An algorithm to invert matrix based on LU decomposition to apply in reactor core analyses

R. S. Dos Santos[1]
E-mail: rsantos@ien.gov.br

[1] *SETER, IEN*

Keywords: matrix calculations, reactor analysis, numerical calculations, condition number.

The analysis of a nuclear reactor, be it for power production, radioisotope production, or even for research, is always preceded by the determination of the neutron flux distribution Ψ in the reactor core, both in space, energy, angular direction, and also in the time variable. Using operators to describe the neutron distribution we have:

$$\Theta\Psi = S \tag{1}$$

where, Θ is an operator describing neutron interactions and spatial dependence, and S represents an external source.

Analytical solution is impractical for Eq.(1). Usually, solutions are based on so-called numerical methods. For that, the operator equation is discretized spatially in such way that we always have an equation system represented by a matrix like this:

$$\underline{\underline{M}}\underline{\Psi} = \underline{S} \tag{2}$$

This system can be analyzed, according to its nature, as well- or ill-conditioned [1]. The first leads to a numerical solution, dependent only on an acceptable error. The second one does not lead to a solution. This matrix condition number, $\kappa(\underline{\underline{M}})$, is defined by:

$$\kappa(\underline{\underline{M}}) = \|\underline{\underline{M}}\|.\|\underline{\underline{M}}^{-1}\| \tag{3}$$

where, $\|\underline{\underline{X}}\|$ represents the norm of matrix $\underline{\underline{X}}$. In Eq.(3), well-conditioned system has $\kappa(\underline{\underline{M}}) \approx 1$. On the hand, large one is ill-one. For determining $\underline{\underline{M}}^{-1}$, the usual method is to use the well-known adjoint matrix $adj(\underline{\underline{M}})$ and associated determinant $|\underline{\underline{M}}|$.

$$\underline{\underline{M}}^{-1} = \frac{1}{|\underline{\underline{M}}|} adj(\underline{\underline{M}}) \tag{4}$$

However, in reactor core calculations, when we consider space and energy, this leads to a very expensive matrix calculations.

In this work, we have developed an algorithm to calculate the $\|\underline{\underline{M}}^{-1}\|$, based on $\underline{\underline{L}}.\underline{\underline{U}}$ decomposition. Here $\underline{\underline{L}}$ is Lower, with unit at principal diagonal, and $\underline{\underline{U}}$ is Upper matrices.

$$\underline{\underline{M}} = \underline{\underline{L}}.\underline{\underline{U}} \tag{5}$$

$$\underline{\underline{M}}^{-1} = .\underline{\underline{U}}^{-1}\underline{\underline{L}}^{-1} \tag{6}$$

We have applied this matrix methodology using a finite difference for a discretization to a 1D diffusion operator

$$\Theta\Psi|_i = -\frac{\partial^2\Psi}{\partial x^2}|_i \approx \frac{1}{(\Delta x)^2}(-\Psi_{i-1}+2\Psi_i-\Psi_{i+1}) \tag{7}$$

For four points, the matrices are:

$$\underline{\underline{M}} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

$$\underline{\underline{L}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1/2 & 1 & 0 & 0 \\ 0 & -2/3 & 1 & 0 \\ 0 & 0 & -3/4 & 1 \end{bmatrix} \quad \underline{\underline{L}}^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 1/3 & 2/3 & 1 & 0 \\ 1/4 & 1/2 & 3/4 & 1 \end{bmatrix}$$

$$\underline{\underline{U}} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ 0 & 3/2 & -1 & 0 \\ 0 & 0 & 4/3 & -1 \\ 0 & 0 & 0 & 5/4 \end{bmatrix} \quad \underline{\underline{U}}^{-1} = \begin{bmatrix} 1/2 & 1/3 & 1/4 & 1/5 \\ 0 & 2/3 & 1/2 & 2/5 \\ 0 & 0 & 3/4 & 3/5 \\ 0 & 0 & 0 & 4/5 \end{bmatrix}$$

$$\underline{\underline{M}}^{-1} = \frac{1}{5}\begin{bmatrix} 4 & 3 & 2 & 1 \\ 3 & 6 & 4 & 2 \\ 2 & 4 & 6 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

Condition numbers are exhited at Tab 1.

Table 1: Condition numbers and norms.

	$\|\underline{\underline{M}}\|$	$\|\underline{\underline{M}}^{-1}\|$	$\kappa(\underline{\underline{M}})$
L_1	4.000	4.500	18;00
L_2	5.292	3.919	20.74
L_∞	4.000	4.500	18.00

Reference

[1] KUO, S.S., Computer Applications of Numerical Methods, Addison-Wesley, 1972.