Assignment 1

Numerical Methods Applications

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Problem 1: Solution of Linear Equations using Gaussian Elimination

Problem Statement

The objective of this problem is to solve a system of linear equations using the Gaussian elimination method. Given a coefficient matrix M and a right-hand side vector R, we apply forward elimination to reduce the system to an upper-triangular form and then use back-substitution to obtain the solution.

Methodology

Gaussian elimination transforms the augmented matrix $[M|R]$ into row-echelon form by successively eliminating variables. For each pivot element, entries below it are zeroed out. The general procedure is:

1. Form the augmented matrix $A = [M|R]$.
2. For each pivot column p:
   - Normalize/eliminate entries below the pivot by subtracting suitable multiples of the pivot row.
3. Once in upper-triangular form, perform back-substitution:

$$x_i = \frac{A_{i,n+1} - \sum_{j=i+1}^{n} A_{i,j} x_j}{A_{i,i}}.$$

Pseudo-code

1. Store M and R.
2. Construct augmented matrix $A = [M|R]$.
3. For each pivot column $p = 1 \to n-1$:
   - For each row $r > p$, eliminate $A(r,p)$ using row operations.
4. Perform back-substitution starting from the last row.
5. Output solution vector $X = [x, y, z]^T$.

Results

The given system is:

$$\begin{aligned} x + y + z &= 0, \\ x - 2y + 2z &= 4, \\ x + 2y - z &= 2. \end{aligned}$$

The augmented matrix is:

$$A = \begin{bmatrix} 1 & 1 & 1 & | & 0 \\ 1 & -2 & 2 & | & 4 \\ 1 & 2 & -1 & | & 2 \end{bmatrix}.$$

After applying forward elimination, the system reduces to an upper-triangular form. Back-substitution yields the solution:

$$x = 4.00, \quad y = -2.00, \quad z = -2.00.$$

Conclusion

Gaussian elimination was successfully applied to solve the system of equations. The method systematically reduces the system to an upper-triangular form, from which the solution can be obtained efficiently via back-substitution. The computed solution verifies the correctness of the algorithm implementation.

Problem 2: Solution of Linear Equations using Gaussian Elimination with Partial Pivoting

Problem Statement

The objective of this problem is to solve a system of linear equations using the Gaussian elimination method with partial pivoting. Partial pivoting improves numerical stability by reducing round-off errors, especially when pivot elements are small or zero.

Methodology

Gaussian elimination with partial pivoting proceeds in two phases:

1. **Pivoting:** At each step, reorder the rows such that the largest (by absolute value) candidate for the pivot element is placed on the diagonal. This avoids division by small numbers.

2. **Forward elimination:** Use the pivot row to eliminate entries below the pivot, reducing the system to an upper-triangular form.

3. **Back-substitution:** Solve for the variables starting from the last equation upwards:
$$x_i = \frac{A_{i,n+1} - \sum_{j=i+1}^{n} A_{i,j}x_j}{A_{i,i}}.$$

Pseudo-code

1. Store M and R.

2. Form augmented matrix $A = [M|R]$.

3. For each pivot index $p = 1 \to n - 1$:

   - Swap rows to place the largest pivot in row p (partial pivoting).
   - For each row $r > p$, eliminate $A(r, p)$ using the pivot row.

4. Apply back-substitution to compute the solution vector.

Results

The given system of equations is:

$$\begin{aligned} 0x + 2y + z &= -8, \\ x - 2y - 2z &= 0, \\ -x + y + 2z &= 3. \end{aligned}$$

The augmented matrix is:

$$A = \begin{bmatrix} 0 & 2 & 1 & | & -8 \\ 1 & -2 & -2 & | & 0 \\ -1 & 1 & 2 & | & 3 \end{bmatrix}.$$

After applying partial pivoting, the sorted augmented matrix becomes:

$$A = \begin{bmatrix} 1 & -2 & -2 & | & 0 \\ 0 & 2 & 1 & | & -8 \\ -1 & 1 & 2 & | & 3 \end{bmatrix}.$$

Forward elimination reduces this system to upper-triangular form, and back-substitution yields:

$$x = -10.00, \quad y = -3.00, \quad z = -2.00.$$

Conclusion

Gaussian elimination with partial pivoting was successfully implemented to solve the given system of equations. The pivoting step ensured stability by preventing division by zero (since the original first pivot was zero). The computed solution confirms that partial pivoting is an essential enhancement to the standard Gaussian elimination method when working with arbitrary systems.

Problem 3: Solution of Linear Equations using Gauss–Jordan Elimination

Problem Statement

The objective of this problem is to solve a system of linear equations using the Gauss–Jordan elimination method. Unlike Gaussian elimination, which reduces the system to an upper-triangular form followed by back-substitution, Gauss–Jordan elimination directly reduces the augmented matrix to a diagonal (row-reduced echelon) form. This makes the solution values explicit without requiring further substitution.

Methodology

The Gauss–Jordan method transforms the augmented matrix $[M|R]$ into reduced row-echelon form (RREF). The steps are:

1. Form the augmented matrix $A = [M|R]$.
2. For each pivot column $p = 1 \to n$:
   - Identify the pivot element $A(p, p)$.
   - For each row $r \neq p$, eliminate $A(r, p)$ by subtracting a multiple of the pivot row.
3. Once all off-diagonal elements are zero, divide each row by its pivot element so that the coefficient matrix becomes the identity.
4. The last column of the reduced matrix contains the solution vector.

Pseudo-code

1. Input coefficient matrix M and right-hand side vector R.
2. Construct augmented matrix $A = [M|R]$.
3. For each pivot index $p = 1 \to n$:
   - For each row $r \neq p$, set
   $$A(r, :) = A(r, :) - \frac{A(r, p)}{A(p, p)} \cdot A(p, :).$$
4. Compute solution as $x_i = A(i, n + 1)/A(i, i)$.
5. Output the solution vector.

Results

The given system of equations is:

$$\begin{aligned}
-76x + 25y + 50z &= -10, \\
25x - 56y + 1z &= 0, \\
50x + y - 106z &= 0.
\end{aligned}$$

The augmented matrix is:

$$A = \begin{bmatrix} -76 & 25 & 50 & | & -10 \\ 25 & -56 & 1 & | & 0 \\ 50 & 1 & -106 & | & 0 \end{bmatrix}.$$

Applying Gauss–Jordan elimination reduces the matrix to diagonal form, from which the solution is read directly:

$$x = 0.2449, \quad y = 0.1114, \quad z = 0.1166.$$

Conclusion

The Gauss–Jordan elimination method was applied to solve the system of three equations. Unlike standard Gaussian elimination, no back-substitution was necessary since the algorithm produced a diagonal system. The obtained values of x, y, and z represent the loop currents in the given electrical circuit (clockwise in loops 1, 2, and 3 respectively), validating the method's application to circuit analysis problems.

Problem 4: Solution of First-order Differential Equation using Gaussian Elimination

Problem Statement

The objective of this problem is to solve a first-order differential equation numerically using the Gauss elimination method. The model describes exponential decay, governed by:

$$\frac{dN}{dt} = -\lambda N, \quad N(0) = N_0,$$

where λ is the decay constant and N_0 is the initial value. The equation is discretized and solved as a linear system.

Methodology

The exponential decay equation is discretized using a finite-difference approximation:

$$N_i - N_{i-1} = -\lambda\, t_{i-1}\, \Delta t, \quad i = 2, 3, \ldots, N,$$

with the initial condition $N_1 = N_0$.

This system can be written in matrix form:

$$M \cdot \vec{N} = \vec{R},$$

where M is a lower bidiagonal matrix and $\vec{R}$ is the right-hand side vector incorporating the initial condition and decay terms.

The steps are:

1. Construct matrix M of size $N \times N$:
   - $M(1, 1) = 1$,
   - $M(i, i) = 1$, $M(i, i-1) = -1$ for $i \geq 2$.
2. Construct vector $\vec{R}$:
   - $R(1) = N_0$,
   - $R(i) = -\lambda(i-1)\Delta t^2$ for $i \geq 2$.
3. Form augmented matrix $A = [M|\vec{R}]$.
4. Apply Gaussian elimination to reduce A to upper-triangular form.
5. Use back-substitution to solve for $\vec{N}$.

Pseudo-code

1. Define parameters: Δt, $t_{\max}$, λ, N_0.
2. Construct M and $\vec{R}$ as above.
3. Form augmented matrix $A = [M|\vec{R}]$.
4. Apply Gaussian elimination:

$$A(r,:) = A(r,:) - \frac{A(r,p)}{A(p,p)}A(p,:), \quad r > p.$$

5. Solve using back-substitution:

$$N_p = \frac{A(p,n+1) - \sum_{j=p+1}^{n} A(p,j)N_j}{A(p,p)}.$$

6. Plot $N(t)$ against time.

Results

The given problem parameters are:

$$\Delta t = 0.01, \quad t_{\max} = 5, \quad \lambda = 0.3, \quad N_0 = 100.$$

The solution vector $\vec{N}$ was obtained numerically using Gaussian elimination. The figure below shows the computed decay curve:

The numerical solution matches the expected exponential decay behavior, decreasing monotonically from $N(0) = 100$.

Conclusion

The Gauss elimination method was successfully applied to solve the discretized form of a first-order decay differential equation. The computed results reproduce the exponential decay curve accurately. This demonstrates the viability of solving differential equations by converting them into linear systems and applying linear algebra techniques.

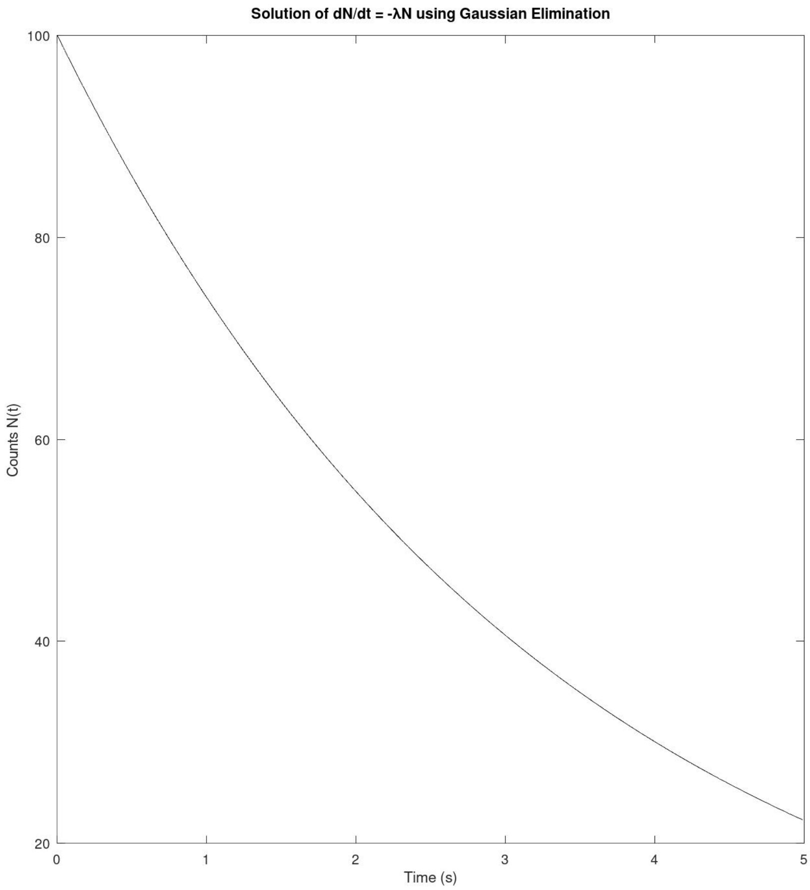

Figure 4.1: Numerical solution of $\frac{dN}{dt} = -\lambda N$ using Gaussian elimination

Problem 5: Solution of the Time-dependent Schrödinger Equation using Gauss–Jordan Elimination

Problem Statement

The objective of this problem is to solve the time-dependent Schrödinger equation numerically using the Gauss–Jordan elimination method. The wavefunction $\psi(t)$ evolves according to:

$$i\hbar\frac{d\psi}{dt} = E\psi,$$

where E is the energy of the system. For a constant energy E, the analytical solution is an exponential function:

$$\psi(t) = \psi(0)\, e^{-iEt/\hbar}.$$

The aim is to discretize this equation, solve the resulting linear system using Gauss–Jordan elimination, and study both the magnitude and phase of $\psi(t)$ over time.

Methodology

The differential equation is discretized using finite differences. With time step Δt, the recursion can be expressed as:

$$\psi_k - \delta\,\psi_{k-1} = R_k, \quad k = 2, 3, \ldots, N,$$

where

$$\delta = \frac{iE\Delta t}{\hbar} - 1.$$

This leads to a system of linear equations $M \cdot \vec{\psi} = \vec{R}$, where:

- M is a bidiagonal matrix with $M(k,k) = 1$ and $M(k,k-1) = \delta$ for $k \geq 2$,
- $\vec{R}$ is the right-hand side vector incorporating the initial condition $\psi(0) = \psi_0$.

Algorithm

1. Define parameters: Δt, $t_{\max}$, $\hbar$, E, and ψ_0.
2. Construct coefficient matrix M and vector $\vec{R}$.
3. Form augmented matrix $A = [M|\vec{R}]$.

4. Apply Gauss–Jordan elimination to reduce A to diagonal form:

$$A(r,:) = A(r,:) - \frac{A(r,p)}{A(p,p)} \cdot A(p,:), \quad r \neq p.$$

5. Extract solution $\psi_k = A(k, end)/A(k,k)$ for all k.

6. Plot $|\psi(t)|$ (magnitude) and $\arg(\psi(t))$ (phase) versus time.

Results

The chosen parameters are:

$$\Delta t = 0.01, \quad t_{\max} = 5.0, \quad \hbar = 6.626 \times 10^{-34}, \quad E = -10\hbar, \quad \psi_0 = 0.5 + 0.5i.$$

The numerical solution $\psi(t)$ was computed at discrete time steps. Figure 5.1 shows the evolution of the wavefunction.

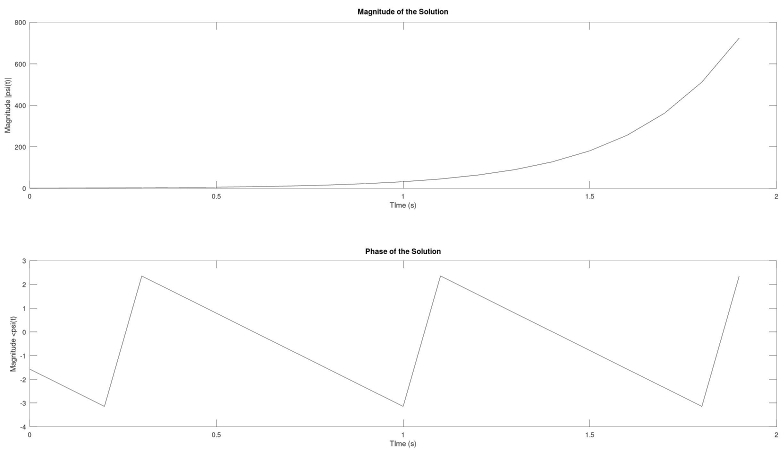

Figure 5.1: Time evolution of the wavefunction $\psi(t)$: (top) magnitude $|\psi(t)|$, (bottom) phase $\arg(\psi(t))$.

The observed behavior is:

- The magnitude $|\psi(t)|$ does not remain perfectly constant, but instead drifts over time.
- The phase $\arg(\psi(t))$ roughly follows a linear increase, though small deviations accumulate.

These deviations are not physical but arise from **numerical round-off errors** introduced by the Gauss–Jordan elimination method and the discretization scheme. Since the matrix system is ill-conditioned, the method does not preserve the unitarity of Schrodinger evolution.

Conclusion

The Gauss–Jordan elimination method was applied to the time-dependent Schrödinger equation for a constant-energy system. While the analytical solution predicts constant magnitude and a linearly increasing phase, the numerical results show noticeable deviations.

This discrepancy highlights a limitation of the chosen numerical scheme: round-off errors accumulate, and the method does not enforce unitarity. Therefore, although Gauss–Jordan elimination demonstrates how linear algebra techniques can be applied.