Problem Set for Module – 06

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Problem 1: Method of Undetermined Coefficients for three-point backward differences

Use the method of undetermined coefficients to find the following numerical derivatives:

$$f'(x_i) = a_1 x_{i-2} + a_2 x_{i-1} + a_3 x_i$$
$$f''(x_i) = a_1 x_{i-2} + a_2 x_{i-1} + a_3 x_i$$

Problem 2: Optimal Δx for Numerical Derivatives

Determine the optimal step size to compute the above two numerical derivatives such that the *total error* is minimized. Assume double precision machine ($\epsilon_{tol} = 2 \times 10^{-16}$).

Problem 3: Numerical Example

Use the three point formulae derived above to compute numerical derivatives $f'(x)$ and $f''(x)$ for:

$$f(x) = xe^{-\frac{1}{x}}$$

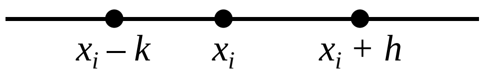
at $x = 1$. Use $h = 0.1$.

Repeat for a range of h values from 10^{-1} to 10^{-10}. Compare with the true value of the derivatives and verify the results of the previous problem.

Problem 4: Numerical Example (continued)

Repeat the previous problem using central difference and two-point forward difference (only $f'(x)$).

Problem 5: Differentiation with Unequal Intervals



In this problem, we derive the central difference formula for unequal segments. Consider three points,

$$x_{i-1} = x_i - k, \qquad x_i, \qquad x_{i+1} = x_i + h$$

which we will use to obtain $f'(x_i)$.

1. One possible approximation is

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

   Find how the truncation error varies with k and h.

2. Use the Taylor's series expansion to derive a second-order accurate numerical approximation. Specifically, the error may be proportional to $(k \pm h)^2$.

Problem 6: Numerical differentiation

The following data was generated for $f(x) = x^2 \ln(x)$. Obtain $[f'(x)]_{x=1}$ and compare with the true value (algebraically differentiate $f(x)$ and obtain the value)

x	0.9	1	1.1	1.2
$f(x)$	-0.0853	0	0.1153	0.2625

1. Use the forward difference method with the above data.
2. Use the central difference method with the above data.
3. Fit a Newton's Forward/Divided difference polynomial and differentiate it. Compare the results.

Problem 7: Numerical differentiation with error in data

Let us repeat the procedure if the data is generated in a similar manner as the previous problem, but with some noise added to it. Repeat the following for the data below.

x	0.9	1	1.1	1.2
$f(x)$	-0.054	-0.04	0.112	0.31

1. Use the central difference method as before. Compare these results to the previous problem.
2. Fit a Newton's Forward/Divided difference polynomial and differentiate it. Contrast these results with what you observed in the previous problem.

Problem 8: Simpson's 3/8$^{\text{th}}$ Rule

Complete the derivation of the Simpson's 3/8$^{\text{th}}$ rule, starting from Newton's polynomial.
Show that this approximation has the same order of error as the 1/3$^{\text{rd}}$ rule.

Problem 9: Method of Undetermined Coefficients – 1/3$^{\text{rd}}$ Rule

Derive the Simpson's 1/3$^{\text{rd}}$ rule using method of undetermined coefficients. Start by expressing

$$\int_{x_1}^{x_3} f(x)dx = c_1 x_1 + c_2 x_2 + c_3 x_3$$

and use the procedure shown in the videos for $f(x) = 1, x, x^2$.

Problem 10: Method of Undetermined Coefficients – 3/8$^{\text{th}}$ Rule

Derive the Simpson's 3/8$^{\text{th}}$ rule as $I = c_1 x_1 + c_2 x_2 + c_3 x_3 + c_4 x_4$.

Problem 11: Limits of Integration

Convert through appropriate change of variables:

$$\int_a^b f(x)dx \rightarrow \int_{-1}^{1} f(\tau)d\tau$$

Problem 12: Indefinite Integral

$$I = \int_a^{\infty} f(x)dx$$

cannot be solved using numerical integration because one of the limits is ∞ (which will require infinite or a very large number of intervals in a numerical integration scheme). The above integral can be converted into an alternate form with finite limits of integral through an appropriate transformation of variables. An example is $\tau = 1/x$.

1. Use an appropriate transformation to convert the above into a numerically tractable method.
2. How will you modify the procedure for:

$$\int_0^{\infty} f(x)dx$$

3. How will you modify the procedure for

$$\int_{-\infty}^{\infty} f(x)dx$$

Problem 13: Numerical Comparison

Find the following integral using (i) Trapezoidal rule; (ii) Simpson's 1/3rd Rule; (iii) Simpson's 3/8th Rule; (iv) Gauss Quadrature. Use six equally spaced intervals for the first three methods.

$$\int_0^6 x^2 e^x \, \mathrm{d}x$$

Compare with the true value of the integral. Comment on accuracy of the various methods.

Problem 14: Richardson's Extrapolation

Re-solve the above example using a single application of the Simpson's 1/3rd rule.
Apply Richardson's extrapolation to the solution just obtained. Compare with the true value.

Problem 15: Some Special Integrals

Two important integrals in engineering are those of the error function and sinc function. Obtain the following using the Trapezoidal rule. Reduce the interval h so that the result is accurate to $\epsilon < 10^{-4}$. (**Hint**: Start with some value of the step-size h. Half the step size each time, so that further reduction in the step size does not change the integral by more than the tolerance value).

$$I_{erf} = \frac{2}{\sqrt{\pi}} \int_0^2 e^{-x^2} \, \mathrm{d}x$$

$$I_{sinc} = \int_0^{4\pi} \frac{\sin(x)}{x} \mathrm{d}x$$

Problem 16: Double Integral using Gauss Quadrature

$$I = \int_{-1}^{1} \int_{-1}^{1} x^2 \sin(y) \, \mathrm{d}x \, \mathrm{d}y$$