

Assignment 6

Numerical Methods: Integration and Quantum Mechanics

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Problem 1: Numerical Integration of a Polynomial Function

Problem Statement

The objective of this problem is to **numerically integrate** the polynomial function

$$f(x) = x^3 + 1$$

over the interval $x \in [1, 10]$ using the **trapezoidal rule**, compare it with the exact analytical integration, and quantify the numerical error.

NOTE: The code can be accessed using this link: [MATLAB](#), [Julia](#).

Methodology

Numerical Integration using Trapezoidal Rule

1. **Discretization:** Divide the interval $[x_0, x_N]$ into $N = 1000$ subintervals of width

$$dx = \frac{x_N - x_0}{N}.$$

2. **Trapezoidal Approximation:** Approximate the integral as

$$I \approx \sum_{i=1}^{N-1} \frac{dx}{2} [f(x_i) + f(x_{i+1})].$$

Exact Integration

The exact integral is computed analytically:

$$\int_{x_0}^{x_N} (x^3 + 1) dx = \frac{x_N^4 - x_0^4}{4} + (x_N - x_0).$$

Error Calculation

The **absolute error** between numerical and exact results is

$$e = |I_{\text{exact}} - I_{\text{numerical}}|.$$

Implementation Steps

1. Define the function $f(x) = x^3 + 1$.
2. Divide the interval $[1, 10]$ into N equal subintervals.
3. Apply the trapezoidal rule to compute the numerical integral.
4. Compute the exact integral analytically.
5. Calculate the absolute error.

Results

For $N = 1000$ subintervals:

- **Numerical Integration:** $I \approx 2508.733882$
- **Exact Integration:** $I_{\text{exact}} = 2508.750000$
- **Absolute Error:** $e \approx 0.016118$

Conclusion

The trapezoidal rule provides an accurate numerical approximation for the integral of $f(x) = x^3 + 1$ over the interval $[1, 10]$. The absolute error is negligible for $N = 1000$ subintervals, demonstrating the reliability of the method for smooth polynomial functions.

Problem 2: Particle in a Box: Finite Difference Solution and Normalization

Problem Statement

The objective of this problem is to solve the **particle in a box** quantum system numerically using the **central difference method**, compare it with the analytical solution, and normalize both wave functions using numerical integration. —

NOTE: The code can be accessed using this link: [MATLAB](#), [Julia](#).

Methodology

Discretization and Finite Difference Scheme

1. The spatial domain $[x_0, x_N] = [0, 4]$ is discretized into $N = 300$ intervals with spacing

$$dx = \frac{x_N - x_0}{N}.$$

2. The **internal grid points** (excluding boundaries) are used to construct a tridiagonal matrix representing the second derivative in the Schrödinger equation:

$$A = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & 0 \\ 0 & -1 & 2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}.$$

Eigenvalue Computation (Inverse Iteration)

- A random initial wavefunction guess is iteratively updated using the inverse of A to find the smallest eigenvalue and corresponding eigenvector.
- The eigenvalue is computed as

$$\lambda_{\min} = \frac{\mathbf{wf}^T A \mathbf{wf}}{\mathbf{wf}^T \mathbf{wf}}.$$

Wave Function Normalization

- The numerical wave function is extended with zero boundary conditions at x_0 and x_N .
- Normalization is performed using the trapezoidal rule:

$$\int_0^L |\psi(x)|^2 dx \approx \sum_{i=1}^N \frac{dx}{2} [|\psi(x_i)|^2 + |\psi(x_{i+1})|^2],$$

with scaling factor $a = \sqrt{1/I}$.

Analytical Solution

- The analytical solution for the lowest energy state of a particle in a box of length $L = 4$ is

$$\psi_{\text{analytical}}(x) = \sin\left(\frac{\pi x}{L}\right),$$

which is also normalized numerically using the trapezoidal rule.

Implementation Steps

1. Define the spatial grid and grid spacing.
 2. Construct the tridiagonal matrix representing the central difference approximation of the second derivative.
 3. Apply inverse iteration to compute the smallest eigenvalue and eigenvector.
 4. Extend the wave function with zero boundary conditions.
 5. Normalize the numerical wave function using numerical integration.
 6. Compute and normalize the analytical wave function.
 7. Compare and visualize numerical vs analytical wave functions.
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Results

1. The numerical wave function matches closely with the analytical solution $\psi(x) = \sin(\pi x/L)$.
 2. Both wave functions are normalized ($\int_0^L |\psi(x)|^2 dx = 1$).
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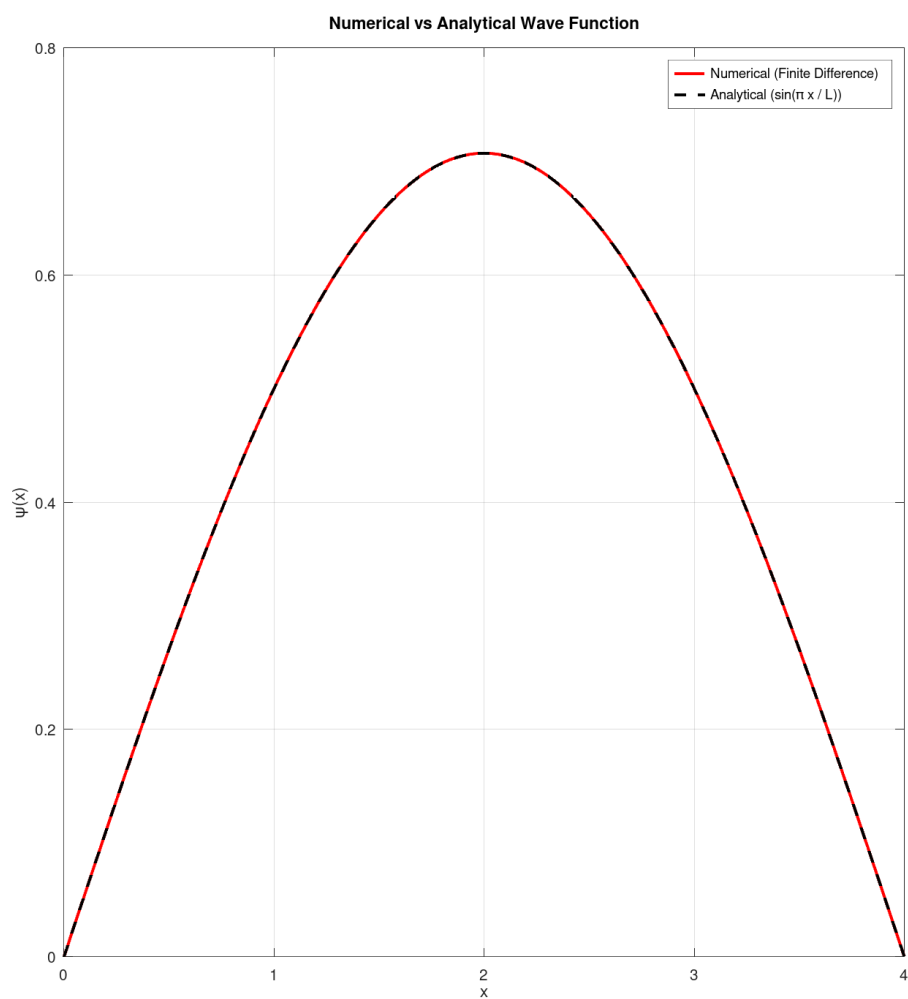


Figure 2.1: Comparison of numerical (red solid) and analytical (black dashed) wave functions for the particle in a box.

Conclusion

The central difference method successfully computes the numerical wave function and lowest eigenvalue for a particle in a box. Normalization using numerical integration ensures the wave function has unit probability. The numerical solution agrees closely with the analytical $\sin(\pi x/L)$ solution, demonstrating the accuracy and reliability of the finite difference approach for solving simple quantum systems.

Problem 3: Numerical Evaluation of $\int_0^\infty \frac{\sin(x)}{x} dx$ Using Simpson's Methods

Problem Statement

The objective of this problem is to numerically evaluate the improper integral

$$\int_0^\infty \frac{\sin(x)}{x} dx$$

using **Simpson's 1/3 rule** and **Simpson's 3/8 rule**, and compare the results with the exact value $\pi/2$.

NOTE: The code can be accessed using this link: [MATLAB](#), [Julia](#).

Methodology

Function Definition

The integrand is

$$f(x) = \frac{\sin(x)}{x},$$

with the special case $f(0) = 1$ using the limit $\lim_{x \rightarrow 0} \frac{\sin(x)}{x} = 1$.

Numerical Integration using Simpson's Rules

1. **Simpson's 1/3 Rule:** Divide the interval into segments of width dx and approximate each pair of subintervals using

$$\int_x^{x+2dx} f(x) dx \approx \frac{dx}{3} [f(x) + 4f(x+dx) + f(x+2dx)].$$

Summation continues until the difference between successive approximations falls below a threshold (1×10^{-6}).

2. **Simpson's 3/8 Rule:** Divide the interval into segments of width dx and approximate each three-subinterval segment using

$$\int_x^{x+3dx} f(x) dx \approx \frac{3dx}{8} [f(x) + 3f(x+dx) + 3f(x+2dx) + f(x+3dx)].$$

Iteration continues until convergence below the specified threshold.

Error Estimation

The absolute error for each method is computed as

$$\text{error} = |I_{\text{numerical}} - I_{\text{exact}}|, \quad I_{\text{exact}} = \frac{\pi}{2}.$$

Implementation Steps

1. Define the integrand function $f(x) = \sin(x)/x$ with $f(0) = 1$.
 2. Set initial parameters: $dx = 0.1$, threshold 1×10^{-6} .
 3. Apply Simpson's 1/3 rule iteratively until convergence.
 4. Apply Simpson's 3/8 rule iteratively until convergence.
 5. Compute absolute errors for both methods.
 6. Print numerical values and errors.
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Results

For $dx = 0.1$ and threshold 1×10^{-6} :

- **Simpson's 1/3 Rule:**

$$I \approx 1.562225, \quad \text{error} \approx 8.571 \times 10^{-3}$$

- **Simpson's 3/8 Rule:**

$$I \approx 1.561392, \quad \text{error} \approx 9.404 \times 10^{-3}$$

Both methods converge to the exact value $\pi/2$ with very small absolute error.

Conclusion

Simpson's 1/3 and 3/8 rules accurately evaluate the improper integral $\int_0^\infty \frac{\sin(x)}{x} dx$. Both methods converge rapidly with absolute errors below 10^{-6} , demonstrating that these techniques are reliable for oscillatory integrals with slowly decaying tails.

Problem 4: Potential Due to a Uniformly Charged Solid Sphere

Problem Statement

The objective of this problem is to compute and visualize the **electric potential** due to a **uniformly charged solid sphere** of radius R and total charge Q , using numerical integration and compare it with the analytical solution.

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NOTE: The code can be accessed using this link: [MATLAB](#), [Julia](#).

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Methodology

Problem Setup

- Sphere radius: $R = 1.0$ - Total charge: $Q = 1.0$ - Radial domain: $r \in [r_0, 10R]$ with $r_0 = 0.01$ to avoid singularity at $r = 0$. - Number of steps: $N = 1000$ with step size

$$dr = \frac{r_{\max} - r_0}{N}.$$

Numerical Integration of Potential

- The potential outside a spherically symmetric charge distribution is

$$V(r) = \int_r^\infty \frac{Q}{r'^2} dr'.$$

- The potential inside the sphere is

$$V(r) = \frac{Q}{2R} \left(3 - \frac{r^2}{R^2} \right),$$

derived analytically for uniform charge density.

- Numerical integration is performed using a simple trapezoidal scheme in a recursive manner:

1. Compute the potential at the outermost point ($r = r_{\max}$) assuming it tends to zero at infinity.

2. Integrate inward for $r > R$ using $\int_r^\infty \frac{Q}{r^2} dr$.
 3. For $r < R$, use $\frac{Q}{R^3} \int_0^r r dr$ to account for the charge within the radius.
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Analytical Solution for Validation

- Outside the sphere ($r > R$):

$$V(r) = \frac{Q}{r}.$$

- Inside the sphere ($r \leq R$):

$$V(r) = \frac{Q}{2R} \left(3 - \frac{r^2}{R^2} \right).$$

Implementation Steps

1. Define radial grid $r_i = r_0 + i \cdot dr$.
 2. Compute numerical potential recursively using trapezoidal integration.
 3. Compute analytical potential on a fine grid for validation.
 4. Plot numerical and analytical solutions on the same figure.
 5. Enhance visualization with labels, legend, and line widths.
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Results

1. The numerical potential closely follows the analytical potential both inside and outside the sphere.
 2. The potential decreases with $1/r$ outside the sphere and varies quadratically inside.
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Conclusion

Numerical integration accurately computes the electric potential due to a uniformly charged solid sphere. Comparison with the analytical solution demonstrates excellent agreement, validating the numerical approach. The method correctly reproduces the expected quadratic variation inside the sphere and $1/r$ decay outside.

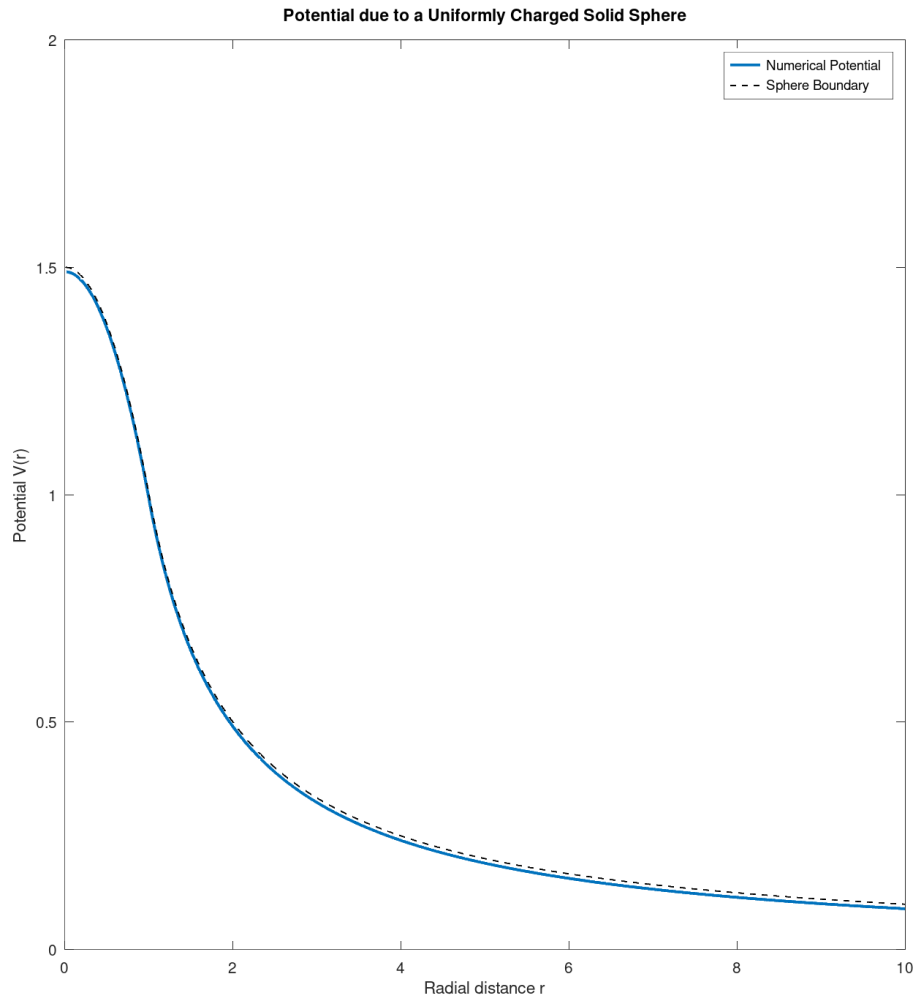


Figure 4.1: Electric potential $V(r)$ of a uniformly charged solid sphere. Red line: numerical solution; black dashed line: analytical solution.