Crout's LU Decomposition of a Matrix

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1 Factoring a matrix to find its determinant and prepare to solve equations

This routine enables one to factor an $n \times n$ nonsingular matrix $\mathbf{A}$ into a product $\mathbf{A} = \mathbf{PLU}$ where $\mathbf{P}$ is a permutation matrix (its rows are the rows of of the $n \times n$ identity matrix in some order), $\mathbf{L}$ is lower triangular, and $\mathbf{U}$ is upper triangular. This factorization makes solving a system of equations $\mathbf{Ax} = \mathbf{b}$ rather easy, where $\mathbf{b}$ is a column of constants. Actually, $\mathbf{b}$ can be any $n \times k$ matrix. The routine also computes the determinant of $\mathbf{A}$.

STEP 1: Initialize

(a) Input (the location of $\mathbf{A}$) and the size of the matrix to a variable N. Also input a tolerance $\varepsilon > 0$ such that anything smaller than it in absolute value will be considered $= 0$.

(b) Create a one-dimensional array IND(I), a variable DET, and temporary variables necessary for indexing, such as I and J, and for storing other variables when necessary. Also identify the location of the variables $\mathbf{U}$ and $\mathbf{L}$ with the location within the variable $\mathbf{A}$. That is, identify $\mathbf{L}_{\mathrm{I,J}} \equiv \mathbf{A}_{\mathrm{IND(I),J}}$ for $1 \leq \mathrm{J} \leq \mathrm{I}$ and $\mathbf{U}_{\mathrm{I,J}} \equiv \mathbf{A}_{\mathrm{IND(I),J}}$ for $\mathrm{I} < \mathrm{J} \leq \mathrm{N}$.

(c) Initialize variables

  (*i*) DET := 1

  (*ii*) IND(I) := I for $1 \leq \mathrm{I} \leq \mathrm{N}$

  (*iii*) J := 1

STEP 2: This is the start of the main loop of the algorithm, and the place where one tests whether to exit.

If $\mathrm{J} > \mathrm{N}$, RETURN from the routine. Where $\mathbf{A}$ was you now have the information to construct $\mathbf{U}$ and $\mathbf{L}$, IND gives you the information to get $\mathbf{P}$, and DET contains the determinant.

STEP 3: Create the J^{th} column of $\mathbf{L}$. (By convention an empty sum is 0.)

For $\mathrm{I} \geq \mathrm{J}$, set

$$\mathbf{L}_{\mathrm{I,J}} := \mathbf{A}_{\mathrm{IND(I),J}} - \sum_{\mathrm{K}=1}^{\mathrm{J}-1} \mathbf{L}_{\mathrm{I,K}} \cdot \mathbf{U}_{\mathrm{K,J}}$$

STEP 4: Look for a pivot. Let R be the smallest integer such that

$$\mathbf{L}_{\mathrm{R,J}} := \max\{|\mathbf{L}_{\mathrm{I,J}}| : \mathrm{J} \le \mathrm{I} \le \mathrm{N}\}.$$

This pivoting strategy is called partial pivoting.

STEP 5: If $|\mathbf{L}_{\mathrm{R,J}}|$ is within ε of zero, RETURN with an error message saying that the determinant of $\mathbf{A} = 0$. Else if $R \neq J$ interchange entries J and R of IND and set DET := − DET. Then multiply DET by the pivot $\mathbf{L}_{J,J}$.

STEP 6: Create the IND(J)th row of $\mathbf{U}$. For $\mathrm{N} \ge \mathrm{L} > \mathrm{J}$ set

$$\mathbf{U}_{\mathrm{J,L}} := \frac{1}{\mathbf{L}_{\mathrm{J,J}}}\left[\mathbf{A}_{\mathrm{IND(J),L}} - \sum_{\mathrm{K}=1}^{\mathrm{J}-1} \mathbf{L}_{\mathrm{J,K}} \cdot \mathbf{U}_{\mathrm{K,L}}\right].$$

STEP 7: Increment J and repeat the loop, that is, set J := J + 1 and GOTO Step 2.

2 Solving a system of n linear equations in n unknown with nonsingular coefficient matrix.

Given the system

$$\mathbf{Ax} = \mathbf{b}$$

of n linear equations in n unknowns, we proceed as follows:

STEP 1: Initialize

(a) Input N = the number of equations, $\mathbf{A}$ = the coefficient matrix, and (the location of) the column of constants $\mathbf{B}$.

(b) Identify the locations of $\mathbf{Z}$ and $\mathbf{Y}$ with the location of $\mathbf{B}$.

(c) Use the previous routine to replace $\mathbf{A}$ with the its factorization into a product $\mathbf{PLU}$ where $\mathbf{L}$ is lower triangular, $\mathbf{U}$ is upper triangular and $\mathbf{P}$ is a permutation matrix obtainable from information contained in the variable IND. If that routine reports that $\mathbf{A}$ is singular, then RETURN an error condition.

(d) Set I := 1.

Now solve the equation $\mathbf{LZ} = \mathbf{P^{-1}B}$ by forward substitution ($\mathbf{L}$ is lower triangular).

STEP 2: Set

$$\mathbf{Z}_{\mathrm{I}} := \frac{1}{\mathbf{L}_{\mathrm{I,I}}}\left[\mathbf{B}_{\mathrm{IND(I)}} - \sum_{\mathrm{K}=1}^{\mathrm{I}-1} \mathbf{L}_{\mathrm{I,K}}\mathbf{Z}_{\mathrm{K}}\right].$$

Set I := I + 1.

STEP 3: IF I $\leq$ N THEN GOTO Step 2. ELSE set I := N and GOTO Step 4.

When the forward substitution has computed $\mathbf{Z}$, we use back substitution. We initialize I to N to compute the solution of $\mathbf{UX} = \mathbf{Z}$.

STEP 4: Set

$$\mathbf{X}_I := \mathbf{Z}_I - \sum_{K=I+1}^{N} \mathbf{U}_{I,K}\mathbf{X}_K$$

Then set I := I − 1.

STEP 5: IF I $\geq$ 1 THEN GOTO Step 4. ELSE RETURN with the solution in $\mathbf{X}$.

3 An Example

Let us illustrate by solving the equations

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 2 & 1 \\ 1 & 1 & 0 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ -2 \end{bmatrix}$$

with coefficient matrix $\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 2 & 1 \\ 1 & 1 & 0 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix}$ which we must factor.

Initialize: Set the variable DET to 1. Set the variable IND to $[1, 2, 3, 4]$. Set the variable J to 1. Input the matrix $\mathbf{A}$ and the size N = 4.

In Step 2, we have not computed anything, so we just have the initial values, and nothing entered for $\mathbf{L}$ or $\mathbf{U}$.

In Step 3, we compute the first column (possibly permuted) of $\mathbf{L}$. In this case, our sums are empty, that is, we just copy over column 1 of $\mathbf{A}$.

$$\mathbf{L} = \begin{bmatrix} 1 & & & \\ 0 & \cdot & & \\ 1 & \cdot & \cdot & \\ -1 & \cdot & \cdot & \cdot \end{bmatrix}$$

We are lucky here that our pivot is that 1 in the 1, 1 position. Steps 4 and 5 change nothing. Again we have empty sums, and we compute the first row of $\mathbf{U}$. Our algorithm 'mentally' sets all the diagonal elements of $\mathbf{U}$ to 1.

$$\mathbf{U} = \begin{bmatrix} (1) & 0 & 1 & 0 \\ & (1) & \cdot & \cdot \\ & & (1) & \cdot \\ & & & (1) \end{bmatrix}$$

We now move on to the second column of $\mathbf{L}$ and the second row of $\mathbf{U}$. The second column of L will look, up to a possible permutation, like $\begin{bmatrix} (0) \\ -1-0\cdot 0 \\ 1-1\cdot 0 \\ 1-(-1)\cdot 0 \end{bmatrix} = \begin{bmatrix} (0) \\ -1 \\ 1 \\ 1 \end{bmatrix}$ and again we pivot on the diagonal. The variable IND does not change, but we multiply DET by the pivot -1. (It saves time to do this now, rather than later recalling the diagonal elements of $\mathbf{L}$. We now get DET $= -1$ and

$$\mathbf{L} = \begin{bmatrix} 1 & & & \\ 0 & -1 & & \\ 1 & 1 & \cdot & \\ -1 & 1 & \cdot & \cdot \end{bmatrix}$$

and the second row of $\mathbf{U} = \begin{bmatrix} (0) & (1) & \frac{2-0\cdot 1}{-1} & \frac{1-0\cdot 0}{-1} \end{bmatrix} = \begin{bmatrix} (0) & (1) & -2 & -1 \end{bmatrix}$ so

$$\mathbf{U} = \begin{bmatrix} (1) & 0 & 1 & 0 \\ & (1) & -2 & -1 \\ & & (1) & \cdot \\ & & & (1) \end{bmatrix}$$

For column 3 of $\mathbf{L}$ we compute $\begin{bmatrix} (0) \\ (0) \\ 0-1\cdot 1-1\cdot(-2) \\ -1-(-1)\cdot 1-1\cdot(-2) \end{bmatrix} = \begin{bmatrix} (0) \\ (0) \\ 1 \\ 2 \end{bmatrix}$ which gives another pivot on the diagonal, so again the variable IND does not change, and DET is multiplied by the pivot 1 so it is still equal to -1.

$$\mathbf{L} = \begin{bmatrix} 1 & & & \\ 0 & -1 & & \\ 1 & 1 & 1 & \\ -1 & 1 & 2 & \cdot \end{bmatrix}$$

and for row 3 of $\mathbf{U}$ we get $\begin{bmatrix} (0) & (0) & (1) & 1-1\cdot 0-1\cdot(-1) \end{bmatrix} = \begin{bmatrix} (0) & (0) & (1) & 2 \end{bmatrix}$ so

$$\mathbf{U} = \begin{bmatrix} (1) & 0 & 1 & 0 \\ & (1) & -2 & -1 \\ & & (1) & 2 \\ & & & (1) \end{bmatrix}$$

and our last pass sets $\mathbf{L}_{4,4} = 1-(-1)\cdot 0 - 1\cdot(-1) - 2\cdot 2 = -2$ giving

$$\mathbf{L} = \begin{bmatrix} 1 & & & \\ 0 & -1 & & \\ 1 & 1 & 1 & \\ -1 & 1 & 2 & -2 \end{bmatrix}, \qquad \text{DET} = (-1)\cdot(-2) = 2, \qquad \text{IND} = [1,2,3,4]$$

with no L satisfying $4 \geq \text{L} > 4$ so we increment J to 5, go back to Step 2, and exit. We have completed the factorization.

Check:

$$\mathbf{L}\cdot\mathbf{U} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ -1 & 1 & 2 & -2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & -2 & -1 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 2 & 1 \\ 1 & 1 & 0 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix} = \mathbf{A}$$

We are now ready to solve the initial equations. To do this, we set $\begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix} = \mathbf{U}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$ and solve

$$\mathbf{L}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ -1 & 1 & 2 & -2 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ -2 \end{bmatrix}$$

by forward substitution. That is,

$$z_1 = 0, \quad z_2 = \tfrac{1-0\cdot z_1}{-1} = -1, \quad z_3 = \tfrac{2-1\cdot z_1-1\cdot z_2}{1} = 3, \quad z_4 = \tfrac{-2-(-1)\cdot z_1-1\cdot z_2-2\cdot z_3}{-2} = \tfrac{-2-(-1)\cdot 0-1\cdot(-1)-2\cdot(3)}{-2} = \tfrac{7}{2}.$$

We then solve $\mathbf{U}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & -2 & -1 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 3 \\ \frac{7}{2} \end{bmatrix}$ for $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$ by back substitution to get:

$$x_4 = \tfrac{7}{2}, \quad x_3 = 3 - 2\cdot\left(\tfrac{7}{2}\right) = -4, \quad x_2 = -1-(-2)\cdot(-4)-(-1)\cdot\left(\tfrac{7}{2}\right) = -\tfrac{11}{2} \quad x_1 = 0 - x_3 = 4$$

which says our solution is $\begin{bmatrix} 4 \\ -\frac{11}{2} \\ -4 \\ \frac{7}{2} \end{bmatrix}$.

As a final operation, check this answer in the original equation:

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 2 & 1 \\ 1 & 1 & 0 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ -\frac{11}{2} \\ -4 \\ \frac{7}{2} \end{bmatrix} = \begin{bmatrix} 4+0-4+0 \\ 0+\frac{11}{2}-8+\frac{7}{2} \\ 4-\frac{11}{2}+0+\frac{7}{2} \\ -4-\frac{11}{2}+4+\frac{7}{2} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ -2 \end{bmatrix}$$