Numerical Methods. Subjects and goals:

Problems:
- Solving systems of linear equations
- Solving systems of non-linear equations
- Numerical integration and integral equations
- Numerical solution of ordinary differential equations
- Numerical solution of partial differential equations

For each problem, we will discuss
- examples of applications in which the problem occur
- outline the most important numerical solution methods including when to apply which method
- pitfalls in numerical solutions

All numerically generated results must have an associated estimate of the accuracy !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

System of linear equations:

$$
\begin{aligned}
a_{00}x_0 + a_{01}x_1 + a_{02}x_2 + \cdots + a_{0,N-1}x_{N-1} &= b_0 \\
a_{10}x_0 + a_{11}x_1 + a_{12}x_2 + \cdots + a_{1,N-1}x_{N-1} &= b_1 \\
a_{20}x_0 + a_{21}x_1 + a_{22}x_2 + \cdots + a_{2,N-1}x_{N-1} &= b_2 \\
\cdots \qquad\qquad &\quad \cdots \\
a_{M-1,0}x_0 + a_{M-1,1}x_1 + \cdots + a_{M-1,N-1}x_{N-1} &= b_{M-1}
\end{aligned}
$$

Here the N unknowns x_j, $j = 0, 1, \ldots, N-1$ are related by M equations. The coefficients a_{ij} with $i = 0, 1, \ldots, M-1$ and $j = 0, 1, \ldots, N-1$ are known numbers, as are the *right-hand side* quantities b_i, $i = 0, 1, \ldots, M-1$.

Matrix-vector notation:

$$
\begin{array}{ccc}
a_{00}x_0 + a_{01}x_1 + a_{02}x_2 + \cdots + a_{0,N-1}x_{N-1} & = & b_0 \\
a_{10}x_0 + a_{11}x_1 + a_{12}x_2 + \cdots + a_{1,N-1}x_{N-1} & = & b_1 \\
a_{20}x_0 + a_{21}x_1 + a_{22}x_2 + \cdots + a_{2,N-1}x_{N-1} & = & b_2 \\
\cdots & & \cdots \\
a_{M-1,0}x_0 + a_{M-1,1}x_1 + \cdots + a_{M-1,N-1}x_{N-1} & = & b_{M-1}
\end{array}
$$

$$
\mathbf{A} = \begin{bmatrix} a_{00} & a_{01} & \cdots & a_{0,N-1} \\ a_{10} & a_{11} & \cdots & a_{1,N-1} \\ & \cdots & & \\ a_{M-1,0} & a_{M-1,1} & \cdots & a_{M-1,N-1} \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} b_0 \\ b_1 \\ \cdots \\ b_{M-1} \end{bmatrix}
$$

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$$

We start with: $N = M$

General Numerical Recipes notation:

$$\mathbf{C} = \mathbf{A} \cdot \mathbf{B} \quad \Longleftrightarrow \quad c_{ik} = \sum_j a_{ij} b_{jk}$$

$$\mathbf{b} = \mathbf{A} \cdot \mathbf{x} \quad \Longleftrightarrow \quad b_i = \sum_j a_{ij} x_j$$

$$\mathbf{d} = \mathbf{x} \cdot \mathbf{A} \quad \Longleftrightarrow \quad d_j = \sum_i x_i a_{ij}$$

$$q = \mathbf{x} \cdot \mathbf{y} \quad \Longleftrightarrow \quad q = \sum_i x_i y_i$$

Boldface capital letters are matrices, boldface small letters are vectors, non-boldface small letters are scalars

LU decomposition:

Suppose we are able to write the matrix $\mathbf{A}$ as a product of two matrices,

$$\mathbf{L} \cdot \mathbf{U} = \mathbf{A} \tag{2.3.1}$$

where $\mathbf{L}$ is *lower triangular* (has elements only on the diagonal and below) and $\mathbf{U}$ is *upper triangular* (has elements only on the diagonal and above). For the case of a 4×4 matrix $\mathbf{A}$, for example, equation (2.3.1) would look like this:

$$\begin{bmatrix} \alpha_{00} & 0 & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\mathbf{L} \cdot \mathbf{y} = \mathbf{b}$$

$$\mathbf{A} \cdot \mathbf{x} = (\mathbf{L} \cdot \mathbf{U}) \cdot \mathbf{x} = \mathbf{L} \cdot (\mathbf{U} \cdot \mathbf{x}) = \mathbf{b}$$

$$\mathbf{U} \cdot \mathbf{x} = \mathbf{y}$$

$$\begin{bmatrix} \alpha_{00} & 0 & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

(N=4)

Solve $\mathbf{L} \cdot \mathbf{y} = \mathbf{b}$ (forward substitution):

$$y_0 = \frac{b_0}{\alpha_{00}}$$

$$y_i = \frac{1}{\alpha_{ii}} \left[b_i - \sum_{j=0}^{i-1} \alpha_{ij} y_j \right] \qquad i = 1, 2, \ldots, N-1$$

$$\begin{bmatrix} \alpha_{00} & 0 & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

(N=4)

Solve $\mathbf{L} \cdot \mathbf{y} = \mathbf{b}$ (forward substitution):

$$y_0 = \frac{b_0}{\cancel{\alpha_{00}}}$$

$$y_i = \cancel{\frac{1}{\alpha_{ii}}}\left[b_i - \sum_{j=0}^{i-1} \alpha_{ij} y_j \right] \qquad i = 1, 2, \ldots, N-1$$

$$\alpha_{ii} \equiv 1 \qquad i = 0, \ldots, N-1$$

Solve $\mathbf{U} \cdot \mathbf{x} = \mathbf{y}$ (back substitution):

$$x_{N-1} = \frac{y_{N-1}}{\beta_{N-1,N-1}}$$

$$x_i = \frac{1}{\beta_{ii}}\left[y_i - \sum_{j=i+1}^{N-1} \beta_{ij} x_j \right] \qquad i = N-2, N-3, \ldots, 0$$

Solve for L and U:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\beta_{00} = a_{00}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\alpha_{10} = \frac{a_{10}}{\beta_{00}}$$

$$\begin{bmatrix} \alpha_{00} & 0 & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\alpha_{20} = \frac{a_{20}}{\beta_{00}}$$

$$\begin{bmatrix} \alpha_{00} & 0 & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\alpha_{30} = \frac{a_{30}}{\beta_{00}}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & \boxed{a_{01}} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\beta_{01} = a_{01}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & \boxed{a_{11}} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\beta_{11} = a_{11} - \alpha_{10}\beta_{01}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & \boxed{a_{21}} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\alpha_{21} = \frac{a_{21} - \alpha_{20}\beta_{01}}{\beta_{11}}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & \boxed{a_{31}} & a_{32} & a_{33} \end{bmatrix}$$

$$\alpha_{31} = \frac{a_{31} - \alpha_{30}\beta_{01}}{\beta_{11}}$$

For each $j = 0, 1, 2, \ldots, N-1$ do these two procedures:

$$\text{for } i = 0, 1, \ldots, j \qquad \beta_{ij} = a_{ij} - \sum_{k=0}^{i-1} \alpha_{ik}\beta_{kj}$$

$$\text{for } i = j+1, j+2, \ldots, N-1 \qquad \alpha_{ij} = \frac{1}{\beta_{jj}}\left(a_{ij} - \sum_{k=0}^{j-1} \alpha_{ik}\beta_{kj}\right)$$

What if $\beta_{jj} = 0$? (also a problem for a ”small” β_{jj}

Pivoting (row swaps) like in Gaussian elimination. Terrible to bookkeep, but implemented in the Numerical Recipes routines Ludcmp.

Computational complexity (big O() notation)

LU decomposition:

For each $j = 0, 1, 2, \ldots, N-1$ do these two procedures:

$$\text{for } i = 0, 1, \ldots, j \qquad \beta_{ij} = a_{ij} - \sum_{k=0}^{i-1} \alpha_{ik}\beta_{kj}$$

$$\text{for } i = j+1, j+2, \ldots, N-1 \qquad \alpha_{ij} = \frac{1}{\beta_{jj}}\left(a_{ij} - \sum_{k=0}^{j-1} \alpha_{ik}\beta_{kj}\right)$$

O(N^3)

Forward substitution:

$$y_0 = \frac{b_0}{\cancel{\alpha_{00}}}$$

$$y_i = \cancel{\frac{1}{\alpha_{ii}}}\left[b_i - \sum_{j=0}^{i-1} \alpha_{ij} y_j\right] \qquad i = 1, 2, \ldots, N-1$$

O(N^2)

Back substitution:

$$x_{N-1} = \frac{y_{N-1}}{\beta_{N-1,N-1}}$$

$$x_i = \frac{1}{\beta_{ii}}\left[y_i - \sum_{j=i+1}^{N-1} \beta_{ij} x_j\right] \qquad i = N-2, N-3, \ldots, 0$$

O(N^2)

Advantage of LU decomposition when comparing to Gaussian elimination ?

Assume we have to solve a system of linear equations with the **same matrix** and a **new right hand side.**

Then we only need to do forward and back substitutions (assuming we stored L and U). Hence O(N^2) rather than O(N^3).

Exercises

1) Consider an NxN matrix A where we have computed L and U. How can we then easily compute the determinant of A ?
2) Assume that we have 2 NxN matrices A and B, and we have LU-decompositions A=LU and B=L'U'. Let now C=AB. How can we solve Cx=b and what is the resulting computational complexity ?
3) Compute by hand the LU decomposition of

$$A = \begin{pmatrix} 1 & 3 & 5 \\ -2 & 0 & -1 \\ 2 & 3 & 1 \end{pmatrix}$$