

High-accuracy reconstruction of a function $f(x)$ when only $\frac{d}{dx}f(x)$ or $\frac{d^2}{dx^2}f(x)$ is known at discrete measurement points

Clemens Elster^a and Ingolf Weingärtner^b

^aPhysikalisch-Technische Bundesanstalt Berlin,
Abbestr. 2-12, 10587 Berlin, Germany

^bPhysikalisch-Technische Bundesanstalt Braunschweig,
Bundesallee 100, 38116 Braunschweig, Germany

ABSTRACT

The task of reconstructing a function $f(x)$ from a set of measurements of the first or second derivative is considered. Methods for numerical integration are briefly outlined and discussed with regard to their potential application to the current task. Furthermore, cubic spline interpolation of the data followed by integration of the interpolation spline is proposed, and the influence of noise on the accuracy of the reconstructed function $f(x)$ is examined.

Results of numerical simulations for several test problems are presented for both noiseless and noisy data, and the efficiency of different methods is compared. Best results were obtained by cubic spline interpolation and subsequent integration of the spline function. The examples presented demonstrate that the reconstruction of a function $f(x)$ from a set of measurements of the first or second derivative can be performed with high accuracy.

Keywords: Numerical integration, spline interpolation, topography reconstruction

1. INTRODUCTION

In the last few years several proposals have been made to determine the topography by measuring first or second derivatives.¹⁻⁶ To reach high accuracy, e.g. determine the profile $f(x)$ of a topography with nanometric uncertainty, high-accuracy reconstruction of $f(x)$ must be performed when the derivatives $\frac{d^2}{dx^2}f(x)$ or $\frac{d}{dx}f(x)$ are known at discrete measurement locations*.

The present paper has the following aims[†]: We wish to demonstrate that the reconstruction of a surface profile using sampled slope data or data of the second derivative can be performed with a very low uncertainty provided that the function is smooth and that the data are of sufficient accuracy. The proposed method is also relevant to other applications where the integration of noisy function values has to be performed. The accurate reconstructions can be determined by application of standard procedures as implemented in many numerical libraries. Furthermore, error propagation is studied and it is shown that numerical integration is insensitive to noise. Results of numerical simulations for some examples are presented in order to determine reconstruction accuracies that can be reached.

In section 2 standard methods of numerical integration are briefly outlined and discussed with regard to their ability to determine the values $f(x_i)$ of a function $f(x)$ at many different locations x_i using sampled slope data or data of the second derivative. Alternatively, in section 3, application of a cubic spline interpolant to the data is proposed; once the spline function is determined, it can be exactly integrated once or twice. The influence of the measurement noise in the values of slope or second derivative on the errors of the estimated function $f(x)$

*Note that without further information $f(x)$ can be reconstructed only up to an arbitrary constant in case $\frac{d}{dx}f(x)$ is known or up to a straight line in case $\frac{d^2}{dx^2}f(x)$ is known.

[†]One of the authors (Ingolf Weingärtner) was asked during many talks and discussions about accuracy of integration routines as obviously many physicists dealing with the determination of slope and topography are not aware that "numerical integration" can be performed with high accuracy.

is studied in section 4. Finally in section 5, results of numerical examples are presented and the efficiency of the different methods is compared.

2. NUMERICAL INTEGRATION

A brief overview of current methods for the numerical calculation of

$$\int_a^b g(x)dx \quad (1)$$

is given. Some of the procedures can be directly applied to a set of measured values of $g(x)$, whereas other procedures are adaptive and the set of locations where $g(x)$ is to be evaluated is not known in advance.

2.1. Newton-Cotes formulas

The Newton-Cotes formulas are obtained by approximation of the integral (1) by

$$\int_a^b p_k(x)dx$$

where $p_k(x)$ is a polynomial of k -th degree which interpolates the values of $g(x)$ at $k + 1$ equidistant locations

$$x_i = a + ih, i = 0, \dots, k, \quad h = (b - a)/k.$$

This leads to estimates

$$\int_a^b g(x) \approx \sum_{i=0}^k \alpha_i g(x_i).$$

For example, for $k = 1$, the trapezoidal rule

$$\int_a^b g(x)dx = \frac{h}{2} [g(a) + g(b)] + O(h^3 g^{(2)}(\zeta))$$

and for $k = 2$, Simpson's rule

$$\int_a^b g(x)dx = \frac{h}{3} [g(a) + 4g[(a + b)/2] + g(b)] + O(h^5 g^{(4)}(\zeta'))$$

with $\zeta, \zeta' \in [a, b]$ are derived.⁷ The use of large values k is not suitable. Instead, one usually divides the interval $[a, b]$ into a number of, say n , subintervals and then applies the Newton-Cotes formulas for some small k to each of the subintervals. For the trapezoidal rule, for example, this leads to

$$\begin{aligned} \int_a^b g(x)dx &= h \left[\frac{g(a)}{2} + g(a + h) + g(a + 2h) + \dots + g(b - h) + \frac{g(b)}{2} \right] \\ &+ O(h^2 g^{(2)}(\zeta)), \end{aligned}$$

see⁷; the step size h is now defined according to $h := (b - a)/n$ where n denotes the number of subintervals. The trapezoidal rule can thus be readily applied to estimate the integral (1) when tabulated, i.e. measured, values of the function $g(x)$ are available at equidistant locations $x_0 < x_1 < \dots < x_n$. Moreover, the values of the integral can be estimated with the upper limit b equal to any of the values x_1, x_2, \dots, x_n .

2.2. Gaussian quadrature

The Newton-Cotes formulas estimate the integral (1) by the integral of a polynomial which interpolates $g(x)$ at $k + 1$ equidistant locations x_i ; hence, these formulas are exact for all polynomials up to degree k . By lowering the demand for equidistant evaluation points of $g(x)$, the number of function values needed to exactly integrate all polynomials up to a certain degree can be reduced. Gaussian quadrature rules allow all polynomials of degree $\leq 2k - 1$ to be integrated using function evaluations at only k suitably chosen locations $x_i, i = 0, \dots, k - 1$.⁷ Hence Gaussian quadrature rules are more efficient than the Newton-Cotes formulas. However, since the locations $x_i, i = 0, \dots, k - 1$, do not show a systematic pattern, Gaussian quadrature rules are not appropriate for evaluating (1) for different values of the upper bound b using tabulated function values.

2.3. Application of extrapolation

Extrapolation can be used to enhance the convergence of application of, for example, the trapezoidal rule. This technique makes use of the fact that the corresponding integral estimation can be modelled by a polynomial in h^2 where coefficients corresponding to low-order terms are independent of the step size h .⁷ By repeated application of the trapezoidal rule for decreasing values of h , this polynomial is estimated and an improved estimate of the integral is obtained by extrapolation $h \rightarrow 0$. However, as for Gaussian quadrature, this technique is not suitable to evaluate (1) for different values of the upper bound b using tabulated function values.

2.4. Adaptive procedures

A powerful method for approximating the integral (1) is to subdivide the interval $[a, b]$ and to obtain an estimate for the integral including an error estimate for all subintervals. Subsequently, the subinterval containing the largest error estimate is again bisected. This is continued until a prescribed tolerance for the approximation of the integral (1) is reached.⁸ Such a globally adaptive scheme is not, however, suitable for integrating tabulated function values in general.

3. NUMERICAL INTEGRATION WHEN ONLY TABULATED FUNCTION VALUES ARE KNOWN

It is assumed that values of the function $f''(x)$, i.e. $\frac{d^2}{dx^2}f(x)$, or $f'(x)$, i.e. $\frac{d}{dx}f(x)$, are available at $n + 1$ equidistant locations $x_i, i = 0, \dots, n$. The task is to estimate $f(x)$ at these locations $x_i, i = 0, \dots, n$. Two different methods are described for carrying out this task; the latter can also be applied to non-equidistant x_i . For ease of notation, $f(x_i)$, $f'(x_i)$ and $f''(x_i)$ will in the following be abbreviated by f_i , f'_i and f''_i , respectively.

3.1. Application of Newton-Cotes formulas

Since the function values are available at equidistant locations, the Newton-Cotes formulas can be applied. Two variants are considered: (i) repeated application of the trapezoidal rule and (ii) application of the trapezoidal rule followed by repeated application of Simpson's rule. If the values of $f'(x)$ are known, this leads to estimates

$$f_0 := 0, \quad f_{i+1} := f_i + \frac{h}{2}(f'_i + f'_{i+1}), \quad i = 0, \dots, n - 1 \quad (2)$$

for the trapezoidal rule and

$$\begin{aligned} f_0 &:= 0, \quad f_1 := \frac{h}{2}(f'_0 + f'_1), \\ f_{i+2} &:= f_i + \frac{h}{3}(f'_i + 4f'_{i+1} + f'_{i+2}), \quad i = 0, \dots, n - 2 \end{aligned} \quad (3)$$

for the trapezoidal and Simpson's rule combined; $h = x_{i+1} - x_i = (x_n - x_0)/n$ denotes the constant spacing between the evaluation points. Note that in (3) f_1 cannot be estimated by Simpson's rule and this estimate is hence obtained using the trapezoidal rule. Note further that the integration constant has been chosen such that $f_0 = 0$ holds. In case values of $f''(x)$ are available, the above procedures are applied twice.

3.2. Application of interpolation and subsequent integration

This approach first furnishes an estimate $\hat{f}'(x)$ or $\hat{f}''(x)$ of the function $f'(x)$ or $f''(x)$ over the interval $[x_0, x_n]$ from the given function values f'_i or f''_i , $i = 0, \dots, n$, and then determines estimates f_i by integrating $\hat{f}'(x)$ or $\hat{f}''(x)$ once or twice, respectively. In order to obtain $\hat{f}'(x)$ or $\hat{f}''(x)$, cubic spline interpolation can be applied.⁷ A cubic spline function consists of piecewise cubic polynomials, and hence integrating the spline function once or twice can be easily and exactly performed.

In order to unambiguously determine the cubic interpolation spline end conditions at x_0 and x_n have to be posed. The results reported in section 5 were obtained by application of the "not-a-knot" condition, see,⁹ as implemented by IMSL.⁸

4. INFLUENCE OF MEASUREMENT NOISE

Integration is a smoothing operation. In contrast to numerical differentiation where small errors in the function can lead to large errors in the estimated derivative, measurement noise is expected to introduce only moderate errors. In the following, the influence of measurement noise on the result of single or double integration of a function is studied when only tabulated noisy function values are available. For ease of discussion, repeated application of the trapezoidal rule (2) is considered. The following relation between the noisy function values $(f''_i)^\sigma$ and the f''_i is assumed:

$$(f''_i)^\sigma = f''_i + \epsilon_i, \quad i = 0, \dots, n,$$

where the ϵ_i are independently distributed with zero mean and variance σ^2 .

Denote by \hat{f}'_i the application of the trapezoidal rule (2) to the $(f''_i)^\sigma$ and by \hat{f}_i the application of the trapezoidal rule to the \hat{f}'_i . Let $\tilde{\Delta}_i^{(1)}$ and $\tilde{\Delta}_i^{(0)}$ denote the statistical part of the error of the \hat{f}'_i and \hat{f}_i . One immediately obtains

$$\tilde{\Delta}_0^{(1)} = 0, \quad \tilde{\Delta}_i^{(1)} = h \sum_{j=0}^i \epsilon_j - h \frac{\epsilon_0 + \epsilon_i}{2}, \quad i = 1, \dots, n \quad (4)$$

and

$$\tilde{\Delta}_0^{(0)} = 0, \quad \tilde{\Delta}_i^{(0)} = h \sum_{j=0}^i \tilde{\Delta}_j^{(1)} - h \frac{\tilde{\Delta}_0^{(1)} + \tilde{\Delta}_i^{(1)}}{2}, \quad i = 1, \dots, n \quad (5)$$

The errors of the first integration are a sum of independent random variables and the $\tilde{\Delta}_i^{(1)}$ can hence be viewed as a random walk. This introduces correlations into the $\tilde{\Delta}_i^{(1)}$, $\tilde{\Delta}_j^{(1)}$ and into the $\tilde{\Delta}_i^{(0)}$, $\tilde{\Delta}_j^{(0)}$. In order to simplify formulas, the behaviour of

$$\Delta_i^{(1)} := h \sum_{j=0}^i \epsilon_j, \quad i = 0, \dots, n$$

and

$$\Delta_i^{(0)} := h \sum_{j=0}^i \Delta_j^{(1)}, \quad i = 0, \dots, n$$

will be outlined, i.e. end conditions in the formulas (4) and (5) will be ignored. One immediately obtains

$$E(\Delta_i^{(1)}) = E(\Delta_i^{(0)}) = 0, \quad i = 0, \dots, n,$$

where E denotes expectation, and

$$\text{var}(\Delta_i^{(1)}) = h^2(i+1)\sigma^2 = \left(\frac{x_n - x_0}{n}\right)^2 (i+1)\sigma^2$$

as well as

$$\begin{aligned} \text{var}(\Delta_i^{(0)}) &= \frac{h^4}{6}(i+1)(i+2)(2i+3)\sigma^2 \\ &= \text{var}(\Delta_i^{(1)}) \left(\frac{h^2}{6}(i+2)(2i+3)\right) \\ &= \text{var}(\Delta_i^{(1)}) \left(\frac{(x_n - x_0)^2}{6} \frac{(i+2)}{n} \frac{(2i+3)}{n}\right) \end{aligned}$$

where i runs from 0 to n and the step size h is given by $h = (x_n - x_0)/n$. From these relations one immediately recognizes a scaling effect: When – for fixed n – the size of the interval $[x_0, x_n]$ is increased by some factor, the variance of $\Delta_i^{(1)}$ increases by the square of this factor and the variance $\Delta_i^{(0)}$ to the power 4.

If we assume that $x_n - x_0$ is of the order of 1, the size of the errors after integration is reduced, i.e. $\text{var}(\Delta_i^{(1)})$ is smaller than σ^2 . Moreover, the size of the maximum errors of $\Delta_i^{(1)}$ and $\Delta_i^{(0)}$ for $i = n$ are of the same order of magnitude, and for smaller values of i the error level decreases when numerical integration is applied twice.

5. EXAMPLE: DETERMINING A FUNCTION WHEN ONLY THE SECOND DERIVATIVE IS KNOWN AT DISCRETE MEASUREMENT LOCATIONS

In this section results of numerical integration of a function are reported when values of the second derivative are given at discrete measurement locations. The following three test functions on $[0, 1]$ are considered:

(i) $f''(x) = f'(x) = f(x) = 0,$

(ii) $f''(x) = x^2 - 2x^4 + x^6, f'(x) = x^3/3 - 2x^5/5 + x^7/7,$

$$f(x) = x^4/12 - x^6/15 + x^8/56,$$

(iii) $f''(x) = \sin(10\pi x), f'(x) = [1 - \cos(10\pi x)]/(10\pi),$

$$f(x) = x/(10\pi) - \sin(10\pi x)/(10\pi)^2.$$

The first function is the zero function and corresponding results will directly show the influence of integration with respect to noise. The second function is a polynomial which is typical of applications in modern optical systems and their testing,^{10,11} and the third function is a highly oscillating trigonometric function chosen to also test the methods on a non-polynomial function. The functions were chosen such that in particular $f(0) = f'(0) = 0$ holds.

Values $(f_i'')^\sigma$ of the second derivative were chosen according to

$$(f_i'')^\sigma = f''(x_i) + \sigma\epsilon_i, \quad i = 0, \dots, n,$$

where $x_i = i/n, i = 0, \dots, n$. The ϵ_i denote Gaussian random numbers with zero mean and unit variance.

Application of the trapezoidal rule (2), trapezoidal and Simpson's rule combined (3) as well as the integration of an interpolating cubic spline were considered. Integration constants were chosen such that the reconstructed

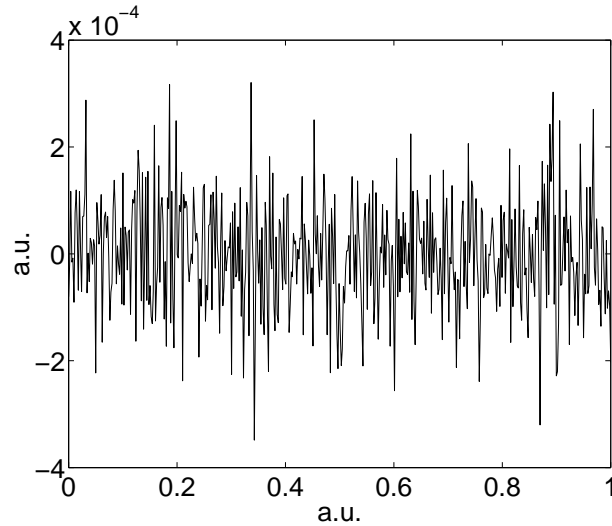


Figure 1: Spline interpolation of test function (i) (purely noise, $\sigma = 1.0 \times 10^{-4}$ a.u.)

functions all satisfy $\hat{f}(0) = \hat{f}'(0) = 0$. The accuracy of the reconstructions was then assessed by the root mean square error and by the maximum of the absolute error

$$rms^{(\nu)} := \sqrt{\frac{1}{n+1} \sum_{i=0}^n \left(\hat{f}_i^{(\nu)} - f_i^{(\nu)} \right)^2}, \quad \delta^{(\nu)} := \max_{i=0}^n \left| \hat{f}_i^{(\nu)} - f_i^{(\nu)} \right|, \quad \nu = 0, 1.$$

For example, $\delta^{(1)}$ denotes the maximum absolute difference between the first derivative of a test function and its estimate, and $\delta^{(0)}$ denotes the maximum absolute difference between a test function and its estimate.

Two values of n , namely $n = 50$ and $n = 500$, as well as two noise levels, namely no noise, i.e. $\sigma = 0$, and $\sigma = 10^{-4}$, were considered. In the case of noisy data the results differ when the simulations are repeated with different random numbers. However, the orders of magnitude of the errors remain the same. Figures 1 and 2 show results of spline interpolation followed by integration(s) of the spline function for test function (i) in the noisy case with $n = 500$. One can see that in this case integration tends to reduce the noise and that it introduces correlations. Table I shows typical results for all cases, where each data set was simultaneously analyzed by all methods.

The results of table I show that excellent accuracies can be reached with noiseless data, and that the errors in the noisy case are comparably small. Obviously, spline interpolation and subsequent integration(s) of the spline function led to the best results. This holds in particular for test function (iii) which is not a simple polynomial. From the results for test function (i) it can directly be seen that the statistical part of the errors in the noisy case becomes smaller when the integration is repeated once. This is in accordance with the discussion of the influence of noise in the last section.

In the case of noiseless data, all methods perfectly treat test function (i), whereas results for test function (ii) and in particular for test function (iii) differ to a large extent. For test functions (ii) and (iii) the difference in the accuracies reached when changing from $n = 50$ to $n = 500$ sampled values of the second derivative, clearly demonstrates the different orders of the procedures. For example, errors of the reconstructed first derivative for the trapezoidal rule for test functions (ii) and (iii) are reduced by a factor of 100 when changing from $n = 50$ to $n = 500$ which is due to the fact that the errors $\hat{f}'(x_n) - f'(x_n)$ of this method are proportional to $h^2 \propto 1/n^2$. For the trapezoidal and Simpson's rule combined, the scaling behaviour also becomes apparent; it is not, however, that clear-cut, since in (3) f_1' (as well as f_1) is obtained by application of the trapezoidal rule

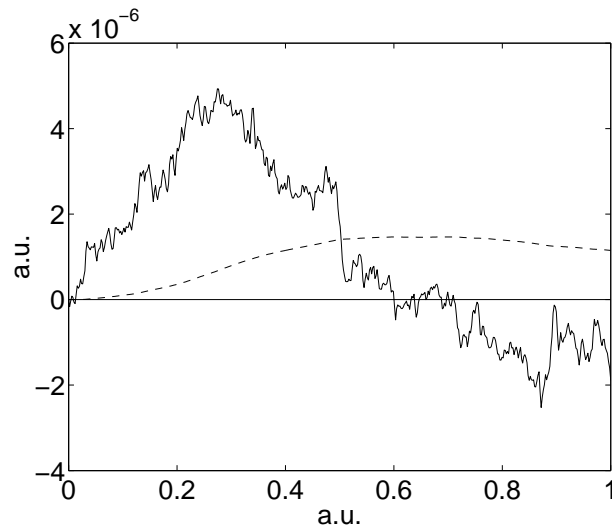


Figure 2. Results of spline interpolation followed by integration of the spline function for test function (i) (purely noise): The solid and dashed lines show the result after single and double integration of the spline function (figure 1), respectively.

and all other estimates are obtained by Simpson's rule which is of a higher order.

The accuracies reached by spline interpolation followed by integration of the spline function are excellent for test function (ii). For test function (iii) the power of the spline interpolation followed by integration of the spline function as compared to the application of the two Newton-Cotes formulas becomes apparent. Note, however, that for this function the accuracy is greatly improved when $n = 500$ instead of $n = 50$ sampled function values are used.

In the case of noisy data, i.e. $\sigma = 10^{-4}$, the following can be observed. For test functions (i) and (ii) all methods perform more or less equally well. In these cases the statistical errors dominate the errors of the estimates. For test function (iii) and $n = 50$, the results of the spline interpolation followed by integration of the spline function are significantly better; hence, in this case, errors due to the integration of the noiseless test function (iii) are still dominant when applying the Newton-Cotes formulas; in the case $n = 500$, both trapezoidal and Simpson's rule combined as well as spline interpolation followed by integration of the spline function perform equally well and still better than the application of the trapezoidal rule. Thus, for the trapezoidal rule errors due to the integration of the noiseless test function (iii) are still relevant, whereas the errors for trapezoidal and Simpson's rule combined as well as for spline interpolation followed by integration of the spline function are dominated by the noise in this case.

6. CONCLUSIONS

The reconstruction of a function $f(x)$ has been considered when only values of the first or second derivative are available at discrete measurement locations. A brief overview of standard methods for numerical integration has been given. From these methods only the application of Newton-Cotes formulas is generally relevant to the task of discretely sampled values. As an alternative, cubic spline interpolation followed by integration(s) of the spline function has been proposed.

The influence of noise has been studied. On the assumption of independent errors in the values of the second derivative, it was shown that for reconstruction on $[0, 1]$ the errors after integration remain small when a numerical integration procedure is applied. Moreover, for repeated integration, the size of the errors of the estimated function obtained tends to be smaller than for the estimated first derivative.

Numerical results have been presented which compare the performance of spline interpolation with subsequent

exact integration(s) of the spline function and application of two Newton-Cotes formulas. The former method clearly outperformed the other two methods in the cases in which errors due to nonlinearities of the functions were larger than those due to statistical errors. In the remaining cases, all methods showed comparable performance. The results also demonstrate that numerical integration can lead to excellent results for smooth functions. It is concluded that spline interpolation with subsequent integration(s) of the spline function can be recommended for integrating a discretely sampled function once or twice.

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Table I: Results of trapezoidal rule, trapezoidal and Simpson's rule combined abbreviated as Simpson's rule, as well as spline interpolation followed by integration of the spline function for typical runs on the three test functions for different noise levels and different numbers of data. The columns headed by $rms^{(1)}$ and $\delta^{(1)}$ show the root mean square error and the maximum absolute error after single integration, and the columns headed by $rms^{(0)}$ and $\delta^{(0)}$ show the root mean square error and the maximum absolute error after double integration.

		$rms^{(1)}/$ a.u.	$rms^{(0)}/$ a.u.	$\delta^{(1)}/$ a.u.	$\delta^{(0)}/$ a.u.
Test function (i) $n = 50$ $\sigma = 0$	Trapezoidal rule	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}
	Simpson's rule	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}
	Spline interpolation	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}
Test function (i) $n = 500$ $\sigma = 0$	Trapezoidal rule	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}
	Simpson's rule	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}
	Spline interpolation	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}	0.0×10^{-0}
Test function (i) $n = 50$ $\sigma = 1.0 \times 10^{-4}$	Trapezoidal rule	4.4×10^{-6}	1.5×10^{-6}	1.0×10^{-5}	3.2×10^{-6}
	Simpson's rule	5.2×10^{-6}	1.6×10^{-6}	1.5×10^{-5}	3.6×10^{-6}
	Spline interpolation	4.6×10^{-6}	1.6×10^{-6}	1.0×10^{-5}	3.5×10^{-6}
Test function (i) $n = 500$ $\sigma = 1.0 \times 10^{-4}$	Trapezoidal rule	2.9×10^{-6}	5.7×10^{-7}	5.4×10^{-6}	1.0×10^{-6}
	Simpson's rule	3.0×10^{-6}	5.8×10^{-7}	6.4×10^{-6}	1.3×10^{-6}
	Spline interpolation	2.9×10^{-6}	5.7×10^{-7}	5.5×10^{-6}	1.1×10^{-6}
Test function (ii) $n = 50$ $\sigma = 0$	Trapezoidal rule	1.1×10^{-5}	6.1×10^{-6}	1.8×10^{-5}	1.0×10^{-5}
	Simpson's rule	9.4×10^{-7}	4.1×10^{-7}	1.4×10^{-6}	8.9×10^{-7}
	Spline interpolation	6.0×10^{-9}	1.1×10^{-9}	2.1×10^{-8}	3.5×10^{-9}
Test function (ii) $n = 500$ $\sigma = 0$	Trapezoidal rule	1.1×10^{-7}	6.1×10^{-8}	1.8×10^{-7}	1.0×10^{-7}
	Simpson's rule	9.4×10^{-10}	4.1×10^{-10}	1.3×10^{-9}	8.9×10^{-10}
	Spline interpolation	5.1×10^{-13}	6.2×10^{-14}	1.6×10^{-12}	1.6×10^{-13}
Test function (ii) $n = 50$ $\sigma = 1.0 \times 10^{-4}$	Trapezoidal rule	2.5×10^{-5}	6.7×10^{-6}	4.8×10^{-5}	1.8×10^{-5}
	Simpson's rule	2.0×10^{-5}	8.9×10^{-6}	3.4×10^{-5}	1.8×10^{-5}
	Spline interpolation	2.1×10^{-5}	9.8×10^{-6}	3.2×10^{-5}	2.0×10^{-5}
Test function (ii) $n = 500$ $\sigma = 1.0 \times 10^{-4}$	Trapezoidal rule	3.3×10^{-6}	9.5×10^{-7}	6.7×10^{-6}	2.4×10^{-6}
	Simpson's rule	4.0×10^{-6}	1.0×10^{-6}	1.1×10^{-5}	3.0×10^{-6}
	Spline interpolation	3.4×10^{-6}	1.1×10^{-6}	6.8×10^{-6}	2.7×10^{-6}
Test function (iii) $n = 50$ $\sigma = 0$	Trapezoidal rule	1.3×10^{-3}	6.2×10^{-4}	2.1×10^{-3}	1.1×10^{-3}
	Simpson's rule	1.3×10^{-4}	4.6×10^{-5}	2.0×10^{-4}	1.1×10^{-4}
	Spline interpolation	2.0×10^{-5}	1.1×10^{-5}	3.3×10^{-5}	1.9×10^{-5}
Test function (iii) $n = 500$ $\sigma = 0$	Trapezoidal rule	1.3×10^{-5}	6.1×10^{-6}	2.1×10^{-5}	1.1×10^{-5}
	Simpson's rule	1.3×10^{-8}	1.4×10^{-8}	2.1×10^{-8}	2.1×10^{-8}
	Spline interpolation	8.2×10^{-10}	3.8×10^{-10}	1.4×10^{-9}	6.6×10^{-10}
Test function (iii) $n = 50$ $\sigma = 1.0 \times 10^{-4}$	Trapezoidal rule	1.3×10^{-3}	6.2×10^{-4}	2.1×10^{-3}	1.1×10^{-3}
	Simpson's rule	1.3×10^{-4}	4.6×10^{-5}	2.1×10^{-4}	1.1×10^{-4}
	Spline interpolation	2.2×10^{-5}	1.1×10^{-5}	3.5×10^{-5}	2.0×10^{-5}
Test function (iii) $n = 500$ $\sigma = 1.0 \times 10^{-4}$	Trapezoidal rule	1.3×10^{-5}	6.5×10^{-6}	2.3×10^{-5}	1.1×10^{-5}
	Simpson's rule	1.0×10^{-6}	3.4×10^{-7}	2.6×10^{-6}	7.3×10^{-7}
	Spline interpolation	9.1×10^{-7}	4.2×10^{-7}	2.4×10^{-6}	6.6×10^{-7}