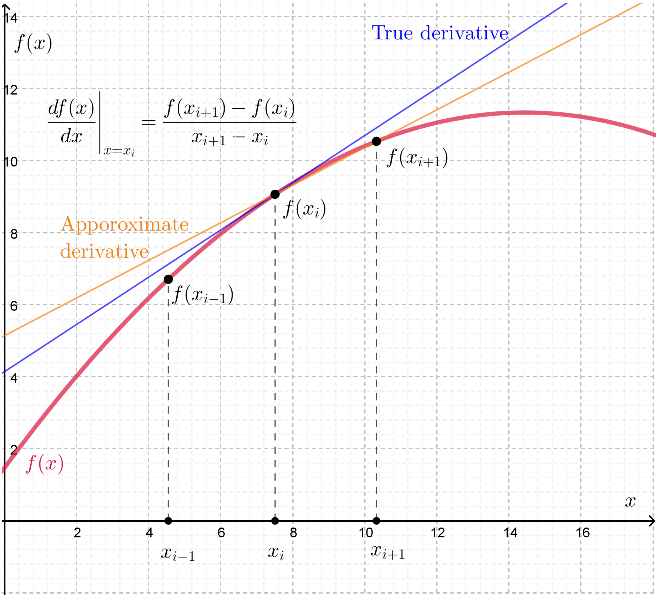
Finite Difference Approximation



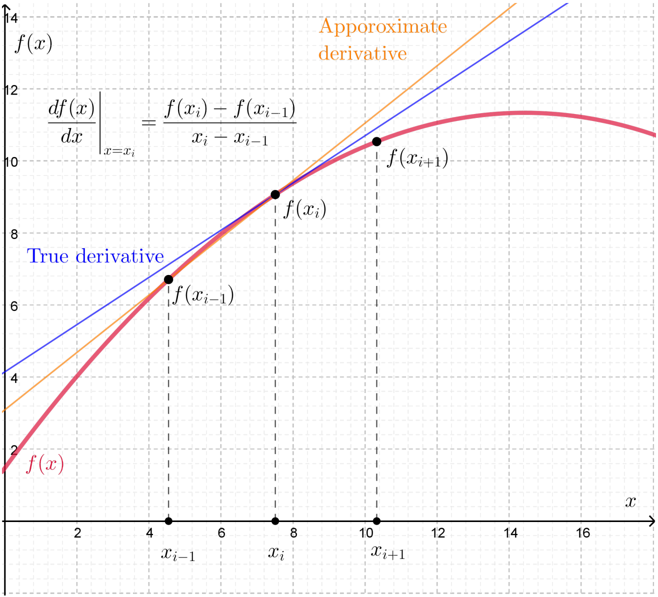
Finite Difference Approximation (F.D.A.)

- The values of the neighborhood of $x = a$ are chosen to estimate the slope.
- The function consists of discrete points.
- A variety of finite difference approximation formulas exist.
- Three of those formulas will be presented. All of them use values of two points.

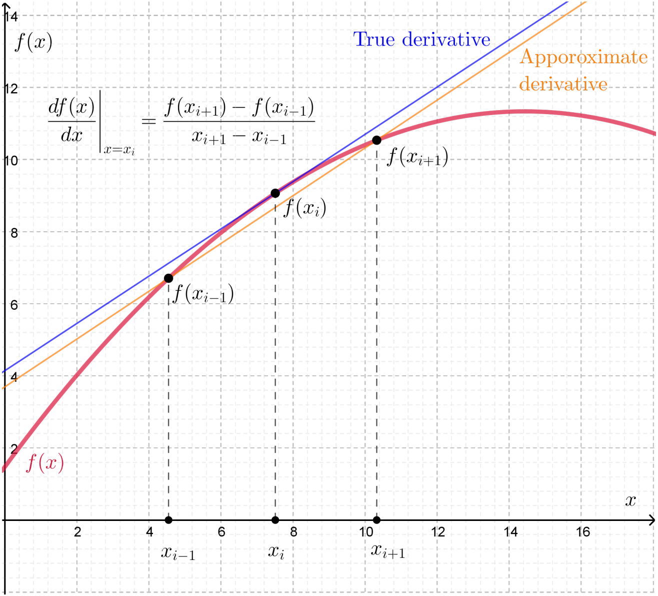
F.D.A. - Forward difference



F.D.A. - Backward difference



F.D.A. - Central difference



F.D.A. - Forward, backward and central difference

- Forward difference is the slope of the line that connects $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$:

$$\left.\frac{df(x)}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

- Backward difference is the slope of the line that connects $(x_{i-1}, f(x_{i-1}))$ and $(x_i, f(x_i))$:

$$\left.\frac{df(x)}{dx}\right|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

- Central difference is the slope of the line that connects $(x_{i-1}, f(x_{i-1}))$ and $(x_{i+1}, f(x_{i+1}))$:

$$\left.\frac{df(x)}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$

Example

F.D.A. - Forward, backward and central difference

In a vibration experiment, a block of mass m is attached to a spring of stiffness k, and a dashpot with damping coefficient c. To start the experiment the block is moved from the equilibrium position and then released from rest. The position of the block as a function of time is recorded at a frequency of 5 Hz (5 times a second). The recorded data for the first 10 s. The data points for $4 \leq t \leq 8$s are given in the table below.
Write a user-defined MATLAB function that calculates the derivative of a function that is given by a set of discrete points. Name the function dx=derivative (x,y) where x and y are vectors with the coordinates of the points, and dx is a vector with the value of the derivative $\frac{dy}{dx}$ at each point. The function should calculate the derivative at the first dx and last points using the forward and backward finite difference formulas, respectively, and using the central finite difference formula for all of the other points. Use the given data points to calculate the velocity of the block for $4 \leq t \leq 8$ s. Calculate the acceleration of the block by differentiating the velocity. Make a plot of the displacement, velocity, and acceleration, versus time for $4 \leq t \leq 8$ s

F.D.A. - Forward, backward and central difference

t(s)	4.0	4.2	4.4	4.6	4.8	5.0	5.2	5.4	5.6	5.8	6.0
x(cm)	-5.87	-4.23	-2.55	-0.89	0.67	2.09	3.31	4.31	5.06	5.55	5.78

t(s)	6.2	6.4	6.6	6.8	7.0	7.2	7.4	7.6	7.8	8
x(cm)	5.77	5.52	5.08	4.46	3.72	2.88	2.00	1.10	0.23	-0.59

Finite Difference - Taylor series

Finite Difference Formulas - Taylor series

- Taylor series expansion can be used to derive the forward, backward, central difference formulas.
- The formulas give an estimation of the derivative at a point from values in the neighborhood.
- The number of points varies with each formula.
- The points can be ahead, behind, or from both sides from which the derivative is calculated.
- An advantage of using Taylor series expansion is that it provides an estimate for the truncation error in the approximation.
- The formulas can be derived for points that are not equally spaced.

Taylor series expansion

The Taylor series (Brook Taylor) is a representation of a function as a `sum of infinite terms`, [5]. The expansion of the Taylor series about point α provides:

$$f(x) = f(\alpha)\frac{(x-\alpha)^0}{0!} + \frac{(x-\alpha)}{1!}\left.\frac{df}{dx}\right|_{x=\alpha} + \frac{(x-\alpha)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=\alpha} + \frac{(x-\alpha)^3}{3!}\left.\frac{d^3f}{dx^3}\right|_{x=\alpha} + \dots + \frac{(x-\alpha)^n}{n!}\left.\frac{d^nf}{dx^n}\right|_{x=\alpha} + R_n(x)$$

note that $(x-\alpha)^0 = 0! = 1$. R_n is called the remainder and can be defined as follows:

$$R_n(x) = \frac{(x-\alpha)^{n+1}}{(n+1)!}\left.\frac{d^{n+1}f}{dx^{n+1}}\right|_{x=\xi}$$

where ξ is a value between x and α.

Taylor series - First derivative - 2 point forward difference

The value of a function at point x_{i+1} can be approximated by a Taylor series of a function and its derivatives at point x_i:

$$f(x_{i+1}) = f(x_i)\frac{(x_{i+1}-x_i)^0}{0!} + \frac{(x_{i+1}-x_i)}{1!}\left.\frac{df}{dx}\right|_{x=x_i} + \frac{(x_{i+1}-x_i)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=x_i} + $$
$$+ \frac{(x_{i+1}-x_i)^3}{3!}\left.\frac{d^3f}{dx^3}\right|_{x=x_i} + \ldots + \frac{(x_{i+1}-x_i)^n}{n!}\left.\frac{d^nf}{dx^n}\right|_{x=x_i} + R_n(x_i)$$

Which can be written as:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f''''(x_i)}{4!}h^4 + \ldots$$

By using the two terms of Taylor series:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \Leftrightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(\xi)}{2!}h$$

If we ignore the second term on the right hand side, we can approximate the derivative (the same as forward difference formula):

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

where $O(h)$ is the truncation error and can be defined as: $O(h) = -\frac{f''(\xi)}{2!}h$

Taylor series - First derivative - 2 point backward difference

The value of a function at point x_{i-1} can be approximated by a Taylor series of a function and its derivatives at point x_i:

$$f(x_{i-1}) = f\,(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2!}(-h)^2 + \frac{f'''(x_i)}{3!}(-h)^3 + \frac{f''''(x_i)}{4!}(-h)^4$$

where $h = x_i - x_{i-1}$ and $x_{i-1} - x_i = -h$. By using the two terms of Taylor series:

$$f(x_{i-1}) = f\,(x_i) - f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \Leftrightarrow f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + \frac{f''(\xi)}{2!}h$$

If we ignore the second term on the right hand side, we can approximate the derivative (the same as backward difference formula):

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

where $O(h)$ is the truncation error and can be defined as: $O(h) = \frac{f''(\xi)}{2!}h$

Taylor series - First derivative - 2 point central difference

To derive the central difference by using three terms and a remainder. The value of the function at x_{i+1} is derived in terms of the function and its derivatives at point x_i:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3$$

The value of the function at point x_{i-1} is derived in terms of the function and its derivatives at point x_i:

$$f(x_{i-1}) = f(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2!}(-h)^2 + \frac{f'''(\xi_2)}{3!}(-h)^3$$

note that $h = x_{i+1} - x_i = x_i - x_{i-1}$ and therefore $x_{i-1} - x_i = -h$. Subtracting the two previous equations:

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\xi_1)}{3!}h^3 - \frac{f'''(\xi_2)}{3!}(-h)^3$$

Finally, the derivative can be derived:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$

Taylor series - First derivative - 3 point forward difference

The equation is the same with the central difference formula with equal intervals

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f'''(\xi_1)}{3!}(x_{i+1} - x_i)^3$$
$$f(x_{i+2}) = f(x_i) + f'(x_i)(x_{i+2} - x_i) + \frac{f''(x_i)}{2!}(x_{i+2} - x_i)^2 + \frac{f'''(\xi_2)}{3!}(x_{i+2} - x_i)^3$$

Noting that $(x_{i+1} - x_i) = h$ and $(x_{i+2} - x_i) = 2h$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3$$
$$f(x_{i+2}) = f(x_i) + f'(x_i)2h + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f'''(\xi_2)}{3!}(2h)^3$$

where ξ_1 is a value between x_{i+1} and x_i and ξ_2 is between x_{i+2} and x_i. Subtracting the second equation from the first one times 4 (so that $f''(x_i)$ disappears):

$$4f(x_{i+1}) - (x_{i+2}) = 3f(x_i) + 2f'(x_i)h + 4\frac{f'''(\xi_1)}{3!}h^3 - \frac{f'''(\xi_2)}{3!}(2h)^3 \Leftrightarrow$$
$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h} + O(h^2)$$

Taylor series - First derivative - 3 point backward difference

The equation is the same with the central difference formula with equal intervals

$$f(x_{i-1}) = f(x_i) + f'(x_i)(x_{i-1} - x_i) + \frac{f''(x_i)}{2!}(x_{i-1} - x_i)^2 + \frac{f'''(\xi_1)}{3!}(x_{i-1} - x_i)^3$$
$$f(x_{i-2}) = f(x_i) + f'(x_i)(x_{i-2} - x_i) + \frac{f''(x_i)}{2!}(x_{i-2} - x_i)^2 + \frac{f'''(\xi_2)}{3!}(x_{i-2} - x_i)^3$$

Noting that $(x_{i-1} - x_i) = -h$ and $(x_{i-2} - x_i) = -2h$:

$$f(x_{i-1}) = f(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2!}(-h)^2 + \frac{f'''(\xi_1)}{3!}(-h)^3$$
$$f(x_{i-2}) = f(x_i) + f'(x_i)(-2h) + \frac{f''(x_i)}{2!}(-2h)^2 + \frac{f'''(\xi_2)}{3!}(-2h)^3$$

where ξ_1 is a value between x_i and x_{i-1} and ξ_2 is between x_i and x_{i-2}. Subtracting the second equation from the first one times 4 (so that $f''(x_i)$ disappears):

$$4f(x_{i-1}) - f(x_{i-2}) = 3f(x_i) - 2f'(x_i)h + 4\frac{f'''(\xi_1)}{3!}h^3 - \frac{f''(\xi_2)}{3!}(2h)^3 \Leftrightarrow$$
$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2)$$

Taylor series - Second derivative - 3 point central difference

The value of a function at point x_{i+1} can be approximated by a Taylor series of a function and its derivatives at point x_i:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f'''(x_i)}{3!}(x_{i+1} - x_i)^3 + \frac{f''''(\xi_1)}{4!}(x_{i+1} - x_i)^4$$

$$f(x_{i-1}) = f(x_i) + f'(x_i)(x_{i-1} - x_i) + \frac{f''(x_i)}{2!}(x_{i-1} - x_i)^2 + \frac{f'''(x_i)}{3!}(x_{i-1} - x_i)^3 + \frac{f''''(\xi_2)}{4!}(x_{i-1} - x_i)^4$$

Noting that $x_{i+1} - x_i = h$ and $x_{i-1} - x_i = -h$ and adding the two equations in order to get rid of the first and third derivative:

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + 2\frac{f''(x_i)}{2!}h^2 + \frac{f''''(\xi_1)}{4!}h^4 + \frac{f''''(\xi_2)}{4!}h^4$$

$$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2} + O(h^2)$$

Example

Example: Second derivative - 5 point central difference

Derive the second derivative by using 5-term Taylor series expansion with 5 points within the central difference scheme.

Solution: Second derivative - 5 point central difference

We need 5 points: $x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}$. Using Taylor series expansion around x_i:

$$(1)\ f(x_{i-2}) = f(x_i) + f'(x_i)(x_{i-2} - x_i) + \frac{f''(x_i)}{2!}(x_{i-2} - x_i)^2 + \\ + \frac{f'''(x_i)}{3!}(x_{i-2} - x_i)^3 + \frac{f''''(\xi_1)}{4!}(x_{i-2} - x_i)^4$$

$$(2)\ f(x_{i-1}) = f(x_i) + f'(x_i)(x_{i-1} - x_i) + \frac{f''(x_i)}{2!}(x_{i-1} - x_i)^2 + \\ + \frac{f'''(x_i)}{3!}(x_{i-1} - x_i)^3 + \frac{f''''(\xi_2)}{4!}(x_{i-1} - x_i)^4$$

$$(3)\ f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \\ + \frac{f'''(x_i)}{3!}(x_{i+1} - x_i)^3 + \frac{f''''(\xi_3)}{4!}(x_{i+1} - x_i)^4$$

$$(4)\ f(x_{i+2}) = f(x_i) + f'(x_i)(x_{i+2} - x_i) + \frac{f''(x_i)}{2!}(x_{i+2} - x_i)^2 + \\ + \frac{f'''(x_i)}{3!}(x_{i+2} - x_i)^3 + \frac{f''''(\xi_4)}{4!}(x_{i+2} - x_i)^4$$

Solution: Second derivative - 5 point central difference

Assuming that the distance between the points is equal. There are different ways to proceed. One way is to add eqs. (1)+(2)+(3)+(4):

$$(5)\ f''(x_i) = \frac{-4f(x_i) + f(x_{i-2}) + f(x_{i-1}) + f(x_{i+1}) + f(x_{i+2})}{5h^2} + O(h^2)$$

Another way is to add eqs. (2)+(3) to get eqs. (6) and eqs. (1)+(4) to get eq. (7) separately:

$$(6)\ 16f(x_{i+1}) + 16f(x_{i-1}) = 32f(x_i) + 16f''(x_i)h^2 + O(h^4)$$

$$(7)\ f(x_{i+2}) + f(x_{i-2}) = 2f(x_i) + 4f''(x_i)h^2 + O(h^4)$$

By subtracting eqs. (6)-(7) we get eq.(8):

$$(8)\ f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2} + O(h^2)$$

Solution: Second derivative - 5 point central difference

We can compare eqs. (5) and (8) for different cases: (i) $f(x) = 0.002x^3 - 0.097x^2 + 1.35x + 3.67$, (ii) $h(x) = \sin(x)$, (iii) $m(x) = \frac{e^x}{300}$. We can select step $h = 0.1$ and evaluate from analytical expressions: $f(x_{i-2}), f(x_{i-1}), f(x_i), f(x_{i+1}), f(x_{i+2})$.

If we take the second derivative for the three functions (i,ii,iii) and use eqs. (5) and (8) and compare them with analytical solution at $x_i = 8.5$ we have:

	cubic (i)	sinusoidal (ii)	exponential (iii)
Analytical	-0.07	-0.8	16.43
Eq.(5)	-0.11	-0.7	13.75
Eq.(8)	-0.18	-0.44	7.09

The errors $\left|\frac{f_{TS} - f_{NS}}{f_{TS}}\right|$ are as follows:

Error	cubic (i)	sinusoidal (ii)	exponential (iii)
Eq.(5)	0.5714	0.1250	0.1631
Eq.(8)	1.5714	0.4500	0.5685

Taylor series-Second derivative-3 point forward difference

The value of a function at point x_{i+1} can be approximated by a Taylor series of a function and its derivatives at point x_i:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f'''(\xi_1)}{3!}(x_{i+1} - x_i)^3$$
$$f(x_{i+2}) = f(x_i) + f'(x_i)(x_{i+2} - x_i) + \frac{f''(x_i)}{2!}(x_{i+2} - x_i)^2 + \frac{f'''(\xi_2)}{3!}(x_{i+2} - x_i)^3$$

Noting that $x_{i+1} - x_i = h$ and $x_{i+2} - x_i = 2h$ and subtracting two times the first equation minus the second in order to get rid of the first derivative:

$$2f(x_{i+1}) - f(x_{i+2}) = 2f(x_i) - 2\frac{f''(x_i)}{2!}h^2 + 2\frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3$$
$$f''(x_i) = \frac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2} + O(h)$$

Taylor series-Second derivative-3 point backward difference

The value of a function at point x_{i+1} can be approximated by a Taylor series of a function and its derivatives at point x_i:

$$f(x_{i-1}) = f(x_i) + f'(x_i)(x_{i-1} - x_i) + \frac{f''(x_i)}{2!}(x_{i-1} - x_i)^2 + \frac{f'''(\xi_1)}{3!}(x_{i-1} - x_i)^3$$
$$f(x_{i-2}) = f(x_i) + f'(x_i)(x_{i-2} - x_i) + \frac{f''(x_i)}{2!}(x_{i-2} - x_i)^2 + \frac{f'''(\xi_2)}{3!}(x_{i-2} - x_i)^3$$

Noting that $x_{i-1} - x_i = -h$ and $x_{i-2} - x_i = -2h$ and subtracting two times the first equation minus the second in order to get rid of the first derivative:

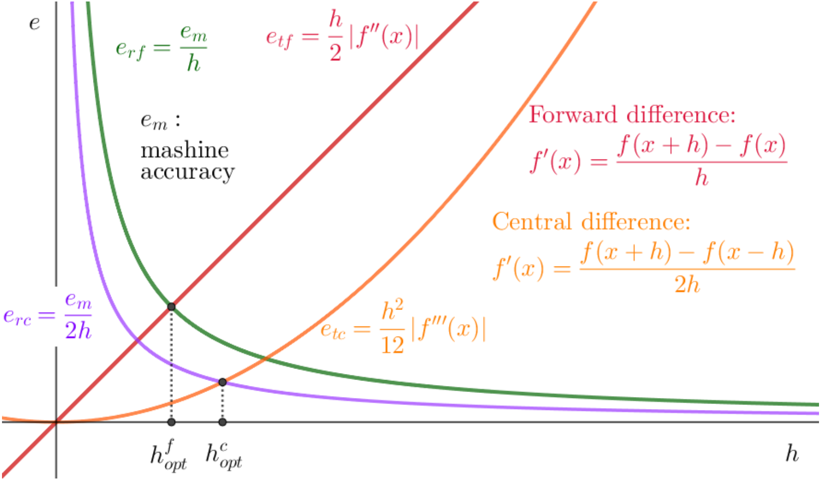
$$2f(x_{i-1}) - f(x_{i-2}) = f(x_i) - 2\frac{f''(x_i)}{2!}h^2 - 2\frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3$$
$$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2} + O(h)$$

Error in Numerical Differentiation

Error in Numerical Differentiation

- All expressions introduce a numerical error, namely truncation error.
- In the finite difference formulas, we can estimate the error as a function of h (spacing between points) raised at some power.
- The smaller the h, the smaller the error.
- For a function with fixed spacing h the truncation error cannot be reduced by reducing the h.
- Alternatively, a finite difference formula with higher order truncation error can be used.
- When the function is given by a mathematical expression, the h could be selected as small as possible to reduce the truncation error.
- BUT the error consists by two parts: truncation and round-off.
- Even if truncation error will be small, the round-off error will remain.

Error in Numerical Differentiation



Error in Numerical Differentiation

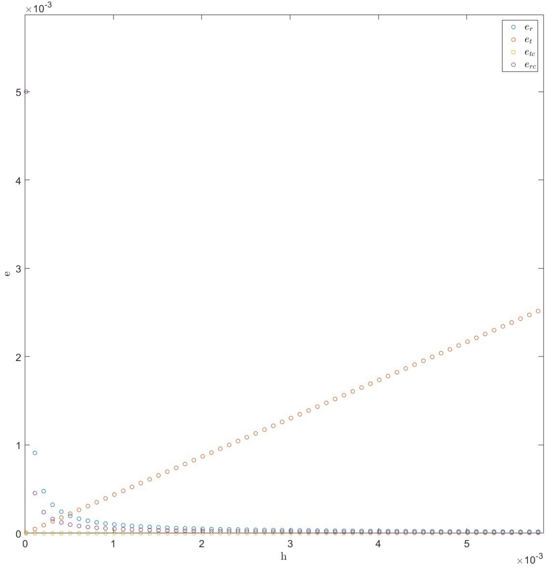
- The round-off error appears in the numerator in the computation of the term (for forward difference): $f(x+h) - f(x)$ and error in the $f'(x)$ is of the order e_m/h, where e_m can be assumed as the machine accuracy (e.g. $1.19 \cdot 10^{-7}$ for single precision, $2.22 \cdot 10^{-16}$ for double precision, [3]).
- For the backward difference the round-off error is the same.
- The round-off error for the central difference: $f(x+h)-f(x-h)$ and error in the $f'(x)$ is of the order $e_m/2h$.
- The smaller the h, the larger the round-off error (chose h so that $x+h$ and x differ by an exactly representative number [3]).
- The truncation error (from Taylor series) for the forward (same for backward) is: $\frac{h}{2}|f''(x)|$, while for the central difference: $\frac{h^2}{12}|f'''(x)|$.
- The smaller the step, the smaller the truncation error.
- There is a region in between where these two functions of errors (round-off and truncation) intersect and the optimal h can be defined.

Example

Example: Error in Numerical Differentiation

Write a script in MatLab, that estimates the errors e (round-off and truncation) for the function $\sin(x)$ for the forward and central difference finite difference scheme at $x = \pi/3$. Vary the step h from $1e-5$ to $1e-1$ with step $1/10000$. Plot the data (use `scatter` in MatLab) in the form h versus e. Identify the optimal steps h for each case.

Example: Error in Numerical Differentiation - Solution



Example: Error in Numerical Differentiation - Solution

The limitations imposed by the finite difference schemes with the growth of round-off errors as the step size h decreases, may be overcome by using methods such as **Richardson extrapolation** or **Ridders method**.

Numerical Differentiation - Lagrange polynomials

Numerical Differentiation - Lagrange polynomials

- The numerical differentiation can also be derived by using Lagrange polynomials.
- To obtain the formulas for the first derivative, the two-point central, three-point forward and three-point backward difference formulas can be obtained by using the points (x_i, y_i), (x_{i+1}, y_{i+1}) and (x_{i+2}, y_{i+2}). Then the polynomial in Lagrange form can be written as:

$$f(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}$$

- The derivative gives:

$$f'(x) = \frac{2x - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{2x - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{2x - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}$$

Numerical Differentiation - Lagrange polynomials

- The following formulas can be derived for the first derivative at values of x as x_i, x_{i+1}, x_{i+2}:

$$f'(x_i) = \frac{2x_i - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{2x_i - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{2x_i - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2}$$

$$f'(x_{i+1}) = \frac{2x_{i+1} - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{2x_{i+1} - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{2x_{i+1} - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2}$$

$$f'(x_{i+2}) = \frac{2x_{i+2} - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{2x_{i+2} - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{2x_{i+2} - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2}$$

Numerical Differentiation - Lagrange polynomials

- By simplifying the numerators of the fractions we get:

$$
\begin{aligned}
f'(x_i) = \frac{2x_i - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} \\
+ \frac{x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}
\end{aligned}
$$

$$
\begin{aligned}
f'(x_{i+1}) = \frac{x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{2x_{i+1} - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} \\
+ \frac{x_{i+1} - x_i}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}
\end{aligned}
$$

$$
\begin{aligned}
f'(x_{i+2}) = \frac{x_{i+2} - x_{i+1}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{x_{i+2} - x_i}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} \\
+ \frac{2x_{i+2} - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}
\end{aligned}
$$

Numerical Differentiation - Lagrange polynomials

- For equally spaced points the following hols true $x_{i+1} - x_i = h$, $x_{i+2} - x_{i+1} = h$ and $x_{i+2} - x_i = 2h$:

$$f'(x_i) = \frac{-h-2h}{(-h)(-2h)}y_i + \frac{-2h}{(h)(-h)}y_{i+1} + \frac{-h}{(2h)(h)}y_{i+2} = \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2h}$$

  which is the forward difference three-point formula
- For the point x_{i+1}:

$$f'(x_{i+1}) = \frac{-h}{(-h)(-2h)}y_i + \frac{h-h}{(h)(-h)}y_{i+1} + \frac{h}{(2h)(h)}y_{i+2} = \frac{y_{i+2} - y_i}{2h}$$

  which is the two-point central difference formula
- For the point x_{i+2}:

$$f'(x_{i+2}) = \frac{h}{(-h)(-2h)}y_i + \frac{2h}{(h)(-h)}y_{i+1} + \frac{2h+h}{(2h)(h)}y_{i+2} = \frac{y_i - 4y_{i+1} + 3y_{i+2}}{2h}$$

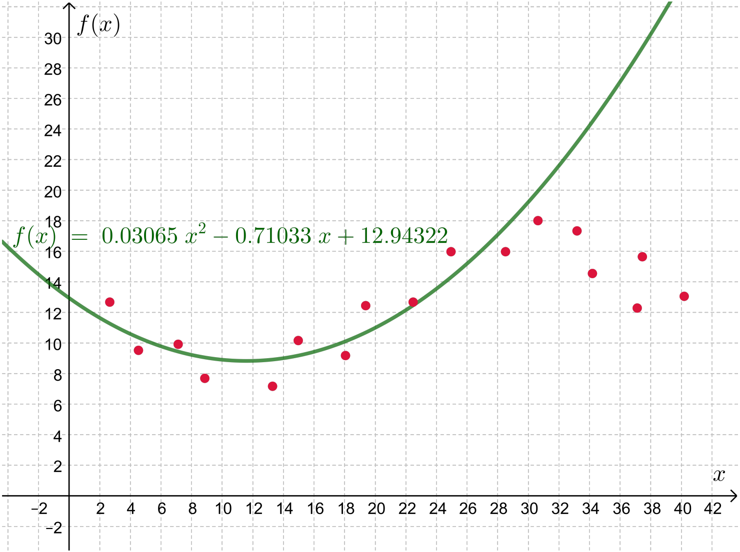
  which is the three-point backward formula

Numerical Differentiation - Lagrange polynomials

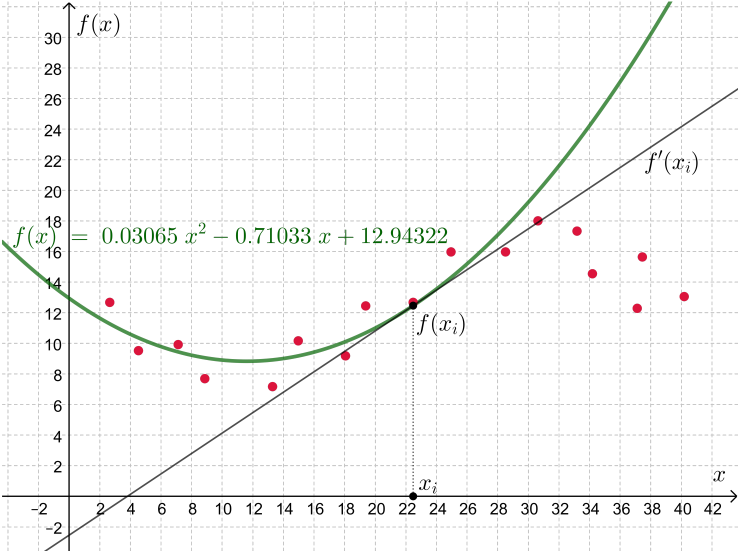
- The equations derived previously by the Lagrange polynomials can be used when the points are not spaced equally.
- Using Lagrange polynomials might be easier to derive the finite difference formulas compared to Taylor series.
- BUT, Taylor series provides estimation of the truncation error.

Numerical Differentiation - Curve fitting

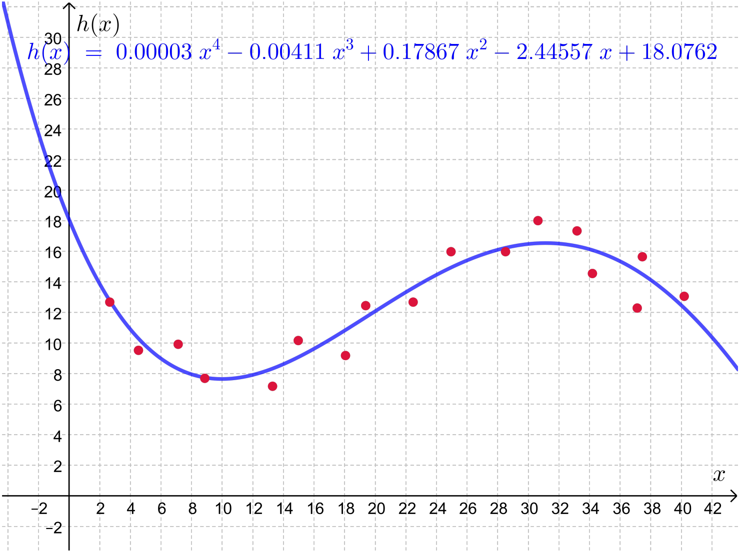
Numerical Differentiation - Curve fitting



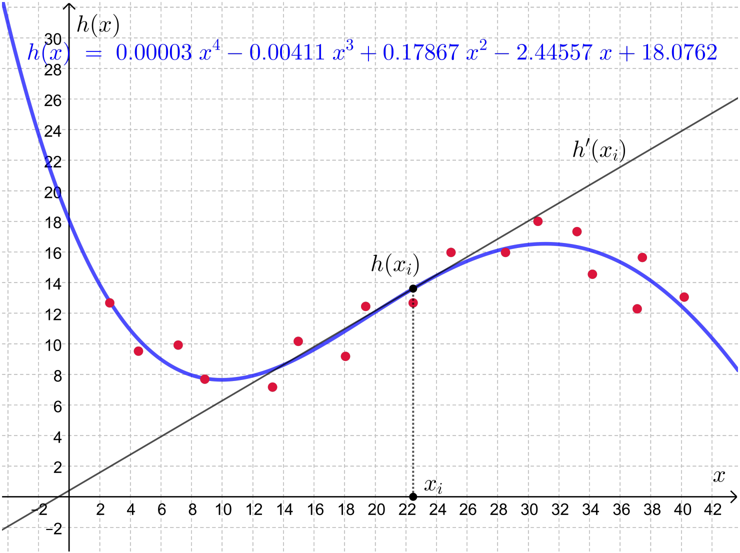
Numerical Differentiation - Curve fitting



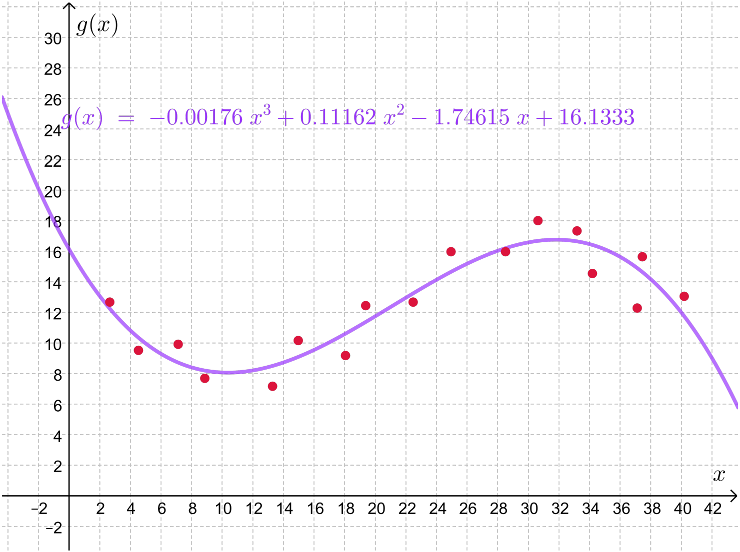
Numerical Differentiation - Curve fitting



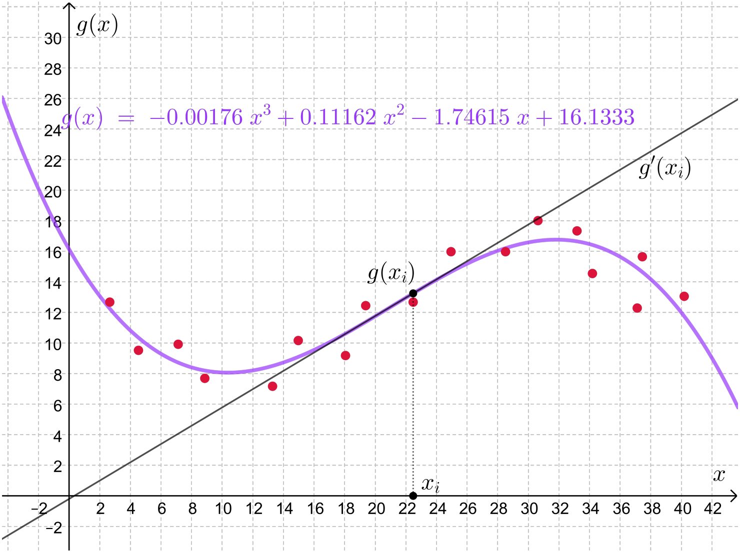
Numerical Differentiation - Curve fitting



Numerical Differentiation - Curve fitting



Numerical Differentiation - Curve fitting

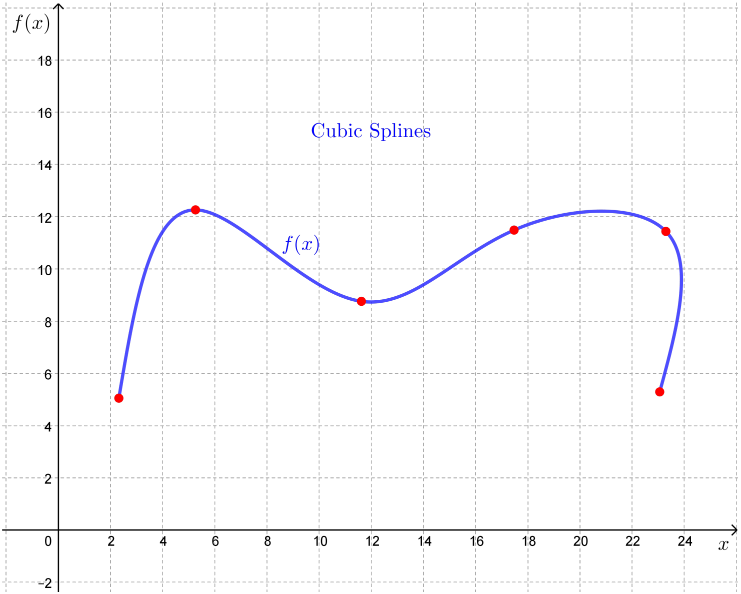


Numerical Differentiation - Curve fitting

- Approximate the data with an analytical function and then differentiate.
- Curve fitting can be used for that.
- Curve fitting for nonlinear relationship with least squares scheme.
- Functions that can be used are: exponential, power, low-order polynomial, or combination of nonlinear functions which are simple to differentiate.
- The process might be used when the data contain scatter or noise.

Numerical Differentiation - Interpolation

Numerical Differentiation - Interpolation



Numerical Differentiation - Interpolation

- Approximate the derivative with the derivative of $f(x)$ by the derivative of the interpolant.
- It can be used for uneven intervals of x.

1. Polynomial interpolant
2. Cubic spline interpolant

Numerical Differentiation - Polynomial interpolant

- The order of the polynomial should preferably be less than six, [2]:

$$P_{n-1}(x) = a_1 x^n + a_2 x^{n-1} + a_{n-1} x + a_n$$

  where n the number of data points.
- For evenly spaced data points interpolation provides the same result with finite difference.
- Least squares fit should be used in determining the coefficients $a_1, a_2, .., a_n$.

Numerical Differentiation - Cubic Spline interpolant

- Cubic spline is easy to differentiate.
- First step is to determine the second derivatives k_i.
- The first and second derivative can be calculated as:

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

$$-\frac{k_{i+1}}{6}\left[\frac{3(x - x_i)^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right] + \frac{y_i - y_{i+1}}{x_i - x_{i+1}}$$

$$f''_{i,i+1}(x) = k_i \frac{x - x_{i+1}}{x_i - x_{i+1}} - k_{i+1} \frac{x - x_i}{x_i - x_{i+1}}$$

Cubic Splines - Lagrange form - Recalling

- The equation of cubic spline for each segment:

$$f_{i,i+1}(x) = \frac{k_i}{6}\left(\frac{(x-x_{i+1})^3}{x_i-x_{i+1}} - (x-x_{i+1})(x_i-x_{i+1})\right) - \frac{k_{i+1}}{6}\left(\frac{(x-x_i)^3}{x_i-x_{i+1}} - (x-x_i)(x_i-x_{i+1})\right) + \frac{y_i(x-x_{i+1}) - y_{i+1}(x-x_i)}{x_i-x_{i+1}}$$

Cubic Splines - Lagrange form - Recalling

- The second derivative k_i of the spline at the internal points (knots) can be obtained from slope continuity $f'_{i,i+1}(x_i) = f'_{i-1,i}(x_i)$, for $i = 2, 3, .., n-1$. The simultaneous equations to be solved are the following:

  $$k_{i-1}(x_{i-1} - x_i) + 2k_i(x_{i-1} - x_{i+1}) + k_{i+1}(x_i - x_{i+1}) = 6\left(\frac{y_{i-1} - y_i}{x_{i-1} - x_i} - \frac{y_i - y_{i+1}}{x_i - x_{i+1}}\right)$$

  where $i = 2, 3, .., n-1$ and the coefficient matrix is tridiagonal.

Numerical Differentiation - MatLab build-in functions

Numerical Differentiation - MatLab build-in functions

- MatLab does not have a function that can perform numerical differentiation.
- There is however the `diff` function that can perform numerical differentiation.
- There is also the function `polyder` that defines the derivative of a polynomial.
- The function `diff` calculates the differences between adjacent elements of a vector.
- In the simplest form the function can be written as: `d=diff(x)`, where `x` is a vector and `d` is a vector with the differences:

$$\begin{aligned} \mathtt{x} &= [x_1, x_2, x_3, x_4, ..., x_{n-1}, x_n]; \\ \mathtt{d} &= [(x_2 - x_1), (x_3 - x_2), (x_4 - x_3), .., (x_n - x_{n-1})] \end{aligned}$$

- The vector `d` is an element shorter than vector `x`

Numerical Differentiation - MatLab build-in functions

- For a function presented by a discrete set of n points (x_1, y_1), (x_2, y_2),...,(x_n, y_n) the first derivative with the two-point forward difference formula can be calculated by using:

```
diff(y)./diff(x)
```

- When the spacing is the same between the points, namely `h`, it can be calculated as:

```
diff(y)./h
```

- The `diff` has an additional option for calculating higher-order derivatives:

```
d=diff(x,n)
```

  where `n` is the number (integer) of the times that `diff` is going to be applied

Numerical Differentiation - MatLab build-in functions

- The command `diff(x)` calculates a vector with $n-1$ elements:

$$x_{i+1} - x_i; \quad \text{for } i = 1, 2, .., n-1$$

- The function `diff(x,2)` provides a vector $n-2$:

$$((x_{i+2} - x_{i+1}) - (x_{i+1} - x_i)) = x_i - 2x_{i+1} + x_{i+2}; \quad \text{for } i = 1, 2, .., n-1$$

  The right hand side of the last equation is the numerator of the three-point forward difference formula for the second derivative at x_i

- For a function that has the same distance h between the points an estimate of the second derivative can be given according to the three-point forward difference formula: `diff(y,2)/h^2`
- Similarly, `diff(y,n)` gives the numerator of the nth derivative in the forward difference formula.

Numerical Differentiation - MatLab build-in functions

- The function `polyder` gives the derivative of a polynomial
- The simplest form of the command can be written as:

  `dp=polyder(p)`

  where `dp` is a vector with the coefficients of the polynomial that is the derivative of the polynomial `p` and `p` is the vector of the coefficients of the polynomial to be differentiated
- In MatLab polynomials can be represented as a row vector where the elements are the coefficients of the polynomial
- if `p` is of order n, then `dp` is of order $n-1$
- Example: the polynomial $f(x) = 4x^3 + 5x + 7$ gives the vector `p=[4 0 5 7]` and then the `df=polyder(p)` will give `df=[12 0 5]`, which means that the derivative is $12x^2 + 5$

Example

Richardson's Extrapolation

Richardson's Extrapolation

- Is a method for calculating a more accurate approximation of a derivative from two less accurate approximations of that derivative
- In general terms, the value D of a derivative (unknown) can be calculated as follows:

  $$D = D(h) + k_2 h^2 + k_4 h^4$$

  where $D(h)$ is the function that approximates the derivative and the terms $k_2 h^2$ and $k_4 h^4$ are error terms in which the coefficients k_2, k_4 are independent of the spacing h.
- Using the same formula for spacing $h/2$:

  $$D = D\left(\frac{h}{2}\right) + k_2\left(\frac{h}{2}\right)^2 + k_4\left(\frac{h}{2}\right)^4 \Leftrightarrow$$

  $$4D = 4D\left(\frac{h}{2}\right) + k_2 h^2 + k_4 \frac{h^4}{4}$$

Richardson's Extrapolation

- Subtracting the first equation from the second equation:

$$D = D(h) + k_2 h^2 + k_4 h^4$$

$$4D = 4D\left(\frac{h}{2}\right) + k_2 h^2 + k_4 \frac{h^4}{4}$$

we get:

$$3D = 4D\left(\frac{h}{2}\right) - D(h) - k_4 \frac{h^4}{4}$$

Solving for D

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) - O(h^4)$$

- The value of D is derived with an error $O(h^4)$ from two lower-order approximations $D(h)$ and $D(\frac{h}{2})$ that were calculated with error $O(h^2)$

Example

Example: Richardson's Extrapolation

Using the 5-term Taylor series using central difference scheme we have for $x_{i+1} = x + h$:

$$f(x_i + h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f''''(x_i)}{4!}h^4 + \frac{f'''''(\xi_1)}{5!}h^5$$

and for $x_{i-1} = x - h$:

$$f(x_i - h) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f''''(x_i)}{4!}h^4 - \frac{f'''''(\xi_2)}{5!}h^5$$

By subtracting the previous two equations:

$$f(x_i + h) - f(x_i - h) = 2f'(x_i)h + 2\frac{f'''(x_i)}{3!}h^3 + \frac{f'''''(\xi_1)}{5!}h^5 + \frac{f'''''(\xi_2)}{5!}h^5$$

Example: Richardson's Extrapolation

Now solving for $f'(x_i)$ we have:

$$(1)\ f'(x_i) = \frac{f(x_i + h) - f(x_i - h)}{2h} - \frac{f'''(x_i)}{3!}h^2 + O(h^4)$$

If we now change the step from h to $h/2$ we get:

$$f'(x_i) = \frac{f(x_i + h/2) - f(x_i - h/2)}{2\frac{h}{2}} - \frac{f'''(x_i)}{3!}\left(\frac{h}{2}\right)^2 + O(h^4) \Leftrightarrow$$

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

By subtracting eq.(2)-eq.(1) we are able to derive Richardson's extrapolation:

$$f'(x_i) = \frac{1}{3}\left[4\underbrace{\frac{f(x_i + h/2) - f(x_i - h/2)}{h}}_{D(h/2)} - \underbrace{\frac{f(x_i + h) - f(x_i - h)}{2h}}_{D(h)}\right] + O(h^4)$$

Richardson's Extrapolation

- Richardson's extrapolation method can also be calculated with approximations that have errors of higher order. Two approximations with an error $O(h^4)$ (one calculated at spacing h and one at spacing $h/2$) can be used for calculating a more accurate approximation with error $O(h^6)$

$$D = \frac{1}{15}\left(16D\left(\frac{h}{2}\right) - D(h)\right) - O(h^6)$$

Example

Richardson's Extrapolation: Example

Consider the function $f(x) = \frac{2^x}{x}$ Calculate the second derivative at $x = 2$ numerically with the x three-point central difference formula using:

(a) Points $x = 1.8$, $x = 2$, and $x = 2.2$.

(b) Points $x = 1.9$, $x = 2$, and $x = 2.1$.

Then use Richardson's extrapolation for a more accurate solution. Compare the results with analytical solution.

Note: The analytical derivative of $f(x)$ is:

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

In MatLab for `ln` (natural logarithm) you need to use function `log`

Ridders Extrapolation

Ridders Extrapolation

- Assume that we have want to calculate the derivative of function $f(x)$.
- According to the scheme we are using the error would be proportional to h^n, where h is the step and n is a real number.
- Assume that we make to applications of the formula with intervals h and $2h$. In this case the errors will be:

$$E_1 \approx C(2h)^n; \quad E_2 \approx C(h)^n$$

- The relationship between the errors can be:

$$\frac{E_1}{E_2} \approx 2^n \rightarrow E_2 \approx \frac{E_1}{2^n}$$

- The solution of $2h$ is given as $A_1 + E_1$ and the solution for h is given by $A_2 + E_2$.

Ridders Extrapolation

- The solution is $I = A_1 + E_1 = A_2 + E_2$.
- We can rewrite the equation as $A_2 - A_1 = E_1 - E_2$.
- We showed that $E_2 \approx \frac{E_1}{2^n}$ and therefore $E_1 - E_2 = E_1 - \frac{E_1}{2^n} = E_1\left(\frac{2^n-1}{2^n}\right)$.
- By dividing $E_1 - E_2$ with E_2 we get $\frac{E_1-E_2}{E_2} = \frac{E_1}{E_2}\left(\frac{2^n-1}{2^n}\right) = 2^n\left(\frac{2^n-1}{2^n}\right) = 2^n - 1$.
- Solving the last equation for E_2 we get $E_2 = \frac{E_1-E_2}{2^n-1}$
- We go back to the equation $I = A_2 + E_2$ and we replace $E_2 = \frac{E_1-E_2}{2^n-1}$ and we have $I = A_2 + \frac{E_1-E_2}{2^n-1}$.
- Recalling that $A_2 - A_1 = E_1 - E_2$ we get that $I = A_2 + \frac{A_2-A_1}{2^n-1}$,
- Finally, by operating in the last equation $I = \frac{A_2(2^n-1)+A_2-A_1}{2^n-1}$

  and therefore $\boxed{I = \dfrac{2^n A_2 - A_1}{2^n - 1}}$

Ridders Extrapolation

- For the case of the first derivative of function $f(x)$ by the central difference formula $(f(x+h)-f(x-h))/2h$, the error is of order h^2.
- Therefore: $f'(x) \approx \frac{4A_2 - A_1}{4-1}$
- Generally, [4]:

For accuracy of h^n with $n = 2$ we have:

$$
\begin{array}{lcccc}
 & A_1 & A_2 & A_3 & A_4 \ldots \\
m = 1 & & B_1 & B_2 & B_3 \ldots \\
m = 2 & & & C_1 & C_2 \ldots \\
m = 3 & & & & D_1 \ldots
\end{array}
$$

$$B_i = \frac{4^m A_{i+1} - A_i}{4^m - 1}, m = 1$$

$$C_i = \frac{4^m B_{i+1} - B_i}{4^m - 1}, m = 2$$

$i = [1, n_{tab}]$ where n_{tab} is the number of the Romberg table

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