Linear Matrix Equations – Part 2

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Overview

Numerical Solution

of

Linear Matrix Equations

Mathematical Viewpoint

Mathematical Viewpoint

Solutions to linear equations is given by theoretical results from linear algebra, namely:

- A unique solution $\{X\} = [A^{-1}] \cdot \{B\}$ exists when $[A^{-1}]$ exists (i.e., $\det [A] \neq 0$).
- The equations are inconsistent when $[A]$ is singular and $\text{rank}\,[A|B] \neq \text{rank}\,[A]$.
- If $\text{rank}\,[A|B]$ equals $\text{rank}\,[A]$, then there are an infinite number of solutions.

We can use these results to guide the design of numerical algorithms for computing solutions to linear equations.

Engineering Viewpoint

Direct Methods:

- Transform the original equations into equivalent equations that can be solved more easily.
- Exact answer results if there are no round-off errors. Finite work. Use on dense matrices containing few zeros.
- Gausss Elimination, LU Decomposition.

Iterative Methods:

- Start with a guess of the the solution and repeatedly refine the solution until convergence criteria are achieved.
- Needs infinite work to get an exact answer. No round-off errors. Use on sparse, large order systems.
- Gauss-Seidel Iteration, Jacobi's Iteration Method.

Engineering Viewpoint

Evaluation Criteria:

- Robustness (i.e., Do the solvers work? When will they work?)
- Accuracy and Efficiency (i.e., How does computatioal effort vary as a function of problem size?).
- Ease of Implementation (i.e., implementation speed and cost).

Common Problems:

- Is A singular (or not)?
- Matrix A might be nearly singular. This is important for finite-precision arithmetic.

The pathway from mathematical analysis to a software implementation requires consideration of ill-conditioned equations and finite precision arithmetic.

Ill-Conditioned Equations

Definition. A system of equations is said to be ill-conditioned if small changes to one or more coefficients of $[A]\,[X] = [B]$ causes large deviations in the solution.

Example: The following pairs of almost parallel equations:

$$\begin{bmatrix} 1.00 & 2.00 \\ 0.48 & 0.99 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3.00 \\ 1.47 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \qquad (1)$$

Let's increment coefficient a_{21} by 2%:

$$\begin{bmatrix} 1.00 & 2.00 \\ 0.49 & 0.99 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3.00 \\ 1.47 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \end{bmatrix}. \qquad (2)$$

Finite-Precision Arithmetic

Example 1. Compute a numerical solution to:

$$\begin{bmatrix} 1.0 \times 10^{-3} & 1.0 \\ 1.0 & 1.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 2.0 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \approx \begin{bmatrix} 1.0 \\ 1.0 \end{bmatrix}. \quad (3)$$

with a computer having 2 digits of precision (mantissa + floating point + rounded).

Method 1: Transform the matrix equations into echelon form.

Step 1: Compute row multiplier m_{21}:

$$m_{21} = \left[\frac{a_{21}}{a_{11}}\right] = \frac{1}{1.0 \times 10^{-3}} = 1.0 \times 10^{3}. \quad (4)$$

Finite-Precision Arithmetic

Step 2: Compute row operation: $r_2 \rightarrow r_2 - m_{21} r_1$.

$$
\begin{aligned}
(1 - 1000 \times 1.0) x_2 &= (2.0 - 1.0 \times 1000) \\
-999 x_2 &= -998 \\
-1.0 \times 10^3 x_2 &= -1.0 \times 10^3 \\
x_2 &= 1.0 \\
x_1 &= 0.0
\end{aligned}
$$

This is completely the wrong answer! The source of the problem is the large multiplier m_{12}.

Finite-Precision Arithmetic

Method 2: Idea: Swap rows 1 and 2. Then transform the matrix equations into echelon form.

Step 1: Compute row multiplier m_{21}:

$$m_{21} = \left[\frac{a_{21}}{a_{11}} \right] = \frac{1.0 \times 10^{-3}}{1.0} = 10^{-3}. \tag{5}$$

Step 2: Compute row operation: $r_2 \rightarrow r_2 - m_{21} r_1$.

$$\begin{aligned} (1 - 0.001 \times 1.0)x_2 &= (1.0 - 0.0001 \times 2.0) \\ 0.999x_2 &= 0.998 \\ 1.0x_2 &= 1.0 \\ x_2 &= 1.0 \end{aligned}$$

Finite-Precision Arithmetic

Step 3: Backsubstitution:

$$x_1 = 1.0 \tag{6}$$

To two decimal places of accuracy $[x_1, x_2] = [1.0, 1.0]$ is correct.

The absolutely correct answer is $[x_1, x_2] = [1.001, 0.999]$.

Recommended Strategy

- Rearrange rows so that the largest coefficient in absolute value in the column is in the pivotal position.
- This process is called partial pivoting.
- Can also row equilibrate – scale individual rows so maximum element value is 1.

Gauss Elimination

(No Pivoting)

Gauss Elimination (No Pivoting)

Elementary Row Operations

- Interchange any two rows.
- Multiply any row by a non-zero number.
- Add to one equation a non-zero multiple of another equation.

Step-by-Step Procedure

- Write $[A]\,[x] = [B]$ in augmented matrix form.
- Apply a sequence of row operations to transform the augmented matrix into echelon form.
- Use back substitution to compute the solution vector.
- Validate answer.

Gauss Elimination (No Pivoting)

Example 1. Consider the family of matrix equations:

$$\begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -4 \end{bmatrix} \tag{7}$$

Step 1. Augmented Matrix Form

$$\left[\begin{array}{ccc|c} 3 & -6 & 7 & 3 \\ 9 & 0 & -5 & 3 \\ 5 & -8 & 6 & -4 \end{array}\right] \tag{8}$$

Gauss Elimination (No Pivoting)

Step 2. Apply Row Operations

Step 2.1: Divide Row 1 by 3 ($r_1 \to r_1/3$)

$$\left[\begin{array}{ccc|c} 3 & -6 & 7 & 3 \\ 9 & 0 & -5 & 3 \\ 5 & -8 & 6 & -4 \end{array}\right] \to \left[\begin{array}{ccc|c} 1 & -2 & 7/3 & 1 \\ 9 & 0 & -5 & 3 \\ 5 & -8 & 6 & -4 \end{array}\right] \tag{9}$$

Step 2.2: Subtract 9 times row 1 from row 2 ($r_2 \to r_2 - 9r_1$) Step 2.3: Subtract 5 times row 1 from row 3 ($r_3 \to r_3 - 5r_1$)

$$\left[\begin{array}{ccc|c} 1 & -2 & 7/3 & 1 \\ 9 & 0 & -5 & 3 \\ 5 & -8 & 6 & -4 \end{array}\right] \to \left[\begin{array}{ccc|c} 1 & -2 & 7/3 & 1 \\ 0 & 18 & -26 & -6 \\ 0 & 2 & -5.667 & -9 \end{array}\right] \tag{10}$$

Gauss Elimination (No Pivoting)

Step 2.4: Divide row 2 by 18 ($r_2 \to r_2/18$)

Step 2.5: Subtract 2 times row 2 from row 3 ($r_3 \to r_3 - 2r_2$)

Step 2.6: Divide row 3 by 2.777 ($r_3 \to r_3/2.777$)

$$\left[\begin{array}{ccr|r} 1 & -2 & 7/3 & 1 \\ 0 & 18 & -26 & -6 \\ 0 & 2 & -5.667 & -9 \end{array}\right] \to \left[\begin{array}{ccr|r} 1 & -2 & 7/3 & 1 \\ 0 & 1 & -26/18 & -1/3 \\ 0 & 0 & 1 & 3 \end{array}\right] \quad (11)$$

Equation 11 is now in echelon form.

Gauss Elimination (No Pivoting)

Step 3. Compute Solution via Back Substitution

Step 3.1: Row 3: $x_3 = 3.0 \rightarrow x_3 = 3.0$.

Step 3.2: Row 2: $x_2 - 26/18x_3 = -1/3 \rightarrow x_2 = 4.0$.

Step 3.3: Row 1: $x_1 - 2x_2 + 7/3x_3 = 1.0 \rightarrow x_1 = 2.0$.

Step 4. Validate the Answer, $X = [2, 4, 3]$.

$$\begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ 4 \\ 3 \end{bmatrix} \rightarrow \begin{bmatrix} 3 \\ 3 \\ -4 \end{bmatrix}. \tag{12}$$

Gauss Elimination (No Pivoting)

Python Source Code: Step-by-Step Row Reduction

```
import math
import numpy as np
import LinearMatrixEquations as lme

def main():
    print("--- Step 1: Create (3x3) matrix A, (3x1) matrix B ... ");

    A = np.array([ [ 3, -6,  7],
                   [ 9,  0, -5],
                   [ 5, -8,  6] ]);
    B = np.array([ [ 3],
                   [ 3],
                   [-4] ]);

    lme.printmatrix("A", A);
    lme.printmatrix("B", B);

    print("--- Step 2: Create (3x4) augmented matrix [ A | B ] (join on vertical axis) .

    AB = np.concatenate((A, B), axis=1)
    lme.printmatrix("Augmented Matrix [A|B] ...", AB );

    print("--- Step 3.1: Scale row 1 by 1/3 ... ");

    gauss01 = lme.rowscale(AB, 0, 1.0/3.0)
    lme.printmatrix("Matrix gauss01 ...", gauss01 );
```

Gauss Elimination (No Pivoting)

Python Source Code: Step-by-Step Row Reduction

```
print("--- Step 3.2: Subtract 9 times row 1 from row 2 ... ");

gauss02 = lme.rowadd( gauss01, 0, 1, -9.0)
lme.printmatrix("Matrix gauss02 ...", gauss02 );

print("--- Step 3.3: Subtract 5 times row 1 from row 3 ... ");

gauss03 = lme.rowadd( gauss02, 0, 2, -5.0)
lme.printmatrix("Matrix gauss03 ...", gauss03 );

print("--- Step 3.4: Scale row 2 by 1/18 ... ");

gauss04 = lme.rowscale(gauss03, 1, 1.0/18.0)
lme.printmatrix("Matrix gauss04 ...", gauss04 );

print("--- Step 3.5: Subtract 2 times row 2 from row 3 ... ");

gauss05 = lme.rowadd( gauss04, 1, 2, -2.0)
lme.printmatrix("Matrix gauss05 ...", gauss05 );

print("--- Step 3.6: Scale row 3 by -1/2.77777778 ... ");

echelon01 = lme.rowscale(gauss05, 2, -1.0/2.77777778 )

print("--- Step 4.0: Print matrix [A|B] in Echelon Form ... ");

lme.printmatrix("Matrix [A|B] in Echelon Form ...", echelon01 );
```

Gauss Elimination (No Pivoting)

Abbreviated Output: See TestLinearMatrixEquations01.py

```
--- Step 1: Create (3x3) matrix A, (3x1) matrix B ...

Matrix: A
   3.0000000e+00   -6.0000000e+00    7.0000000e+00
   9.0000000e+00    0.0000000e+00   -5.0000000e+00
   5.0000000e+00   -8.0000000e+00    6.0000000e+00

Matrix: B
   3.0000000e+00
   3.0000000e+00
  -4.0000000e+00

--- Step 2: Create (3x4) augmented matrix [ A | B ] (join on vertical axis) ...

Matrix: Augmented Matrix [A|B] ...
   3.0000000e+00   -6.0000000e+00    7.0000000e+00    3.0000000e+00
   9.0000000e+00    0.0000000e+00   -5.0000000e+00    3.0000000e+00
   5.0000000e+00   -8.0000000e+00    6.0000000e+00   -4.0000000e+00
```

Gauss Elimination (No Pivoting)

Abbreviated Output: Continued ...

```
--- Step 3.1: Scale row 1 by 1/3 ...

Matrix: Matrix gauss01 ...
   1.0000000e+00  -2.0000000e+00   2.3333333e+00   1.0000000e+00
   9.0000000e+00   0.0000000e+00  -5.0000000e+00   3.0000000e+00
   5.0000000e+00  -8.0000000e+00   6.0000000e+00  -4.0000000e+00

--- Step 3.2: Subtract 9 times row 1 from row 2 ...
--- Step 3.3: Subtract 5 times row 1 from row 3 ...
--- Step 3.4: Scale row 2 by 1/18 ...
--- Step 3.5: Subtract 2 times row 2 from row 3 ...
--- Step 3.6: Scale row 3 by -1/2.77777778 ...
--- Step 4.0: Print matrix [A|B] in Echelon Form ...

Matrix: Matrix [A|B] in Echelon Form ...
   1.0000000e+00  -2.0000000e+00   2.3333333e+00   1.0000000e+00
   0.0000000e+00   1.0000000e+00  -1.4444444e+00  -3.3333333e-01
  -0.0000000e+00  -0.0000000e+00   1.0000000e+00   3.0000000e+00
```

Gauss Elimination

(with Partial Pivoting)

Gauss Elimination (with Partial Pivoting)

Step-by-Step Procedure:

- Find largest element in absolute value in 1st column. Interchange rows so that it is the pivotal equation.
- Compute multipliers: $m_{i1} = [a_{i1}/a_{11}]$ for i = 2, 3, $\cdots$ n.
- Compute new coefficients in rows 2, 3, $\cdots$ n.

  For example, $a_{22}^{'} = a_{22} - m_{21}a_{12}$, $a_{23}^{'} = a_{23} - m_{21}a_{13}$, $a_{32}^{'} = a_{32} - m_{31}a_{12}$, etc.

  The partially transform matrix is:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}^{'} & a_{23}^{'} \\ 0 & a_{32}^{'} & a_{33}^{'} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2^{'} \\ b_3^{'} \end{bmatrix}. \qquad (13)$$

Gauss Elimination (with Partial Pivoting)

Step-by-Step Procedure:

- Repeat process for 2nd column.
- After (n-1) column calculations the A matrix will be in upper-triangular (echelon) form.
- Solve for unknowns through backsubstitution.

Key Points:

- If the pivotal coeffient is small, then the row multiplier will be very large, and errors magnified due to finite arithmetic.
- Row reduction and back substitution require $O(n^3/3)$ and $O(n^2)$ operations, respectively.

Gauss Elimination (with Partial Pivoting)

Example 2. Consider the following set of equations:

$$\begin{aligned} 2x_1 + 6x_2 - x_3 &= -12 \\ 5x_1 - x_2 + 2x_3 &= 29 \\ -3x_1 - 4x_2 + x_3 &= 5 \end{aligned}$$

Steps 1 and 2: Augmented matrix form, then row equilibration.

$$\left[\begin{array}{rrr|r} 2 & 6 & -1 & -12 \\ 5 & -1 & 2 & 29 \\ -3 & -4 & 1 & 5 \end{array}\right] \rightarrow \left[\begin{array}{rrr|r} 2/6 & 1 & -1/6 & -2.0 \\ 1 & -1/5 & 2/5 & 29/5 \\ -3/4 & -1 & 1/4 & 5/4 \end{array}\right]. \tag{14}$$

Gauss Elimination (with Partial Pivoting)

Step 3: Partial pivoting (swap rows 1 and 2):

$$\left[\begin{array}{rrr|r} 1 & -1/5 & 2/5 & 29/5 \\ 2/6 & 1 & -1/6 & -2.0 \\ -3/4 & -1 & 1/4 & 5/4 \end{array}\right] \tag{15}$$

Step 4: Compute row multipliers:

$$m_{21} = [a_{21}/a_{11}] = 2/6, \quad m_{31} = [a_{31}/a_{11}] = -3/4. \tag{16}$$

Step 5: Compute new coefficients for rows 2 and 3:

$$\left[\begin{array}{lrr|r} 1 & -1/5 & 2/5 & 29/5 \\ 0 & 32/30 & -9/30 & -118/30 \\ 0 & -23/20 & 11/20 & 118/20 \end{array}\right] \tag{17}$$

Gauss Elimination (with Partial Pivoting)

Step 6: Compute multiplier for row 3, columm 2.

$$m_{32} = [a_{32}/a_{22}] = -64/69. \tag{18}$$

Step 7: Eliminate elements below diagonal in column 2.

$$\left[\begin{array}{ccc|c} 1 & -1/5 & 2/5 & 29/5 \\ 0 & 32/30 & -9/30 & -118/30 \\ 0 & 0 & 145/690 & 870/690 \end{array}\right] \tag{19}$$

Step 8: Solve for x_1 through x_3 via back substitution.

$$x_3 = [870/690] \,/\, [145/690] = 6.0, \;\; x_2 = -2.0, \;\; x_1 = 3.0. \tag{20}$$

Step 9: Check solution by substitution.

Gauss Elimination (with Partial Pivoting)

Python Source Code: Row Reduction + Back Substitution

```
# ===============================================================================
# TestLinearMatrixEquations02.py: Gauss Elimination with row reduction, partial
# pivoting, and back substitution.
# ===============================================================================

import math
import numpy as np
import LinearMatrixEquations as lme

def main():
    n = 3  # <--- size of the matrix equations ...

    print("--- Problem 1: Create (3x3) matrix A, (3x1) matrix B ... ");

    A = np.array([ [ 3, -6,  7],
                   [ 9,  0, -5],
                   [ 5, -8,  6] ]);

    B = np.array([ [ 3], [ 3], [-4] ]);

    lme.printmatrix("A", A);
    lme.printmatrix("B", B);

    print("--- Step 2: Compute augmented matrix equations ... ");

    AB = np.concatenate((A, B), axis=1)
    lme.printmatrix("Augmented Matrix [A|B] ...", AB );
```

Gauss Elimination (with Partial Pivoting)

Python Source Code: Continued ...

```python

    print("--- Step 3: Compute row reduction operations to echelon form ... ");

    echelon01 = lme.rowreduction( AB );
    lme.printmatrix("Matrix echelon01 ...", echelon01 );

    print("--- Step 4: Split echelon01 back to (nxn) piece and (nx1) pieces ... ");

    B_reduced = echelon01[:,n:n+1]
    A_reduced = echelon01[:,0:n]

    lme.printmatrix("Matrix A (reduced) ...", A_reduced );
    lme.printmatrix("Matrix B (reduced) ...", B_reduced );

    print("--- Step 5: Compute back substitution ... ");

    soln01 = lme.backsubstitution( A_reduced, B_reduced)
    lme.printmatrix("Matrix X (solution) ...", soln01 );

    print("--- Problem 2: Create (3x3) matrix A, (3x1) matrix B ... ");

    A = np.array([ [  2,  6, -1],
                   [  5, -1,  2],
                   [ -3, -4,  1] ]);

    B = np.array([ [-12], [ 29], [  5] ]);

    lme.printmatrix("A", A);
    lme.printmatrix("B", B);
```

Gauss Elimination (with Partial Pivoting)

Python Source Code: Continued ...

```
    print("--- Step 2: Compute augmented matrix equations ... ");

    AB = np.concatenate((A, B), axis=1)
    lme.printmatrix("Augmented Matrix [A|B] ...", AB );

    print("--- Step 3: Compute row reduction operations to echelon form ... ");

    echelon01 = lme.rowreduction( AB );
    lme.printmatrix("Matrix echelon01 ...", echelon01 );

    print("--- Step 4: Split echelon01 back to (nxn) piece and (nx1) pieces ... ");

    B_reduced = echelon01[:,n:n+1]
    A_reduced = echelon01[:,0:n]

    lme.printmatrix("Matrix A (reduced) ...", A_reduced );
    lme.printmatrix("Matrix B (reduced) ...", B_reduced );

    print("--- Step 5: Compute back substitution ... ");

    soln01 = lme.backsubstitution( A_reduced, B_reduced)
    lme.printmatrix("Matrix X (solution) ...", soln01 );

# call the main method ...

main()
```

Gauss Elimination (with Partial Pivoting)

Abbreviated Output: Problem 1 ...

```
Matrix: A                                                    Matrix: B
   3.0000000e+00   -6.0000000e+00    7.0000000e+00             3.0000000e+00
   9.0000000e+00    0.0000000e+00   -5.0000000e+00             3.0000000e+00
   5.0000000e+00   -8.0000000e+00    6.0000000e+00            -4.0000000e+00

--- Step 2: Compute augmented matrix equations ...

Matrix: Augmented Matrix [A|B] ...
   3.0000000e+00   -6.0000000e+00    7.0000000e+00    3.0000000e+00
   9.0000000e+00    0.0000000e+00   -5.0000000e+00    3.0000000e+00
   5.0000000e+00   -8.0000000e+00    6.0000000e+00   -4.0000000e+00

--- Step 3: Compute row reduction operations to echelon form ...

Matrix: Matrix echelon01 ...
   1.0000000e+00   -2.0000000e+00    2.3333333e+00    1.0000000e+00
   0.0000000e+00    1.0000000e+00   -1.4444444e+00   -3.3333333e-01
  -0.0000000e+00   -0.0000000e+00    1.0000000e+00    3.0000000e+00
```

Gauss Elimination (with Partial Pivoting)

Abbreviated Output: Problem 1 continued ...

```
--- Step 4: Split echelon01 back to (nxn) piece and (nx1) pieces ...

Matrix: Matrix A (reduced) ...

   1.0000000e+00   -2.0000000e+00    2.3333333e+00
   0.0000000e+00    1.0000000e+00   -1.4444444e+00
  -0.0000000e+00   -0.0000000e+00    1.0000000e+00

Matrix: Matrix B (reduced) ...
   1.0000000e+00
  -3.3333333e-01
   3.0000000e+00

--- Step 5: Compute back substitution ...

Matrix: Matrix X (solution) ...
   2.0000000e+00
   4.0000000e+00
   3.0000000e+00
```

Gauss Elimination (with Partial Pivoting)

Abbreviated Output: Problem 2 ...

```
Matrix: A                                                    Matrix: B
   2.0000000e+00    6.0000000e+00   -1.0000000e+00           -1.2000000e+01
   5.0000000e+00   -1.0000000e+00    2.0000000e+00            2.9000000e+01
  -3.0000000e+00   -4.0000000e+00    1.0000000e+00            5.0000000e+00

--- Step 2: Compute augmented matrix equations ...

Matrix: Augmented Matrix [A|B] ...
   2.0000000e+00    6.0000000e+00   -1.0000000e+00   -1.2000000e+01
   5.0000000e+00   -1.0000000e+00    2.0000000e+00    2.9000000e+01
  -3.0000000e+00   -4.0000000e+00    1.0000000e+00    5.0000000e+00

--- Step 3: Compute row reduction operations to echelon form ...

Matrix: Matrix echelon01 ...
   1.0000000e+00    3.0000000e+00   -5.0000000e-01   -6.0000000e+00
  -0.0000000e+00    1.0000000e+00   -2.8125000e-01   -3.6875000e+00
   0.0000000e+00    0.0000000e+00    1.0000000e+00    6.0000000e+00
```

Gauss Elimination (with Partial Pivoting)

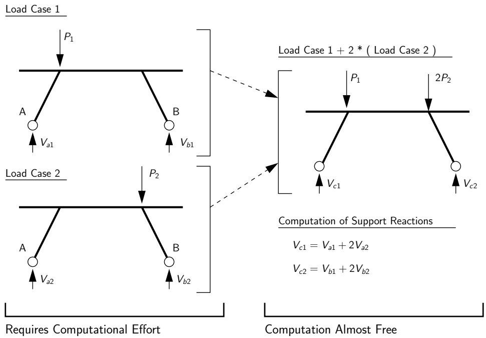
Abbreviated Output: Problem 2 continued ...

```
--- Step 4: Split echelon01 back to (nxn) piece and (nx1) pieces ...

Matrix: Matrix A (reduced) ...
   1.0000000e+00    3.0000000e+00   -5.0000000e-01
  -0.0000000e+00    1.0000000e+00   -2.8125000e-01
   0.0000000e+00    0.0000000e+00    1.0000000e+00

Matrix: Matrix B (reduced) ...
  -6.0000000e+00
  -3.6875000e+00
   6.0000000e+00

--- Step 5: Compute back substitution ...

Matrix: Matrix X (solution) ...
   3.0000000e+00
  -2.0000000e+00
   6.0000000e+00
```

LU Decomposition

LU Decomposition

Motivation. Suppose AX = B needs to be solved for a multiplicity of B vectors (e.g., A $X_1 = B_1$, A $X_2 = B_2$, etc).



Solving AX = B requires $O(n^3)$ computational work. Can we do better? ...

LU Decomposition

Objective. We want to solve $[A]\,[X] = [B]$, where A, X, and B are $(n \times n)$, $(n \times 1)$ and $(n \times n)$ matrices, respectively.

Idea. Factor $[A]$ into the product:

$$[A] = [L]\,[U] \to [L]\,[U]\,[X] = [B]\,. \tag{21}$$

and then solve in two steps.

Step 1: Foward Substitution to get $Z = [z_1, z_2, \cdots, z_n]$.

$$\begin{bmatrix} L_{11} & 0 & \cdots & 0 \\ L_{21} & L_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ L_{n1} & L_{n2} & \cdots & L_{nn} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}. \tag{22}$$

LU Decomposition

Step 2: Back Substitution to get $X = [x_1, x_2, \cdots, x_n]$.

$$\begin{bmatrix} U_{11} & U_{12} & \cdots & U_{1n} \\ 0 & U_{22} & \cdots & U_{2n} \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & U_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}. \qquad (23)$$

Observation: There are n^2 elements in matrix A, and $n(n+1)$ unknowns in equations 22 and 23.

We need to impose n additional constraints to make the method work.

LU Decomposition

Row Reduction Strategies:

- Assume upper diagonal elements are unity, i.e., $U_{ii} = 1$ (Crout Reduction).
- Assume $L_{ii} = I$ (Doolittle's Method).
- Assume $U_{ii} = L_{ii}$ (Cholesky Decomposition).

Step-by-Step Solution Procedure:

- Compute A = LU (this requires $O(n^3)$ work).
- Solve LU $X_1 = B_1$ (only requires $O(n^2)$ work).
- Solve LU $X_2 = B_2$ (only requires $O(n^2)$ work).
- Solve LU $X_3 = B_3$ (only requires $O(n^2)$ work), etc ...

LU Decomposition

General Equations. For a $(n \times n)$ set of equations $[L]\,[U] = [A]$,

$$a_{ij} = \sum_{k=min(i,j)}^{n} \left(L_{ik} U_{kj} \right). \tag{24}$$

Three cases:

$$i \le j \quad U_{ij} = \left[A_{ij} - \sum_{k=1}^{i-1} L_{ik} U_{kj} \right] / U_{ii}$$

$$i = j \quad U_{jj} = \left[A_{ij} - \sum_{k=1}^{j-1} L_{ik} U_{kj} \right] / L_{jj}$$

$$i \ge j \quad L_{ij} = \left[A_{ij} - \sum_{k=1}^{j-1} L_{ik} U_{kj} \right] / U_{jj}$$

LU Decomposition

Example 1. Consider the matrix equations:

$$\begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -4 \end{bmatrix}. \tag{25}$$

Assume $[L][U] = [A]$ with values of unity along the upper diagonal (Crout Reduction).

$$\begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} 1 & U_{12} & U_{13} \\ 0 & 1 & U_{23} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix}. \tag{26}$$

LU Decomposition

Equating terms (1st row of L):

$$
\begin{aligned}
L_{11} \cdot 1 = 3 \quad &\rightarrow \quad L_{11} = 3. \\
L_{11} \cdot U_{12} = -6 \quad &\rightarrow \quad U_{12} = -2. \\
L_{11} \cdot U_{13} = -7 \quad &\rightarrow \quad U_{13} = 7/3.
\end{aligned}
$$

Equating terms (2nd row of L):

$$
\begin{aligned}
L_{21} \cdot U_{11} = 9 \quad &\rightarrow \quad L_{21} = 9. \\
L_{21} \cdot U_{12} + L_{22} \cdot 1 = 0 \quad &\rightarrow \quad L_{22} = 18. \\
L_{21} \cdot U_{13} + L_{22} \cdot U_{23} = 0 \quad &\rightarrow \quad U_{23} = -13/9.
\end{aligned}
$$

LU Decomposition

Equating terms (3rd row of L):

$$\begin{aligned} L_{31} \cdot U_{11} = 5 \quad &\rightarrow \quad L_{31} = 5. \\ L_{31} \cdot U_{12} + L_{32} = -8 \quad &\rightarrow \quad L_{32} = 2. \\ L_{31} \cdot U_{13} + L_{32} \cdot U_{23} + L_{33} = 6 \quad &\rightarrow \quad L_{33} = -25/9. \end{aligned}$$

Hence:

$$\begin{bmatrix} 3 & 0 & 0 \\ 9 & 18 & 0 \\ 5 & 2 & -25/9 \end{bmatrix} \begin{bmatrix} 1 & -2 & 7/3 \\ 0 & 1 & -13/9 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix}. \tag{27}$$

LU Decomposition

Forward Substitution:

$$\begin{bmatrix} 3 & 0 & 0 \\ 9 & 18 & 0 \\ 5 & 2 & -25/9 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -4 \end{bmatrix} \to \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1.0 \\ -1/3 \\ 3.0 \end{bmatrix}. \tag{28}$$

Backward Substitution:

$$\begin{bmatrix} 1 & -2 & 7/3 \\ 0 & 1 & -13/9 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -1/3 \\ 3.0 \end{bmatrix} \to \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.0 \\ 4.0 \\ 3.0 \end{bmatrix}. \tag{29}$$

LU Decomposition

Example 2. Consider $[L]\,[U] = [A]$ with values of unity along the lower diagonal (Doolittle's Method).

$$\begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix} = \begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix}. \quad (30)$$

Can show:

$$\begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 5/3 & 1/9 & 1 \end{bmatrix} \begin{bmatrix} 3 & -6 & 7 \\ 0 & 18 & -26 \\ 0 & 0 & -25/9 \end{bmatrix} = \begin{bmatrix} 3 & -6 & 7 \\ 9 & 0 & -5 \\ 5 & -8 & 6 \end{bmatrix}. \quad (31)$$

Working Examples

Example 3: LU Decomposition with Symbolic Python

Problem Statement: Let's try to use SymPy to compute algebraic representations for LU decomposition for matrices

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = LU, \tag{32}$$

and

$$A = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = LU. \tag{33}$$

Then, we will check the results by assigning numerical values to the symbols to match equation 25. Note: det(A) = det(L).det(U) = -150.

Example 3: LU Decomposition with Symbolic Python

Python Source Code: Compute $A = LU$.

```
# ===============================================================
# TestMatrixLUDecomposition01.py: Compute symbolic descriptions
# of matrix LU decomposition ....
# ===============================================================

import sympy as sp
from sympy import Integral, Matrix, pi, pprint

def main():
    # Define symbolic representation of matrix ...

    print("--- Part 1: Compute LU decomposition of 2x2 matrix equations ...");

    a, b, c, d, e, f = sp.symbols('a,b,c,d,e,f')

    A = sp.Matrix(([a,b],[c,d]))
    B = sp.Matrix([e,f])

    pprint(A)

    L, U, P = A.LUdecomposition()

    print("--- Lower triangular matrix ...\n");

    pprint(L)

    print("--- Upper triangular matrix ...\n");
```

Example 3: LU Decomposition with Symbolic Python

Python Source Code: Continued ...

```

    pprint(U)

    print("--- Check matrix product L*U ...\n");

    pprint(L*U)

    print("--- Part 2: Symbolic LU decomposition of 3x3 matrix equations ...");

    g, h, i = sp.symbols('g,h,i')
    j, k, l = sp.symbols('j,k,l')

    A = sp.Matrix(([a,b,c],[d,e,f], [g,h,i] ))
    B = sp.Matrix([j,k,l])

    pprint(A)

    L, U, P = A.LUdecomposition()

    print("--- Lower triangular matrix ...\n");

    pprint(L)

    print("--- Upper triangular matrix ...\n");

    pprint(U)
```

Example 3: LU Decomposition with Symbolic Python

Python Source Code: Continued ...

```
    print("--- Check matrix product L*U ...\n");

    pprint(L*U)

    print("--- Part 3: LU decomposition for sample 3x3 matrix equations ...");

    print("--- Set values in L ...");
    print("---   L = L.subs( {a:3, b:-6, c:7, d:9, e:0, f:-5, g:5, h:-8, i:6 } ) \n")

    L = L.subs( {a:3, b:-6, c:7, d:9, e:0, f:-5, g:5, h:-8, i:6 } )

    pprint(L)

    print("--- L.det() = {:s} ...".format( str( sp.det(L) ) ))

    print("--- Set values in U ...");
    print("---   U = U.subs( {a:3, b:-6, c:7, d:9, e:0, f:-5, g:5, h:-8, i:6 } ) \n")

    U = U.subs( {a:3, b:-6, c:7, d:9, e:0, f:-5, g:5, h:-8, i:6 } )

    pprint(U)

    print("--- U.det() = {:s} ...".format( str( sp.det(U) ) ))

# call the main method ...

main()
```

Example 3: LU Decomposition with Symbolic Python

Abbreviated Output: Part 1: decomposition of 2x2 matrices

```
| a   b |
|       |
| c   d |

--- Lower triangular matrix    --- Upper triangular matrix

| 1   0 |                      | a      b     |
|       |                      |              |
| c     |                      |        b.c   |
| -   1 |                      | 0   d - ---  |
| a     |                      |        a     |

--- Check matrix product L*U ...

| a   b |
|       |
| c   d |
```

Example 3: LU Decomposition with Symbolic Python

Abbreviated Output: Part 2: decomposition of 3x3 matrices

```
| a  b  c |
|         |
| d  e  f |
|         |
| g  h  i |

--- Lower triangular matrix    --- Upper triangular matrix ...

| 1     0     0 |         | a     b                   c                  |
|               |         |                                            |
| d             |         |        b.d                 c.d             |
| -     1     0 |         | 0  e - ---             f - ---             |
| a             |         |         a                   a              |
|               |         |                                            |
|        b.g    |         |                 (    c.d) (    b.g)        |
|    h - ---    |         |                 (f - ---).(h - ---)        |
| g       a     |         |                 (     a ) (     a )   c.g  |
| -  -------  1 |         | 0     0     i - ------------------- - ---  |
| a       b.d   |         |                       b.d              a   |
|     e - ---   |         |                   e - ---                  |
|          a    |         |                        a                   |
```

Example 3: LU Decomposition with Symbolic Python

Abbreviated Output: Part 2: decomposition of 3x3 matrices

```
| a   b   c |   # <--- Check matrix product L*U ...
|           |
| d   e   f |
|           |
| g   h   i |

--- Check results with sample (3x3) matrix (see equation 25) ...

--- Set values in L ...                     --- Set values in U ...
--- L = L.subs( { a:3, b:-6,   c:7,         --- U = U.subs( { a:3, b:-6,   c:7,
                  d:9,   e:0,  f:-5,                          d:9,   e:0,  f:-5,
                  g:5, h:-8,   i:6 } )                        g:5, h:-8,   i:6 } )

|  1    0    0 |                            |  3   -6     7   |
|              |                            |                 |
|  3    1    0 |                            |  0   18    -26  |
|              |                            |                 |
| 5/3  1/9   1 |                            |  0    0   -25/9 |

--- L.det() = 1,                            --- U.det() = -150
```

Example 3: LU Decomposition with Symbolic Python

Points to note:

- Theoretical analysis indicates:

$$det(A) = det(L)det(U) = 1 * -150 = -150. \tag{34}$$

  The symbolic analysis works!

- The analysis only works when the parameter "a" is non-zero.
- To avoid division-by-zero, we need a way to shuffle the matrix rows.

Example 4: LU Decomposition with Row Permutations

Problem Statement: Compute LU decomposition with row permutation matrix P, i.e.,

$$A = PLU, \tag{35}$$

then solve matrix equations 25:

Note: Here, P is an orthogonal matrix (i.e., $P^T = P^{-1}$). Thus, solving AX = B translates to LUX = P^T B.

Solution Procedure:

- Create matrices A and B.
- Use scipy.linalg to compute A = PLU.
- Solve LY = P^T B (forward substitution).
- Solve UX = Y (backward substitution).

Example 4: LU Decomposition with Row Permutations

Python Source Code:

```
# ================================================================================
# TestLUDecomposition01.py: Use scipy.linalg to compute LU decomposition with
# row permutation matrix P.
# ================================================================================

import math
import numpy as np
import scipy.linalg as la
import LinearMatrixEquations as lme

def main():
    print("--- Problem 1: Create (3x3) matrix A, (3x1) matrix B ... ");

    print("--- Step 1: Define A and B matrices ... ");

    A = np.array([ [ 3, -6,  7], [ 9,  0, -5], [ 5, -8,  6] ]);
    B = np.array([ [3], [3], [-4] ]);

    lme.printmatrix("A", A);
    lme.printmatrix("B", B);

    print("--- Step 2: Compute A = PLU Decomposition ... ");

    P, L, U = la.lu(A)

    lme.printmatrix("P", P);
    lme.printmatrix("L", L);
```

Example 4: LU Decomposition with Row Permutations

Python Source Code: Continued ...

```
    lme.printmatrix("U", U);

    print("--- Step 3: Check decomposition A = PLU ... ");

    lme.printmatrix("np.dot(P,np.dot(L,U))", np.dot(P,np.dot(L,U)) );

    print("--- Step 4: Compute Z = P^T.B (note: matrix P is orthogonal) ... ");

    Z = np.dot(P.T,B);
    lme.printmatrix("Z", Z);

    print("--- Step 5: Compute forward substitution ... ");

    Y = la.solve_triangular(L, Z, lower=True)

    print("--- Step 6: Compute backward substitution ... ");

    X = la.solve_triangular(U, Y, lower=False)

    lme.printmatrix("Solution: X", X);

# call the main method ...

main()
```

Example 4: LU Decomposition with Row Permutations

Abbreviated Output: ...

```
--- Problem 1: Create (3x3) matrix A, (3x1) matrix B ...
--- Step 1: Define A and B matrices ...

Matrix: A                                    Matrix: B
   3.0e+00 -6.0e+00  7.0e+00                    3.0e+00
   9.0e+00  0.0e+00 -5.0e+00                    3.0e+00
   5.0e+00 -8.0e+00  6.0e+00                   -4.0e+00

--- Step 2: Compute A = PLU Decomposition ...

Matrix: P
   0.0e+00  0.0e+00  1.0e+00
   1.0e+00  0.0e+00  0.0e+00
   0.0e+00  1.0e+00  0.0e+00

Matrix: L                                    Matrix: U
   1.0e+00  0.0e+00  0.0e+00                    9.0e+00  0.0e+00 -5.0e+00
   5.5e-01  1.0e+00  0.0e+00                    0.0e+00 -8.0e+00  8.7e+00
   3.3e-01  7.5e-01  1.0e+00                    0.0e+00  0.0e+00  2.0e+00
```

Example 4: LU Decomposition with Row Permutations

Abbreviated Output: Continued ...

```
--- Step 3: Check decomposition A = PLU ...

Matrix: np.dot(P,np.dot(L,U))
   3.0000000e+00   -6.0000000e+00    7.0000000e+00    <---  It works !!!
   9.0000000e+00    0.0000000e+00   -5.0000000e+00
   5.0000000e+00   -8.0000000e+00    6.0000000e+00

--- Step 4: Compute Z = P^T.B (note: matrix P is orthogonal) ...

Matrix: Z
   3.0000000e+00
  -4.0000000e+00
   3.0000000e+00

--- Steps 5-6: Compute forward/backward substitution ...

Matrix: Solution: X   <---  It works !!!
   2.0000000e+00
   4.0000000e+00
   3.0000000e+00
```

Python Code Listings

Code 1: Matrix Row Operations for Gauss Elimination

```
# ======================================================================
# LinearMatrixEquations.py: Functions to compute operations on linear matrix
#                           equations.
# ======================================================================

import math
import numpy as np

# ==================================================================
# LinearMatrixEquations.printmatrix(): Print two-dimensional matrices.
#
# Args: name: string description of matrix.
#       A (nxn) matrix.
#
# Returns: void.
# ==================================================================

def printmatrix(name, a):
    print("");
    print("Matrix: {:s} ".format(name) );
    for row in a:
        for col in row:
            print("{:16.7e}".format(col), end=" ")
        print("")

# ===============================================================
# LinearMatrixEquations.rowswap(): Create duplicate of matrix, then
#                                  swap rows.
```

Code 1: Matrix Row Operations for Gauss Elimination

```
#
# Args: A (nxn) numpy array.
#       k: row to be swapped.
#       l: row to be swapped.
#
# Returns: B (nxn) copy of A with rows swapped.
# =================================================================

def rowswap(A,k,l):
    m = A.shape[0]   # m is number of rows in A
    n = A.shape[1]   # n is number of columns in A

    B = np.copy(A).astype('float64')

    for j in range(n):
        temp = B[k][j]
        B[k][j] = B[l][j]
        B[l][j] = temp

    return B

# ==================================================================
# LinearMatrixEquations.rowscale(): Create duplicate of matrix, then
#                                   scale specified row.
#
# Args: A (nxn) numpy array.
#     : k (int: is matrix row number to be scaled.
#     : scale (double): scale factor.
```

Code 1: Matrix Row Operations for Gauss Elimination

```
#
# Returns: B (nxn) copy of A with row k multiplied by scale ...
# ==================================================================

def rowscale(A,k,scale):

    m = A.shape[0]   # m is number of rows in A
    n = A.shape[1]   # n is number of columns in A

    B = np.copy(A).astype('float64')

    for j in range(n):
        B[k][j] *= scale

    return B

# ======================================================================
# LinearMatrixEquations.rowadd(): Add multiple of a row to another row.
#
# Args: A (nxn) numpy array.
#     : k (int: is matrix row number to be added to.
#     : l (int: is matrix row number to be scaled.
#     : scale (double): scale factor.
#
# Returns: B (nxn) copy of A with row k multiplied by scale ...
# ======================================================================

def rowadd(A,k,l,scale):
    m = A.shape[0]   # m is number of rows in A
    n = A.shape[1]   # n is number of columns in A
```

Code 1: Matrix Row Operations for Gauss Elimination

```
    B = np.copy(A).astype('float64')

    for j in range(n):
        B[l][j] += B[k][j]*scale

    return B
```

Code 2: Gauss Elimination with Partial Pivoting

```
# ========================================================================
# LinearMatrixEquations.py: Functions to compute operations on linear matrix
#                           equations.
# ========================================================================

import math
import numpy as np

# ===========================================================================
# LinearMatrixEquations.rowreduction(): Computes row reduction to echelon form.
#
# Args: A: an augmented matrix of dimension n x (n+1) associated with a
#          linear system.
#
# Returns: B, a numpy array that represents the row echelon form of A.
#
# Note: RowReduction may not return correct results if the the matrix A does
# not have a pivot in each column (i.e., the matrix is rank deficient).
# ===========================================================================

def rowreduction(A):

    m = A.shape[0]   # A has m rows
    n = A.shape[1]   # It is assumed that A has m+1 columns

    B = np.copy(A).astype('float64')

    # For each step of elimination, we find a suitable pivot, move it into
```

Code 2: Gauss Elimination with Partial Pivoting

```
    # position and create zeros for all entries below.

    for k in range(m):
        # Set pivot as (k,k) entry
        pivot = B[k][k]
        pivot_row = k

        # Find a suitable pivot if the (k,k) entry is zero

        while(pivot == 0 and pivot_row < m-1):
            pivot_row += 1
            pivot = B[pivot_row][k]

        # Swap row if needed

        if (pivot_row != k):
            B = rowswap(B,k,pivot_row)

        # If pivot is nonzero, carry on with elimination in column k

        if (pivot != 0):
            B = rowscale(B,k,1./B[k][k])
            for i in range(k+1,m):
                B = rowadd(B,k,i,-B[i][k])
        else:
            print("Pivot could not be found in column",k,".")

    return B
```

Code 2: Gauss Elimination with Partial Pivoting

```

# ==============================================================================
# LinearMatrixEquations.backsubstitution(): Returns an (nx1) vector that is the
# solution to the matrix system UX = B.
#
# Args: U: A numpy array that represents an upper triangular square mxm matrix.
#       B: A numpy array that represents an nx1 vector
#
# Returns: X, A (nx1) numpy array representing the solution to UX = B.
# ==============================================================================

def backsubstitution(U,B):

    # m is number of rows and columns in U

    m = U.shape[0]
    X = np.zeros((m,1))

    # Calculate entries of X backward from m-1 to 0

    for i in range(m-1,-1,-1):
        X[i] = B[i]
        for j in range(i+1,m):
            X[i] -= U[i][j]*X[j]
        if (U[i][i] != 0):
            X[i] /= U[i][i]
        else:
            print("Zero entry found in U pivot position",i,".")
    return X
```

Code 2: Gauss Elimination with Partial Pivoting

```
# =============================================================================
# LinearMatrixEquations.backsubstitution(): Returns an (nx1) vector that is the
# solution to the matrix system AX = B.
#
# Args: A: A numpy array that represents a matrix of dimension n x n.
#       B: A numpy array that represents a matrix of dimension n x 1.
#
# Returns: X, A (nx1) numpy array representing the solution to AX = B.
#
# Note: Computational procedure will fail if AX = B does not have a
#       unique solution.
# =============================================================================

def solvesystem(A,B):

    # Step 1: Check shape of A

    if (A.shape[0] != A.shape[1]):
        print("--- ERROR: solvesystem accepts only square arrays ...")
        return
    n = A.shape[0]  # n is number of rows and columns in A

    # Step 2: Join A and B to make the augmented matrix

    A_augmented = np.hstack((A,B))

    # Step 3: Carry out elimination
```

Code 2: Gauss Elimination with Partial Pivoting

```

    R = rowreduction(A_augmented)

    # Step 4: Split R back to nxn piece and nx1 piece

    B_reduced = R[:,n:n+1]
    A_reduced = R[:,0:n]

    # Step 5: Compute back substitution

    X = backsubstitution( A_reduced, B_reduced)

    return X
```