# Solution of the N x N problem
# LU decomposition

- Write **A** as a product of two triangular matrices

  (non-unique: we discuss how to do this later)

$$\mathbf{A} = \mathbf{L}\ .\ \mathbf{U} = \begin{pmatrix} L_{11} & 0 & 0 \dots & 0 \\ L_{21} & L_{22} & 0 \dots & 0 \\ L_{31} & L_{32} & L_{33} .. & 0 \\ . & . & & \\ L_{N1} & L_{N2} & \dots\dots & L_{NN} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & \dots\dots & U_{1N} \\ 0 & U_{22} & \dots\dots & U_{2N} \\ 0 & 0 & U_{33} .. & U_{3N} \\ . & . & & \\ 0 & 0 & 0 & \dots U_{NN} \end{pmatrix}$$

# Once **L** and **U** are known, **x** can easily be found

- The problem **A . x = b** can be written
  $\mathbf{L} \, . \mathbf{y} = \mathbf{b}$, with $\mathbf{y} \equiv \mathbf{U} \, . \, \mathbf{x}$

We solve first for **y** by "forward-substitution"

$L_{11} \, \mathbf{y_1} = b_1$ ➔ $y_1 = L_{11}^{-1} \, b_1$

$L_{21} \, y_1 + L_{22} \, \mathbf{y_2} = b_2$ ➔ $y_2 = L_{22}^{-1} \, [b_2 - L_{21} \, y_1]$

…

$L_{i1} \, y_1 + L_{i2} \, y_2 + ..L_{ii} \, \mathbf{y_i} = b_N$

**The unknowns ("not-yet-knowns") appear in red – only one in each eqn**

➔ $y_i = L_{ii}^{-1} \, [b_i - L_{i1}y_1 - L_{i2}y_2 - L_{i3}y_3 - \ldots L_{i,i-1}y_{i-1} \,]$

KEY POINT: Each component of y can be written easily in terms of components already computed

# Solution of the N x N problem LU decomposition

- Once we have **y**, we solve **U** . **x** = **y** just as easily by "backsubstitution"

  (essentially the same method, but starting with the bottom row: $U_{NN} x_N = y_N$ )

  Again, whenever we come to a particular component of x, we get an equation that involves only components that have already been computed.

# So how do we find the LU decomposition of matrix **A?**

A has $N^2$ elements, each of which can be written

$$A_{ij} = L_{i1}U_{1j} + L_{i2}U_{2j} + \ldots + L_{ik}U_{jk}$$

Need only go up to $k = \min(i,j)$, since $L_{ik} = 0$ for $k > i$ and $U_{jk} = 0$ for $k > j$

L and U each have ½ N(N+1) non-zero elements, for a total of $N^2 + N$ unknowns

But there are only $N^2$ constraints, so the problem is underdetermined ➔ we can *choose* N of the elements

# So how do we find the LU decomposition of matrix **A**

Convention: choose $L_{ii} = 1$ for $i = 1,N$

Can now solve all the others in such a way that each element can be written in terms of elements already computed

$$A_{11} = L_{11}\mathbf{U_{11}} \Rightarrow U_{11} = A_{11}/L_{11} = A_{11}$$

$$A_{1j} = L_{11}\mathbf{U_{1j}} \Rightarrow U_{1i} = A_{1i}/L_{11} = A_{1i}$$

$$A_{i1} = \mathbf{L_{i1}}U_{11} \Rightarrow L_{i1} = A_{i1}/U_{11} = A_{i1}/A_{11}$$

# So how do we find the LU decomposition of matrix **A**?

We continue

$A_{2j} = L_{21}U_{1j} + L_{22}\mathbf{U_{2j}} \Rightarrow U_{2j} = A_{2j} - L_{21}U_{1j}$

$A_{i2} = L_{i1}U_{12} + \mathbf{L_{i2}}U_{22} \Rightarrow L_{i2} = U_{22}^{-1}\,(A_{i2} - U_{12}L_{i1})$

In general: $U_{ij} = A_{ij} - \sum_{k=1}^{i-1} L_{ik}\,U_{kj}$ go upward in i

$L_{ij} = U_{jj}^{-1}\,(A_{ij} - \sum_{k=1}^{j-1} L_{ik}\,U_{kj}\,)$ go upward in j

# Computational cost of solving linear system

- To find any $U_{ij}$ requires $2(i-1)$ operations
  (1 addition plus 1 multiplication per term in the sum)

  Total computation of U requires $\sum_{j=1}^{N} \sum_{i=1}^{j} 2(i-1) \sim {}^{1}/_{3}\, N^3$ operations

- Similarly, to find any $L_{ij}$ requires $2(j-1) + 1$ operations ➔ total computation of L also requires $\sim {}^{1}/_{3}\, N^3$ operations

  Extra division

- The final substitutions require $\sim N^2$ operations
  (negligible additional amount for large N)

# Summary of solution to **A**.**x** = **b** using LU decomposition

1) Find **L**.**U** = **A** (~ $^{2}/_{3}$ $N^3$ operations)
2) Solve **L**.**y** = **b** for **y** (~ $^{1}/_{2}$ $N^2$ operations)
3) Solve **U**.**x** = **y** for **x** (~ $^{1}/_{2}$ $N^2$ operations)

# How do we minimize roundoff error?

- Very important trick: reorder rows of **A** before starting so that column 1 elements decrease with increasing i

- This minimizes roundoff error in the early stages and keeps its growth to a minimum

# Iterative improvement

## (correcting the solution for residual roundoff error)

- Let $\mathbf{x}$ be the exact solution to $\mathbf{A}.\mathbf{x} = \mathbf{b}$ and let $\mathbf{x} + \delta\mathbf{x}$ be the result of our numerical calculation

- When we actually substitute $\mathbf{x} + \delta\mathbf{x}$ into the original equation, we get something that isn't exactly $\mathbf{b}$; call the result $\mathbf{b} + \delta\mathbf{b}$

$$\mathbf{A}.(\mathbf{x} + \delta\mathbf{x}) = \mathbf{b} + \mathbf{A}.\ \delta\mathbf{x} = \mathbf{b} + \delta\mathbf{b}$$

- Thus we can estimate the error $\delta\mathbf{x}$ by solving $\mathbf{A}.\ \delta\mathbf{x} = \delta\mathbf{b}$

  This can be done very quickly since we already have the LU decomposition of **A** !

# Matrix inversion and determinants

- Once we have LU-decomposed **A**, it is straightforward to obtain $\mathbf{A}^{-1}$, which is just the solution to

$$\mathbf{A}\,\mathbf{A}^{-1} = \mathbf{I}$$

We can obtain this column by column by solving $\mathbf{A}.\mathbf{x} = \mathbf{b}$ with

$$\mathbf{b} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{etc}$$

- The determinant of **A** is simply

$$|A| = |L|.|U| = (\Pi\, L_{ii})\,(\Pi\, U_{ii}) = (\Pi\, U_{ii})$$