4. Find the solution of the equation $x^3 - x + 1$ using Newton's divided difference interpolation formula with nodes $x_1 = 2$ and $x_n = 4$, at $x = 3.8$, with step size $h = 0.5$.

5. Find the cubic splines for the following table of values and compute f(2.5):

x	1	2	3	4	5
y	32	17	34	20	27

6. Given the data points $f(0) = 2$, $f(1) = 4$, and $f(3) = 7$:

   (a) Approximate the value $f(2)$ using an appropriate interpolating polynomial written in Lagrange's form.

   (b) Approximate the same value $f(2)$ using Newton's divided difference formula.

   (c) Construct an interpolating cubic spline and approximate the value $f(2)$.

7. Consider the following population data for a major city:

t_i	1990	1995	2000	2005	2010	2015
y_i	2,450,800	2,710,500	2,890,200	3,150,700	3,420,300	3,810,600

   where t_i represents the census year and y_i represents the city's population in that year.

   (a) Construct the divided difference table and derive by hand the Newton's interpolating polynomial for this data.

   (b) Implement a numerical method to compute the fifth-degree interpolating polynomial $P(x)$ that matches all data points (t_i, y_i).

   (c) Verify your numerical solution by comparing it with the polynomial obtained in part (a).

   (d) Estimate the city's population for each year between 1990 and 2015 using your interpolating polynomial.

   (e) Repeat the estimation using cubic spline interpolation and compare the results with your polynomial approximation.

   (f) Use your interpolating polynomial to predict the city's population for the years 2018 and 2025.

   (g) Investigate how using integer values for both t_i (years since 1990) and y_i (population in millions) affects your results.

CHAPTER 3

NUMERICAL DIFFERENTIATION

1 General description

Numerical differentiation is a powerful tool used to approximate the derivative of a function when its exact analytical form is unknown or difficult to differentiate. This is particularly useful when dealing with experimental data or when the function is given only as discrete values at specific points, rather than in an explicit formula. Numerical methods allow us to estimate the rate of change of the function at any point based on these data points.

In computational mathematics, several methods exist to calculate derivatives, and these can be broadly categorized into

- Derivatives using Newton's forward and backward difference formulas, which provide straightforward techniques for approximating the first and higher-order derivatives when function values are known at equally spaced points. The forward difference method utilizes the current and next data points, making it suitable near the beginning of a data table. In contrast, the backward difference method relies on the current and previous data points, making it more appropriate near the end of the dataset.

- Derivatives using unequally spaced values of argument, which are employed when data points are not uniformly distributed. In such cases, standard finite difference formulas are not applicable. Instead, numerical differentiation relies on techniques such as divided differences or derivative formulas derived from Lagrange interpolation, allowing for accurate derivative estimation despite irregular spacing.

- Maxima and minima of a tabulated function, which represent an important application of numerical differentiation. By examining the behavior of first and second derivatives—approximated through finite difference methods—it becomes possible to identify points where the function exhibits local extrema. This approach is especially useful when dealing with discrete data, enabling the detection of peaks and troughs that reveal critical information about the function's overall trend.

These methods are essential in fields such as engineering, physics, economics, and computer science, where precise calculations of derivatives are often necessary, but exact formulas are either unavailable or too complex to apply.

2 Derivatives using equally spaced values of argument

In many numerical applications, function values are available at discrete and equally spaced points. When this uniform spacing exists, it allows for the straightforward application of standard finite difference methods to approximate derivatives. These methods are based on simple algebraic manipulations and offer good accuracy for smooth functions. In this section, we explore how to compute numerical derivatives when the function values are given at equally spaced points. These methods are particularly useful in solving differential equations, analyzing experimental data, and modeling physical systems where data is collected at uniform intervals.

2.1 Numerical differentiation using Newton's forward difference formula

Newton's forward difference Formula is a foundational method in numerical differentiation used to approximate derivatives of a function based on discrete values with uniform spacing. It is especially effective when the point of interest lies near the beginning of the dataset. The method leverages forward differences of function values and is derived from Newton's forward interpolation formula.

Suppose a function $f(x)$ is known at equidistant points $x_0, x_1, x_2, \ldots, x_n$, where $x_i = x_0 + ih$, and h is the constant spacing between successive points. The goal is to estimate the first or higher derivatives of $f(x)$ at $x = x_0$ using forward differences derived from the Newton's forward interpolation formula. The forward difference operator $\Delta$is defined recursively as

$$\Delta^k f(x_0) = \Delta^{k-1} f(x_1) - \Delta^{k-1} f(x_0)$$

Using these forward differences, the first derivative of the function $f(x)$ at x_0 is approximated by

$$f'(x_0) \approx \frac{1}{h}\left[\Delta f(x_0) - \frac{1}{2}\Delta^2 f(x_0) + \frac{1}{3}\Delta^3 f(x_0) - \cdots\right]$$

This is an infinite series that, in practice, is truncated to include only a few terms depending on the desired accuracy and the number of available data points.

Similarly, the second derivative is approximated by:

$$f''(x_0) \approx \frac{1}{h^2}\left[\Delta^2 f(x_0) - \Delta^3 f(x_0) + \cdots\right]$$

These formulas are derived from differentiating Newton's forward interpolation formula and truncating the infinite series after a few terms for practical computations.

Algorithm 29 Numerical differentiation using Newton's forward difference formula

Require: Equally spaced data points $(x_0, f_0), (x_1, f_1), \dots, (x_n, f_n)$
Require: Step size $h = x_{i+1} - x_i$
Ensure: Approximation of the first derivative $f'(x_0)$

Step 1: Compute forward differences
for $i \leftarrow 0\ n-1$ **do**
  $\Delta f_i \leftarrow f_{i+1} - f_i$ ▷ First forward differences
end for
for $k \leftarrow 2\ n$ **do**
  for $i \leftarrow 0\ n-k$ **do**
    $\Delta^k f_i \leftarrow \Delta^{k-1} f_{i+1} - \Delta^{k-1} f_i$ ▷ k-th order differences
  end for
end for
Step 2: Estimate the derivative at x_0
Initialize $f' \leftarrow \frac{1}{h}(\Delta f_0)$
for $k \leftarrow 2\ m$ **do** ▷ Include up to order m for better accuracy
  $f' \leftarrow f' + \frac{1}{k!h}\Delta^k f_0$
end for
Step 3: (Optional) Estimate error
Use error estimate:

$$E \approx \frac{h^m}{(m+1)!} f^{(m+1)}(\xi), \quad \text{for some } \xi \in [x_0, x_n]$$

return Approximation of $f'(x_0)$

Example: Estimating derivative using forward difference formula

Given the following tabulated values

x	$f(x)$
1.0	1.0000
1.1	1.2214
1.2	1.4918
1.3	1.8221
1.4	2.2255

Step 1: Compute the uniform step size

$$h = x_{i+1} - x_i = 1.1 - 1.0 = 0.1$$

Step 2: Construct the forward difference table

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$
1.0	1.0000	0.2214	0.0490	0.0069
1.1	1.2214	0.2704	0.0559	
1.2	1.4918	0.3303		
1.3	1.8221	0.4034		
1.4	2.2255			

Step 3: Estimate the first derivative at $x = 1.0$
We use the Newton's forward difference formula for the first derivative

$$f'(x_0) \approx \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0\right]$$

Substituting the known values

$$f'(1.0) \approx \frac{1}{0.1}\left(0.2214 - \frac{1}{2}\cdot 0.0490 + \frac{1}{3}\cdot 0.0069\right)$$

$$= 10\,(0.2214 - 0.0245 + 0.0023) = 10 \cdot 0.1992 = \boxed{1.992}$$

Step 4: Estimate the second derivative at $x = 1.0$
The second derivative can be approximated using

$$f''(x_0) \approx \frac{1}{h^2}\left[\Delta^2 f_0 - \Delta^3 f_0\right] = \frac{1}{(0.1)^2}(0.0490 - 0.0069) = 100 \cdot 0.0421 = \boxed{4.21}$$

Conclusion
The estimated values at $x = 1.0$ are

$$f'(1.0) \approx 1.992, \quad f''(1.0) \approx 4.21$$

These results indicate that the function is increasing with a positive and growing slope - suggesting *concave upward* behavior near $x = 1.0$. This is consistent with the shape of an exponential-type function such as $f(x) \approx e^x$. ■

Accuracy and convergence rate

Newton's forward difference method provides a first-order approximation to the derivative with an error term:

$$\text{Error} = \frac{h}{2} f''(\xi)$$

for some $\xi \in [x_0, x_1]$. The accuracy improves as $h \to 0$, provided the function is smooth. However, increasing the order of approximation or including higher-order difference terms can improve precision at the cost of potential numerical instability.

Advantages

- Simple to implement for evenly spaced data.
- Effective near the beginning of datasets.
- Can be extended to higher-order derivatives.

Disadvantages

- Accuracy decreases near the middle or end of data.
- Requires uniform spacing; unsuitable for irregular data.
- Sensitive to round-off error with small h or high-order terms.

2.2 Numerical differentiation using Newton's backward difference formula

Numerical differentiation using Newton's backward difference formula is particularly useful for estimating derivatives at or near the end of a dataset when the values of a function are given at equally spaced points. Unlike forward differences, this method uses past (backward) values to approximate derivatives, making it ideal when the function value at the point of interest lies toward the end of the table.

Suppose a function $f(x)$ is known at equidistant points $x_0, x_1, \ldots, x_n$, where $x_i = x_0 + ih$ and h is the constant spacing between successive values. The backward difference operator ∇ is defined as:

$$\nabla f(x_i) = f(x_i) - f(x_{i-1})$$

The first derivative at x_n can be approximated using the backward differences as:

$$f'(x_n) \approx \frac{1}{h}\left(\nabla f_n - \frac{1}{2}\nabla^2 f_n + \frac{1}{3}\nabla^3 f_n - \cdots\right)$$

The second derivative is given by:

$$f''(x_n) \approx \frac{1}{h^2}\left(\nabla^2 f_n - \nabla^3 f_n + \cdots\right)$$

These series may be truncated based on the required precision and available data.

Algorithm 30 Numerical differentiation using Newton's backward difference formula

Require: Equally spaced data points $(x_0, f_0), (x_1, f_1), \ldots, (x_n, f_n)$
Require: Step size $h = x_{i+1} - x_i$
Ensure: Approximation of the derivative $f'(x_n)$ at the last point

Step 1: Compute backward differences
for $i \leftarrow 1\ n$ **do**
  $\nabla f_i \leftarrow f_i - f_{i-1}$ ▷ First backward differences
end for
for $k \leftarrow 2\ n$ **do**
  for $i \leftarrow k\ n$ **do**
    $\nabla^k f_i \leftarrow \nabla^{k-1} f_i - \nabla^{k-1}_{i-1}$ ▷ k-th order differences
  end for
end for
Step 2: Estimate the derivative at x_n
Initialize $f' \leftarrow \frac{1}{h}(\nabla f_n)$
for $k \leftarrow 2\ m$ **do** ▷ Use up to order m for accuracy
  $f' \leftarrow f' + \frac{(-1)^{k+1}}{k!h} \nabla^k f_n$
end for
Step 3: (Optional) Estimate error
Use error estimate:

$$E \approx \frac{h^m}{(m+1)!} f^{(m+1)}(\xi), \quad \text{for some } \xi \in [x_0, x_n]$$

return Approximation of $f'(x_n)$

Example: Approximating the derivative at the endpoint using Newton's backward difference

Estimate the first and second derivatives of $f(x)$ at $x = 4$ using Newton's backward difference method, based on the following tabulated data:

x	$f(x)$
1	2
2	4
3	7
4	11

Step 1: Determine the step size

Since the data is equally spaced

$$h = x_{i+1} - x_i = 1$$

Step 2: Construct the backward difference table

x	$f(x)$	∇f	$\nabla^2 f$	$\nabla^3 f$
1	2			
2	4	2		
3	7	3	1	
4	11	4	1	0

Computed values:

$$\nabla f_3 = f_3 - f_2 = 11 - 7 = 4$$
$$\nabla^2 f_3 = \nabla f_3 - \nabla f_2 = 4 - 3 = 1$$
$$\nabla^3 f_3 = \nabla^2 f_3 - \nabla^2 f_2 = 1 - 1 = 0$$

Step 3: Apply Newton's backward difference formulas
First derivative at $x_3 = 4$:

$$f'(x_3) \approx \frac{1}{h}\left(\nabla f_3 - \frac{1}{2}\nabla^2 f_3 + \frac{1}{3}\nabla^3 f_3\right)$$

$$= \frac{1}{1}\left(4 - \frac{1}{2}(1) + \frac{1}{3}(0)\right) = 4 - 0.5 = \boxed{3.5}$$

Second derivative at $x_3 = 4$:

$$f''(x_3) \approx \frac{1}{h^2}\left(\nabla^2 f_3 - \nabla^3 f_3\right) = \frac{1}{1^2}(1 - 0) = \boxed{1}$$

Step 4: Interpretation
The estimates for the derivatives of $f(x)$ at $x = 4$ are:

$$f'(4) \approx 3.5, \quad f''(4) \approx 1$$

This means the function has a slope of approximately 3.5 and a concavity (upward curvature) of 1 at the endpoint. Newton's backward difference method is especially useful when estimating derivatives near the end of a tabulated dataset. ■

Convergence rate and accuracy

In numerical differentiation, the accuracy of an approximation is determined by how closely the numerical result matches the exact derivative, while the convergence rate indicates how rapidly this approximation improves as the step size h decreases. Finite difference methods are derived from Taylor series expansions and produce a truncation error that depends on the step size. For example, the forward difference formula for the first derivative,

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

is a first-order method, meaning its error is proportional to h, expressed as $O(h)$. In contrast, the central difference formula,

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h},$$

is a second-order method with error $O(h^2)$, making it more accurate for smaller values of h. The second derivative can also be approximated using the central difference formula,

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2},$$

which is also second-order accurate. In general, a method is said to have order p if its error behaves like Ch^p, where C is a constant. The convergence rate increases with the order: for a first-order method, halving h roughly halves the error, while for a second-order method, the error is reduced by a factor of four. However, while reducing h improves accuracy, it also increases the effect of round-off errors in finite-precision arithmetic. Higher-order methods offer better theoretical accuracy but may be more sensitive to noise and require more data points. Therefore, choosing an appropriate method involves balancing the trade-offs between accuracy, stability, and computational efficiency.

Advantages

– Well-suited for computing derivatives near the end of the dataset.

– Straightforward extension of the finite difference method.

– Compatible with tabular and experimental data.

Disadvantages

– Less accurate when used far from the boundary point x_n.

– Assumes uniformly spaced data.

– Accuracy decreases for higher-order derivatives or if higher-order differences are unstable.

3 Derivatives using unequally spaced values of argument

In practical applications, the data points may not always be equally spaced. When dealing with such cases, the standard forward and backward difference formulas (which assume constant spacing between data points) cannot be directly applied. Instead, we use modified methods that account for the unequal spacing between data points. These methods are based on weighted finite differences and employ interpolation techniques such as Lagrange interpolation or divided differences.

The derivative approximation for unequally spaced values of x can be derived by adjusting the forward and backward difference formulas. In these cases, the differences between successive data points are no longer constant, so we need to adjust the calculation accordingly. In this section, we discuss how to compute derivatives using unequally spaced values of the argument.

3.1 Unequally Spaced Forward Difference

In many practical numerical problems, the values of the independent variable x are not equally spaced. This situation arises in experimental data, irregular sampling, or adaptive meshing. When the spacing between points is non-uniform, standard forward difference formulas cannot be used directly, as they assume constant step size. In such cases, we rely on interpolation-based methods to approximate derivatives. One widely used approach is to construct a polynomial interpolant-typically using the Lagrange form—through a set of points near the point of interest and differentiate this polynomial to estimate the derivative. To estimate the first derivative at x_0, we consider three points x_0, x_1, x_2, where $x_0 < x_1 < x_2$ and the intervals $h_1 = x_1 - x_0$, $h_2 = x_2 - x_1$ are not equal. Using the Lagrange interpolation polynomial of degree two and differentiating it, we arrive at an expression for $f'(x_0)$ as a weighted sum of the function values at the given points. Specifically, the formula takes the form:

$$f'(x_0) \approx f(x_0)\cdot\left(\frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right)+f(x_1)\cdot\left(\frac{2x_0 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right)+f(x_2)\cdot\left(\frac{2x_0 - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right)$$

This formula allows us to compute the derivative even when the spacing between points is irregular. If only two points are available, a simpler first-order approximation is used:

$$f'(x_0) \approx \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

The accuracy in this case is lower, but the formula still provides a valid estimate. These approximations are especially valuable when only a few data points are available near the point of interest, and regular spacing cannot be assumed.

Algorithm 31 Numerical differentiation using unequally spaced forward differences

Require: Tabulated data points $(x_1, f_1), (x_2, f_2), \ldots, (x_n, f_n)$, where x_i are unequally spaced
Ensure: Approximate derivative $f'(x_1)$

Step 1: Compute the first-order forward difference

$$f'(x_1) \approx \frac{f_2 - f_1}{x_2 - x_1} = \frac{\Delta f_1}{h_1}$$

This gives a first-order approximation of the derivative at the first point using the forward difference quotient.

Step 2: Compute higher-order differences (optional)

For better accuracy, construct a forward divided difference table. The second-order forward divided difference is:

$$\Delta^2 f_1 = \frac{\frac{f_3 - f_2}{x_3 - x_2} - \frac{f_2 - f_1}{x_2 - x_1}}{x_3 - x_1}$$

Step 3: Use the extended Taylor form for unequally spaced points

To improve accuracy, include the second divided difference:

$$f'(x_1) \approx \frac{f_2 - f_1}{x_2 - x_1} + \frac{(x_2 - x_1)}{2} \cdot \Delta^2 f_1$$

Step 4: Output the derivative estimate

Return the numerical value of $f'(x_1)$ from Step 1 or Step 3 depending on desired accuracy.

Step 5: (Optional) Estimate the truncation error

If a smooth $f(x)$ is assumed, the truncation error can be approximated as:

$$E \approx \frac{(x_2 - x_1)(x_3 - x_2)}{3(x_3 - x_1)} f''(\xi), \quad \text{for some } \xi \in (x_1, x_3)$$

Example: Estimating $f'(1.0)$ using unequally spaced forward differences

We are given the following unequally spaced data points

x	$f(x)$
1.00	2.000
1.20	2.450
1.55	3.010

Step 1: Assign variables

$$x_0 = 1.00, \quad x_1 = 1.20, \quad x_2 = 1.55$$

$$f_0 = f(x_0) = 2.000, \quad f_1 = 2.450, \quad f_2 = 3.010$$

Step 2: Apply the general three-point forward difference formula for unequal spacing

$$f'(x_0) \approx f_0 \cdot \left(\frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} \right) + f_1 \cdot \left(\frac{2x_0 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \right) + f_2 \cdot \left(\frac{2x_0 - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \right)$$

Step 3: Substitute numerical values

$$\begin{aligned} f'(1.0) \approx 2.000 \cdot & \left(\frac{2(1.0) - 1.2 - 1.55}{(1.0 - 1.2)(1.0 - 1.55)} \right) \\ + 2.450 \cdot & \left(\frac{2(1.0) - 1.0 - 1.55}{(1.2 - 1.0)(1.2 - 1.55)} \right) \\ + 3.010 \cdot & \left(\frac{2(1.0) - 1.0 - 1.2}{(1.55 - 1.0)(1.55 - 1.2)} \right) \end{aligned}$$

$$\begin{aligned} &= 2.000 \cdot \left(\frac{-0.75}{(-0.2)(-0.55)} \right) + 2.450 \cdot \left(\frac{-0.55}{(0.2)(-0.35)} \right) + 3.010 \cdot \left(\frac{-0.2}{(0.55)(0.35)} \right) \\ &= 2.000 \cdot (-6.8182) + 2.450 \cdot (7.8571) + 3.010 \cdot (-1.0390) \\ &= -13.6364 + 19.2489 - 3.1264 = \boxed{2.4861} \end{aligned}$$

Final Result

$$\boxed{f'(1.0) \approx 2.486}$$

Conclusion: The derivative of $f(x)$ at $x = 1.0$ has been estimated using a second-degree forward interpolant suitable for unequally spaced data. This method provides higher accuracy by incorporating curvature from all three data points.

Convergence rate and accuracy

The convergence rate of the unequally spaced forward difference method is influenced by both the smoothness of the underlying function and the distribution of the data points. When a second-degree interpolating polynomial is used, the method typically achieves first-order accuracy, meaning the error is proportional to $O(h)$, where h denotes the average distance between the points. However, due to the non-uniform nature of the spacing, the local error constant can vary significantly, and the accuracy may degrade if the data points are unevenly spaced or if the function exhibits rapid changes. In general, the more irregular the spacing, the more difficult it becomes to control the error, especially near boundaries or sharp gradients in the function.

Advantages

– Applicable to datasets with non-uniform spacing between the independent variable values.

- Allows for derivative estimation when standard finite difference formulas are inapplicable due to irregular data distribution.
- Provides flexibility in modeling real-world or experimental data where equally spaced sampling is uncommon.
- By using more data points, higher-order accuracy can be achieved if the function is smooth.

Disadvantages

- More algebraically complex than standard finite difference formulas for equally spaced points.
- Sensitive to the irregularity of spacing, which can affect numerical stability and error behavior.
- Requires symbolic differentiation of the interpolating polynomial, which can be computationally intensive for larger datasets.
- Generally less accurate than central difference methods when points on both sides of the evaluation location are available.

3.2 Unequally spaced backward difference

In cases where data points are not equally spaced and the derivative is required near the end of a data set, the standard backward difference formula (which assumes constant step size) cannot be used directly. Instead, we apply an interpolation-based approach that accommodates unequal spacing. By constructing a Lagrange interpolating polynomial through a set of points ending at the target location, and then differentiating the polynomial analytically, we obtain an approximation for the derivative at the last point. Typically, a three-point backward difference using unequally spaced values x_n, x_{n-1}, x_{n-2} is used. These points are not required to be uniformly spaced, and we denote the spacing as $h_1 = x_n - x_{n-1}$, $h_2 = x_{n-1} - x_{n-2}$. This method is particularly useful when only previous values are known, such as in time-dependent simulations or sequential data processing.

Using the Lagrange interpolation polynomial and differentiating it at $x = x_n$, the backward difference approximation for the first derivative becomes:

$$\begin{aligned} f'(x_n) \approx f(x_n) \cdot & \left(\frac{2x_n - x_{n-1} - x_{n-2}}{(x_n - x_{n-1})(x_n - x_{n-2})} \right) \\ & + f(x_{n-1}) \cdot \left(\frac{2x_n - x_n - x_{n-2}}{(x_{n-1} - x_n)(x_{n-1} - x_{n-2})} \right) \\ & + f(x_{n-2}) \cdot \left(\frac{2x_n - x_n - x_{n-1}}{(x_{n-2} - x_n)(x_{n-2} - x_{n-1})} \right) \end{aligned}$$

When only two points are available, the formula simplifies to

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Algorithm 32 Numerical Differentiation Using Unequally Spaced Backward Difference

Require: Tabulated data points $(x_1, f_1), (x_2, f_2), \ldots, (x_n, f_n)$, where $x_1 < x_2 < \cdots < x_n$ are unequally spaced

Ensure: Approximate derivative $f'(x_n)$ at the last point using backward differences

Step 1: Define step sizes

Compute the local step sizes between the last three points:

$$h_1 = x_n - x_{n-1}, \quad h_2 = x_{n-1} - x_{n-2}$$

Step 2: Compute backward difference quotients

$$\Delta_1 = \frac{f_n - f_{n-1}}{h_1}$$
$$\Delta_2 = \frac{f_{n-1} - f_{n-2}}{h_2}$$

Step 3: Estimate the derivative at x_n

Use the unequal-spacing backward difference formula (second-order accurate):

$$f'(x_n) \approx \Delta_1 + \left(\frac{h_1 + h_2}{h_1 + h_2 + h_1 h_2/(x_n - x_{n-2})} \right) (\Delta_1 - \Delta_2)$$

Or alternatively, use an interpolated Lagrange-based expression if exact structure is needed.

Step 4: Output result

return Estimated value $f'(x_n)$

(Optional) Step 5: Estimate truncation error

If $f''(x)$ is known or can be approximated:

$$E \approx \frac{(h_1^2 + h_2^2)}{2} f''(x_n)$$

This provides an estimate of local truncation error due to discretization.

Example: Estimate the derivative using unequally spaced backward difference
Estimate $f'(2.0)$ using the three-point backward difference method for unequally spaced data. The given table is

x	$f(x)$
1.2	3.320
1.7	4.380
2.0	5.800

We denote

$$x_{n-2} = 1.2, \quad x_{n-1} = 1.7, \quad x_n = 2.0$$

$$f_{n-2} = 3.320, \quad f_{n-1} = 4.380, \quad f_n = 5.800$$

Step 1: Use the general backward difference formula for unequally spaced points

$$f'(x_n) \approx f_n \cdot \left(\frac{2x_n - x_{n-1} - x_{n-2}}{(x_n - x_{n-1})(x_n - x_{n-2})} \right) + f_{n-1} \cdot \left(\frac{2x_n - x_n - x_{n-2}}{(x_{n-1} - x_n)(x_{n-1} - x_{n-2})} \right) + f_{n-2} \cdot \left(\frac{2x_n - x_n - x_{n-}}{(x_{n-2} - x_n)(x_{n-2} -} \right.$$

Step 2: Compute the required differences and intermediate values

$h_1 = x_n - x_{n-1} = 0.3, \quad h_2 = x_{n-1} - x_{n-2} = 0.5$
$d_1 = 2x_n - x_{n-1} - x_{n-2} = 1.1, \quad d_2 = 2x_n - x_n - x_{n-2} = 0.8, \quad d_3 = 2x_n - x_n - x_{n-1} = 0.3$
$D_1 = h_1 \cdot (x_n - x_{n-2}) = 0.3 \cdot 0.8 = 0.24$
$D_2 = (x_{n-1} - x_n)(x_{n-1} - x_{n-2}) = (-0.3)(0.5) = -0.15$
$D_3 = (x_{n-2} - x_n)(x_{n-2} - x_{n-1}) = (-0.8)(-0.5) = 0.4$

Step 3: Substitute all values into the formula

$$f'(2.0) \approx 5.800 \cdot \left(\frac{1.1}{0.24} \right) + 4.380 \cdot \left(\frac{0.8}{-0.15} \right) + 3.320 \cdot \left(\frac{0.3}{0.4} \right)$$

$$\approx 5.800 \cdot 4.5833 - 4.380 \cdot 5.3333 + 3.320 \cdot 0.7500$$

$$\approx 26.5829 - 23.3600 + 2.4900 = 5.7129$$

Final Answer

$$\boxed{f'(2.0) \approx 5.713}$$

Conclusion: Using the backward difference method for unequally spaced data, we estimate that the derivative of $f(x)$ at $x = 2.0$ is approximately 5.713. This method is valuable for non-uniform data, particularly when only the most recent values are available.

Convergence rate and accuracy

The convergence rate of the unequally spaced backward difference method is generally first-order when based on a second-degree interpolant. The error behaves as $O(h)$, where h is the average spacing between the data points. However, due to non-uniform spacing, the actual error constant can vary significantly. Unevenly spaced points may lead to reduced accuracy or numerical instability, especially near boundaries or where the function exhibits rapid variation.

Advantages

- Suitable for cases where data is only available behind the point of interest.
- Applicable to datasets with irregular spacing.
- Straightforward to implement using Lagrange polynomial differentiation.
- Useful in time-dependent problems or post-processed data analysis.

Disadvantages

- More complex algebraically than uniform backward difference formulas.
- May be less accurate if the point distribution is highly irregular.
- Requires at least two or three preceding data points for meaningful accuracy.
- Accuracy can be significantly affected by noise or non-smooth behavior in the data.

4 Analysis of tabulated functions

In many scientific and engineering applications, a function is known not through a formula but only at discrete data points, often presented in tabulated form. In such cases, the traditional analytical approach for locating maxima or minima (i.e., solving $f'(x) = 0$) is not directly applicable. Instead, interpolation techniques are applied to estimate the derivative, and the critical points are then found numerically.

This section discusses methods for analyzing tabulated functions, including finding maxima and minima, and the procedures for approximating derivatives using finite differences and interpolation techniques.

4.1 Maxima and Minima of a tabulated function

In many practical applications, we deal with functions whose values are available at discrete points, or tabulated data. These functions may have **local maxima** or **minima**, and it is often necessary to determine the points where these occur. Finding the maxima and minima of tabulated functions is important for optimization problems, engineering, and data analysis.

To identify local maxima and minima from tabulated data, we use finite difference methods, such as checking the behavior of the function values in the table. Specifically, we examine the relative behavior of the function at each point with respect to its neighbors.

Note

- The accuracy of this method depends on the degree of the interpolating polynomial and the smoothness of the underlying function.
- Using more points can improve accuracy but may lead to oscillations (Runge's phenomenon) if the polynomial degree becomes too high.

Algorithm 33 Finding Maxima and Minima of a tabulated function (Equally spaced data)

Require: A set of tabulated data points $(x_0, f_0), (x_1, f_1), \ldots, (x_n, f_n)$, with uniform spacing $h = x_{i+1} - x_i$

Ensure: Approximate location x_{ext} and value $f(x_{\text{ext}})$ of a local extremum

Step 1: Select surrounding points.
Identify 3 to 5 points around the suspected extremum. These will be used for interpolation.
Step 2: Construct the interpolating polynomial.
if the points are equally spaced **then**
    Use Newton's forward or backward interpolation formula (depending on where in the table the extremum lies).
else
    Use Lagrange's interpolation formula:

$$P(x) = \sum_{i=0}^{k} f_i \prod_{\substack{j=0 \\ j \neq i}}^{k} \frac{x - x_j}{x_i - x_j}$$

end if
Step 3: Differentiate the interpolating polynomial.
Obtain the derivative $f'(x) = \frac{d}{dx} P(x)$
Step 4: Solve for critical points.
Solve $f'(x) = 0$ numerically or symbolically to find candidate extremum point(s) x_{ext}
Step 5: Evaluate the extremum value.
Substitute x_{ext} into the interpolated polynomial:

$$f(x_{\text{ext}}) = P(x_{\text{ext}})$$

Step 6: (Optional) Determine the nature of the extremum.
Compute the second derivative:

$$f''(x_{\text{ext}}) = \frac{d^2}{dx^2} P(x)$$

if $f''(x_{\text{ext}}) > 0$ **then**
    Local minimum
else if $f''(x_{\text{ext}}) < 0$ **then**
    Local maximum
else
    Inconclusive – test higher derivatives or inspect neighboring values
end if

4.2 First derivative test for Maxima and Minima

Given a function $f(x)$ with tabulated values $f(x_0), f(x_1), \ldots, f(x_n)$, the following methods can be used to approximate the maxima and minima of the function.

The general rule for identifying maxima and minima is based on the first derivative of the function, as follows:

$$f'(x) = 0$$

- A point x_0 is a local maximum if

$$f'(x_0) = 0 \quad \text{and} \quad f''(x_0) < 0$$

- A point x_0 is a local minimum if

$$f'(x_0) = 0 \quad \text{and} \quad f''(x_0) > 0$$

For tabulated data, we approximate the first derivative using finite differences. The following finite difference formulas are used to compute $f'(x_0)$:

1. **Forward difference formula for the first point** x_0:

$$f'(x_0) \approx \frac{f(x_1) - f(x_0)}{h_0}$$

   where $h_0 = x_1 - x_0$.

2. **Backward difference formula for the last point** x_n:

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{h_{n-1}}$$

   where $h_{n-1} = x_n - x_{n-1}$.

3. **Central difference formula for interior points** $x_1, x_2, \ldots, x_{n-1}$:

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h_i}$$

   where $h_i = x_{i+1} - x_i$ is the spacing between the points.

The first derivative test is used to analyze the sign change of the first derivative around a point x_i to determine whether it corresponds to a local maximum or minimum.

4.3 Second derivative test for Maxima and Minima

For tabulated data, the second derivative $f''(x)$ can be approximated using the central difference method:

$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h_i^2}$$

- If $f''(x_i) < 0$, then x_i is a *local maximum.* - If $f''(x_i) > 0$, then x_i is a *local minimum.*

For endpoints, we typically rely on the first derivative approximation, as we do not have data points on both sides of the point in question.

Example: Identifying local extrema from tabulated function values
Given a set of equally spaced tabulated values

x	$f(x)$
0	1
1	3
2	5
3	4
4	2

We aim to estimate the locations and types (maximum or minimum) of any local extrema using numerical differentiation.

Step 1: Confirm Step Size
The step size is constant

$$h = x_{i+1} - x_i = 1$$

Step 2: Compute First Derivatives Using Central Differences
The first derivative at interior points x_i is estimated as

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

$$\begin{aligned} f'(1) &\approx \frac{f(2) - f(0)}{2} = \frac{5-1}{2} = 2.0 \\ f'(2) &\approx \frac{f(3) - f(1)}{2} = \frac{4-3}{2} = 0.5 \\ f'(3) &\approx \frac{f(4) - f(2)}{2} = \frac{2-5}{2} = -1.5 \end{aligned}$$

Step 3: Compute Second Derivatives Using Central Differences
The second derivative is approximated as

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

$$\begin{aligned} f''(1) &\approx \frac{f(2) - 2f(1) + f(0)}{1} = 5 - 6 + 1 = 0 \\ f''(2) &\approx \frac{f(3) - 2f(2) + f(1)}{1} = 4 - 10 + 3 = -3 \\ f''(3) &\approx \frac{f(4) - 2f(3) + f(2)}{1} = 2 - 8 + 5 = -1 \end{aligned}$$

Step 4: Interpret the Results
We use the signs of $f'(x)$ and $f''(x)$ to classify the extrema

– At $x = 1$: $f'(1) = 2.0$, $f''(1) = 0$
  Derivative not zero → not an extremum

- At $x = 2$: $f'(2) = 0.5$, $f''(2) = -3$
  First derivative is small and second negative → **local maximum**
- At $x = 3$: $f'(3) = -1.5$, $f''(3) = -1$
  First derivative not zero → function is still decreasing → not a local extremum

Conclusion: From the numerical derivatives, we identify that $x = 2$ corresponds to a local maximum of the function $f(x)$. Other points do not satisfy the standard conditions for extremum classification.

5 Tasks

1. Given the following tabulated data for the function $f(x)$:

x	$f(x)$
1	2
2	4
3	9
4	16
5	25

   - Use the **forward difference formula** to compute the derivative at $x_1 = 2$ and $x_2 = 3$.
   - Use the **backward difference formula** to compute the derivative at $x_3 = 4$ and $x_4 = 5$.
   - Compare the results with the analytical derivative of $f(x) = x^2$, which is $f'(x) = 2x$, and discuss the accuracy of the numerical results.

2. Given the following tabulated data for the function $f(x)$ at unequally spaced points:

x	$f(x)$
1.0	2.5
1.3	3.4
2.2	6.0
3.5	12.8
4.8	21.6

   - Use a forward difference approximation to compute the derivative at $x_1 = 1.3$.
   - Use a backward difference approximation to compute the derivative at $x_4 = 3.5$.
   - Use a central difference approximation to compute the derivative at $x_2 = 2.2$.
   - Discuss how the unequal spacing affects the accuracy of the derivative compared to using equally spaced data points.

3. Given the following tabulated data for $f(x)$:

x	$f(x)$
0	0.1
1	1.4
2	3.9
3	2.8
4	1.0
5	0.5

   – Compute the first derivative at the interior points using the **central difference formula**.

   – Compute the second derivative at the interior points using the **central difference formula**.

   – Identify any local maxima and minima based on the first and second derivatives.

   – Interpret the results and discuss the accuracy of identifying local extrema from tabulated data.

4. Given the following tabulated data for $f(x)$:

x	$f(x)$
1.0	1.0
1.2	1.8
1.4	2.5
1.6	3.2
1.8	3.8

   – Compute the first derivative at $x = 1.4$ using the following methods:

      - Forward difference
      - Backward difference
      - Central difference

   – Calculate the exact derivative (if possible), or compare the results with the analytical derivative of the function (if known). For example, if the function is $f(x) = x^2$, the derivative is $f'(x) = 2x$.

   – Discuss the accuracy and effectiveness of each method (forward, backward, central) for calculating derivatives, especially when the data points are not equally spaced.

– Given the following tabulated data for $f(x)$:

x	$f(x)$
0.5	1.8
1.0	3.2
1.5	5.0
2.0	4.7
2.5	3.1
3.0	2.0

– Compute the first derivative using a **central difference method** at the interior points.

– Compute the second derivative using a **central difference method** at the interior points.

– Identify any local maxima and minima using the first and second derivatives.

– Discuss how the uneven spacing of the data points affects the derivative calculations and how it may influence the accuracy of identifying extrema.

5. Suppose you are tasked with optimizing a cost function for a manufacturing process, where the function values are given at different time intervals. The data is given as follows:

Time (hours)	Cost ($)
0	100
1	95
2	90
3	88
4	92
5	100

– Use finite differences to compute the first and second derivatives at the interior points.

– Identify the local minimum (if any) based on the first and second derivative tests.

– Interpret the result: what is the best time to optimize cost, and why?

6. Given a set of data points representing the temperature at various times of the day:

Time (hours)	Temperature (°C)
0	20
2	22
4	24
6	25
8	26
10	27
12	28

7. Use the forward and backward difference formulas to approximate the temperature derivative at various points.

8. Use the central difference formula for the interior points.

9. Analyze: At what time does the temperature change most rapidly? When is the temperature rate of change zero, and what does that indicate about the temperature trend?