Preconditioning

- Introduction to preconditoning
- Preconditioned iterations
- Preconditioned CG and GMRES.
- Basic preconditioners.
- ILU(0), ILU(p), ILUT preconditioners
- See Chapters 9, 10 of text for details.

Preconditioning – Basic principles

Basic idea: Use Krylov subspace method on a modified system such as:

$$M^{-1}Ax = M^{-1}b.$$

- The matrix $M^{-1}A$ need not be formed explicitly; only need to solve $Mw = v$ whenever needed.
- Consequence: fundamental requirement is that it should be easy to compute $M^{-1}v$ for an arbitrary vector v.
- We want: M close to A (system easier to solve) but operation $v \rightarrow M^{-1}v$ inexpensive (added cost not too high).

Left, Right, and Split preconditioning

Left preconditioning

$$\boldsymbol{M^{-1}Ax = M^{-1}b}$$

Right preconditioning

$$\boldsymbol{AM^{-1}u = b}, \text{ with } \boldsymbol{x = M^{-1}u}$$

Split preconditioning: M is factored as $M = M_L M_R$.

$$\boldsymbol{M_L^{-1}AM_R^{-1}u = M_L^{-1}b}, \text{ with } \boldsymbol{x = M_R^{-1}u}$$

Preconditioned CG (PCG)

- Assume: A and M are both SPD.
- Can apply CG directly to systems

$M^{-1}Ax = M^{-1}b$ or $AM^{-1}u = b$

- Problem: loss of symmetry
- Alternative: when $M = LL^T$ use split preconditioner option
- Second alternative: Observe that $M^{-1}A$ is self-adjoint with respect to M inner product:

$$(M^{-1}Ax, y)_M = (Ax, y) = (x, Ay) = (x, M^{-1}Ay)_M$$

ALGORITHM : 1. Preconditioned CG

1. Compute $r_0 := b - Ax_0$, $z_0 = M^{-1}r_0$, and $p_0 := z_0$
2. For $j = 0, 1, \ldots$, until convergence Do:
3. $\quad \alpha_j := (r_j, z_j)/(Ap_j, p_j)$
4. $\quad x_{j+1} := x_j + \alpha_j p_j$
5. $\quad r_{j+1} := r_j - \alpha_j Ap_j$
6. $\quad z_{j+1} := M^{-1} r_{j+1}$
7. $\quad \beta_j := (r_{j+1}, z_{j+1})/(r_j, z_j)$
8. $\quad p_{j+1} := z_{j+1} + \beta_j p_j$
9. EndDo

Note $M^{-1}A$ is also self-adjoint with respect to $(.,.)_A$:

$$(M^{-1}Ax, y)_A = (AM^{-1}Ax, y) = (x, AM^{-1}Ay) = (x, M^{-1}Ay)_A$$

- Can obtain a similar algorithm
- Assume that M = Cholesky product $M = LL^T$.

Then, another possibility: Split preconditioning option, which applies CG to the system

$$L^{-1}AL^{-T}u = L^{-1}b, \text{ with } x = L^T u$$

- Notation: $\hat{A} = L^{-1}AL^{-T}$. All quantities related to the preconditioned system are indicated by $\hat{\ }$.

ALGORITHM : 2. *CG with Split Preconditioner*

1. Compute $r_0 := b - Ax_0$; $\hat{r}_0 = L^{-1}r_0$; $p_0 := L^{-T}\hat{r}_0$.
2. For $j = 0, 1, \ldots,$ until convergence Do:
3. $\quad \alpha_j := (\hat{r}_j, \hat{r}_j)/(Ap_j, p_j)$
4. $\quad x_{j+1} := x_j + \alpha_j p_j$
5. $\quad \hat{r}_{j+1} := \hat{r}_j - \alpha_j L^{-1}Ap_j$
6. $\quad \beta_j := (\hat{r}_{j+1}, \hat{r}_{j+1})/(\hat{r}_j, \hat{r}_j)$
7. $\quad p_{j+1} := L^{-T}\hat{r}_{j+1} + \beta_j p_j$
8. EndDo

➤ The x_j's produced by the above algorithm and PCG are identical (if same initial guess is used).

✍1 Show this

1. Start: Choose x_0 and a dimension m

2. Arnoldi process:

- Compute $r_0 = b - Ax_0$, $\beta = \|r_0\|_2$ and $v_1 = r_0/\beta$.
- For $j = 1, ..., m$ do
  - Compute $z_j := M^{-1}v_j$
  - Compute $w := Az_j$
  - for $i = 1, \ldots, j$, do : $\left\{ \begin{array}{l} h_{i,j} := (w, v_i) \\ w := w - h_{i,j}v_i \end{array} \right\}$
  - $h_{j+1,1} = \|w\|_2; v_{j+1} = w/h_{j+1,1}$
- Define $V_m := [v_1, ..., v_m]$ and $\bar{H}_m = \{h_{i,j}\}$.

3. *Form the approximate solution:* $x_m = x_0 + M^{-1} V_m y_m$ *where* $y_m = \text{argmin}_y \|\beta e_1 - \bar{H}_m y\|_2$ *and* $e_1 = [1, 0, \ldots, 0]^T$.

4. *Restart: If satisfied stop, else set* $x_0 \leftarrow x_m$ *and goto 2.*

Remark: M is assumed to be the same at each step j. Situations may arise where M varies: $M \rightarrow M_j$. We need a 'Flexible' accelerator that allows this. Changes needed:

1) Save each z_j into matrix $Z_m = [z_1, \cdots, z_m]$.

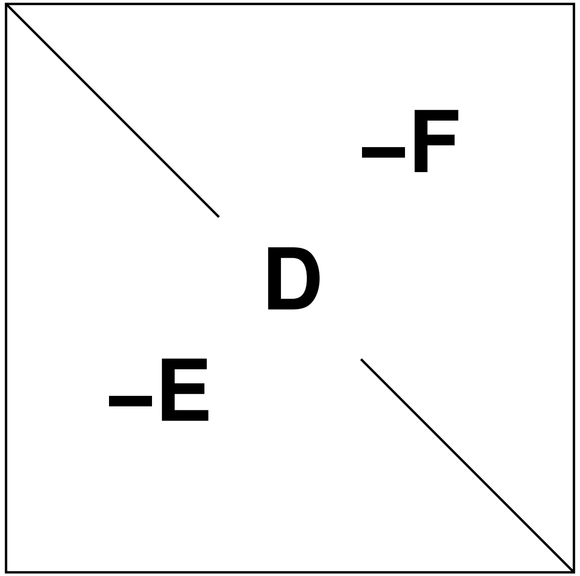
2) Replace $M^{-1} V_m$ by Z_m to form solution in step 3.

✍2 What optimality property is satisfied with (1) Left Preconditioned GMRES, (2) Right Preconditioned GMRES; (3) Flexible GMRES?

Standard preconditioners

- Simplest preconditioner: M = Diag(A) ➤ poor convergence.
- Next to simplest: SSOR. $M = (D - \omega E)D^{-1}(D - \omega F)$
- Still simple but often more efficient: ILU(0).
- ILU(p) – ILU with level of fill p – more complex.
- Class of ILU preconditioners with threshold
- Class of approximate inverse preconditioners
- Class of Multilevel ILU preconditioners
- Algebraic Multigrid Preconditioners

The SOR/SSOR preconditioner



- SOR preconditioning

$$M_{SOR} = (D - \omega E)$$

- SSOR preconditioning

$$M_{SSOR} = (D - \omega E)D^{-1}(D - \omega F)$$

- $M_{SSOR} = LU$, L = lower unit matrix, U = upper triangular. One solve with $M_{SSOR} \approx$ same cost as a MAT-VEC.

- k-step SOR (resp. SSOR) preconditioning:

$$\boxed{k \text{ steps of SOR (resp. SSOR)}}$$

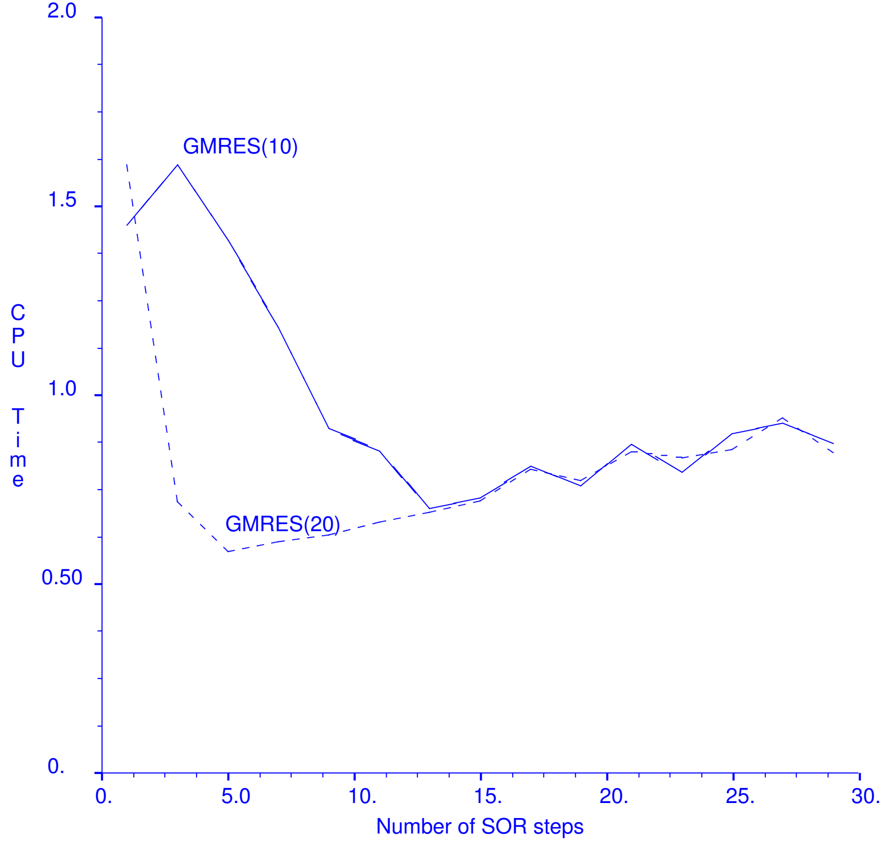
- Questions: Best ω? For preconditioning can take $\omega = 1$

$$\boxed{M = (D - E)D^{-1}(D - F)}$$

Observe: $M = LU + R$ with $R = ED^{-1}F$.

- Best k? $k = 1$ is rarely the best. Substantial difference in performance.

Iteration times versus k for SOR(k) preconditioned GMRES



ILU(0) and IC(0) preconditioners

- **Notation:** $NZ(X) = \{(i,j) \mid X_{i,j} \neq 0\}$
- Formal definition of ILU(0):

$$A = LU + R$$
$$NZ(L) \bigcup NZ(U) = NZ(A)$$
$$r_{ij} = 0 \text{ for } (i,j) \in NZ(A)$$

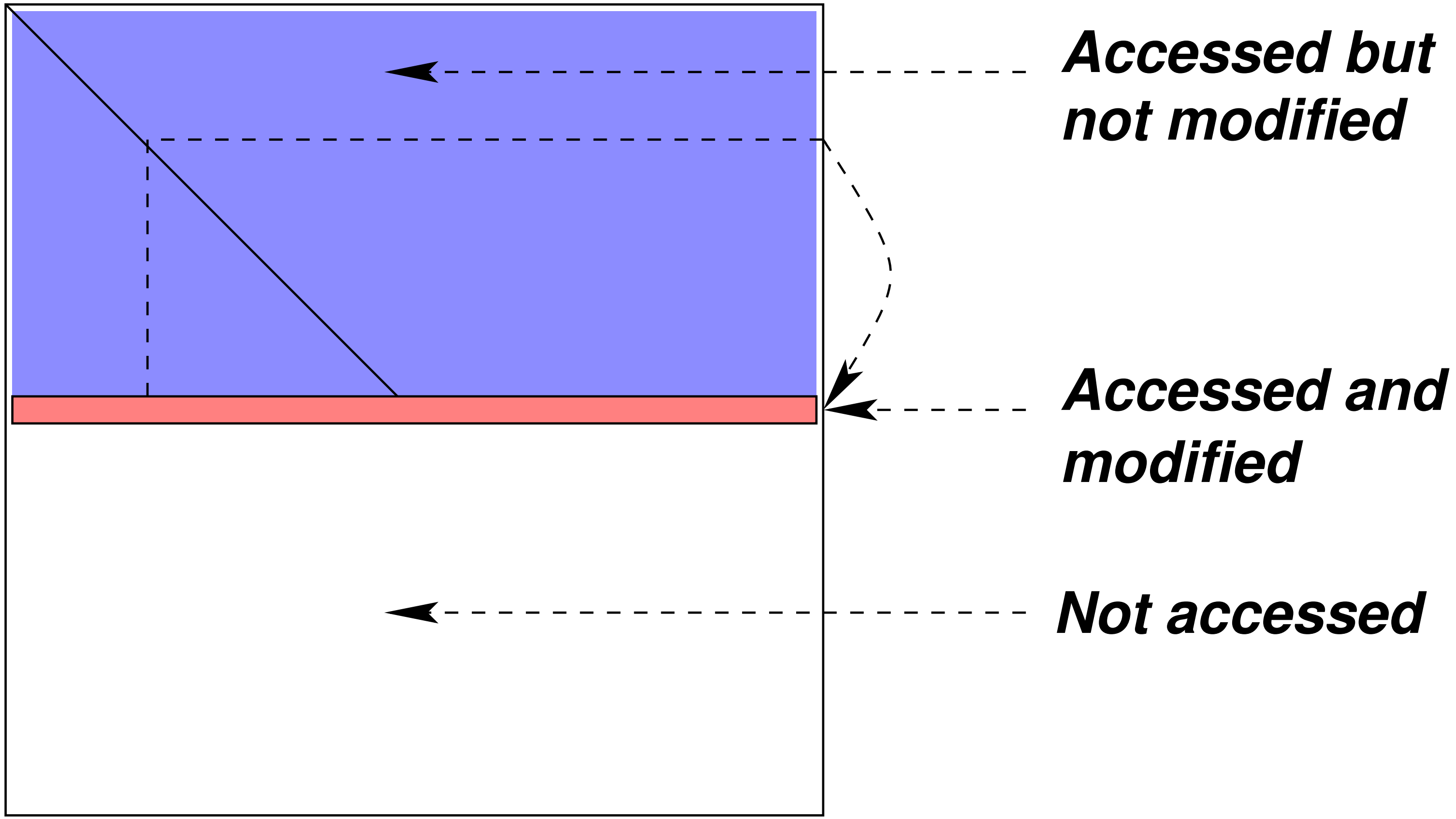
Constructive definition: Compute the LU factorization of A but drop any fill-in in L and U outside of Struct(A).

- ILU factorizations are often based on i, k, j version of GE.

What is the IKJ version of GE?

ALGORITHM : 4. *Gaussian Elimination – IKJ Variant*

1. For $i = 2, \ldots, n$ Do:
2.   For $k = 1, \ldots, i - 1$ Do:
3. $a_{ik} := a_{ik} / a_{kk}$
4.   For $j = k + 1, \ldots, n$ Do:
5. $a_{ij} := a_{ij} - a_{ik} * a_{kj}$
6.   EndDo
7.   EndDo
8. EndDo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ILU(0) – zero-fill ILU

ALGORITHM : 5. *ILU(0)*

For $i = 1, \ldots, N$ *Do:*

For $k = 1, \ldots, i-1$ *and if* $(i,k) \in NZ(A)$ *Do:*

Compute $a_{ik} := a_{ik}/a_{kj}$

For $j = k+1, \ldots$ *and if* $(i,j) \in NZ(A)$, *Do:*

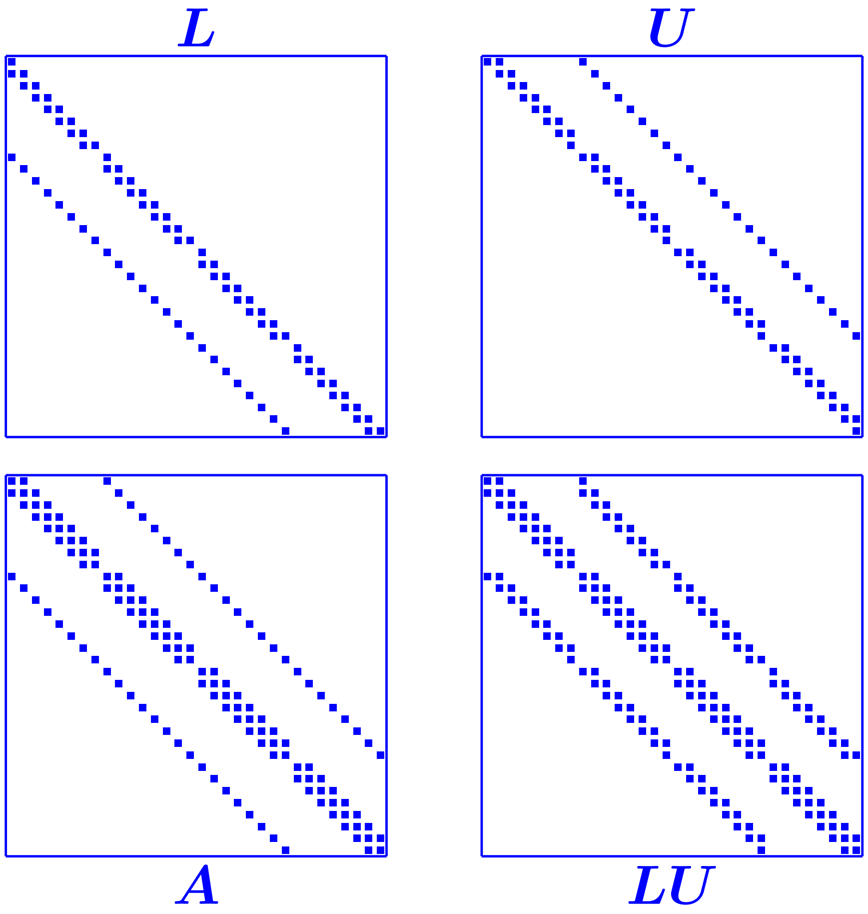
compute $a_{ij} := a_{ij} - a_{ik}a_{k,j}$.

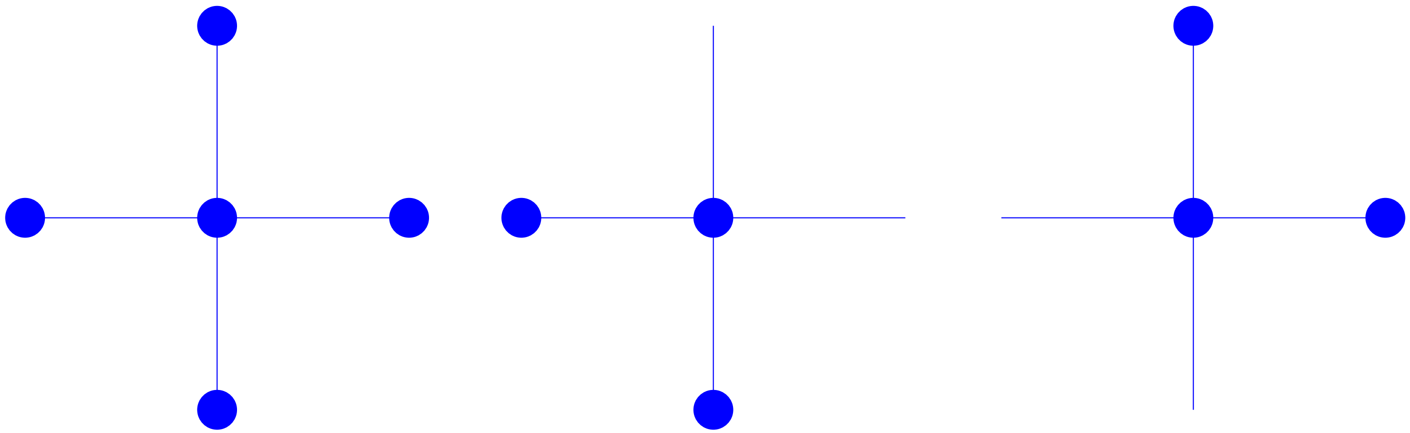
EndFor

EndFor

➤ When A is SPD then the ILU factorization = Incomplete Choleski factorization – IC(0). Meijerink and Van der Vorst [1977].

Pattern of ILU(0) for 5-point matrix. 'Stencil' viewpoint





Stencil of A Stencil of L Stencil of U

➤ Stencil: local connectivity for a graph with a regular pattern.

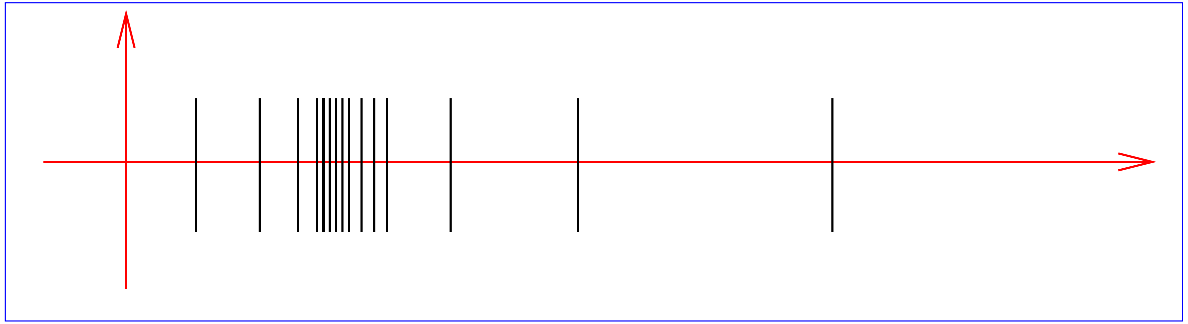
➤ Example: For 5-point matrix A each node is coupled with its East, West, North, South neighbors (when then exist)

✍3 Interpret fill-ins in the ILU(0) and ILU(1) preconditioners using only stencils/

Typical eigenvalue distribution

➤ More than anything else, what determines the convergence of an iterative method is the distribution of the eigenvalues of the matrix.

➤ Need to consider eigenvalues of preconditioned matrix $M^{-1}A$



➤ Clustering around 1 results in fast convergence

✍4 If A is SPD with only k distinct eigenvalues, what is the minimal polynomial p of A? Show that $p(0) \neq 0$. How many steps will it take CG to converge for any linear system $Ax = b$?

Higher order ILU factorization

➤ Higher accuracy incomplete Choleski: for regularly structured problems, IC(p) allows p additional diagonals in L.

➤ Can be generalized to irregular sparse matrices using the notion of level of fill-in [Watts III, 1979]

- Initially $Lev_{ij} = \begin{cases} 0 & \text{for } a_{ij} \neq 0 \\ \infty & \text{for } a_{ij} == 0 \end{cases}$
- At a given step i of Gaussian elimination:

$$\boxed{Lev_{ij} = \min\{Lev_{ij}; Lev_{ik} + Lev_{kj} + 1\}}$$

ALGORITHM : 6. *ILU(p)*

For $i = 2, N$ *Do*

For each $k = 1, \ldots, i-1$ *and if* $a_{ij} \neq 0$ *do*

Compute $a_{ik} := a_{ik}/a_{jj}$

Compute $a_{i,*} := a_{i,*} - a_{ik}a_{k,*}$.

Update the levels of $a_{i,*}$

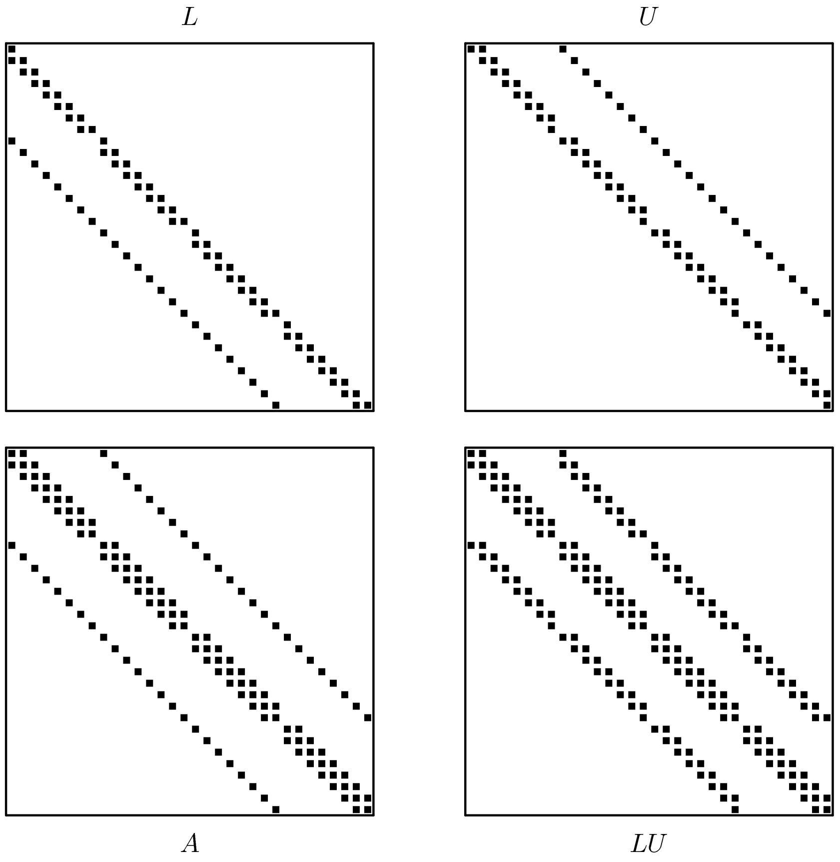
In row i*: if* $lev(a_{ij}) > p$ *set* $a_{ij} = 0$

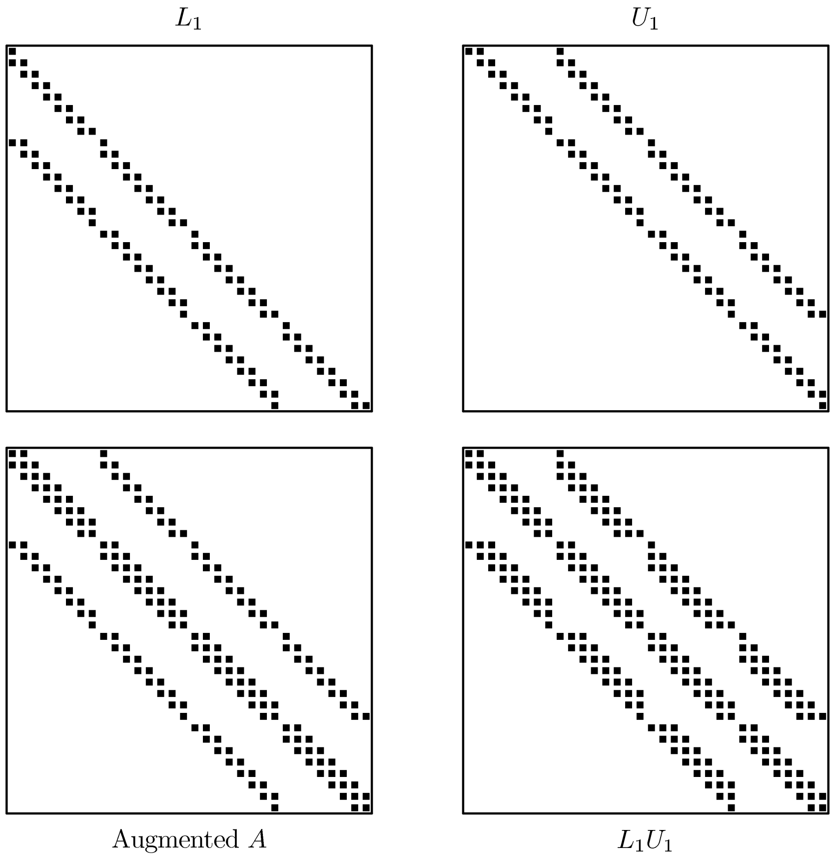
EndFor

EndFor

- Algorithm can be split into symbolic and a numerical phase.
- Higher level of fill-in $\rightarrow$ typically fewer iterations - but more expensive set-up cost

➤ Augmented pattern used for ILU(1) = pattern of L U from ILU(0)





ILU(0)

ILU(1)

ILU with threshold: ILUT(k, ϵ)

ILU(p) factorizations are based on structure only and not numerical values

➤ potential problems for non M-matrices.

Alternative: ILU with Threshold, ILUT

- During each i-th step in GE (i, k, j version), discard pivots or fill-ins whose value is below $\epsilon \|row_i(A)\|$.
- Once the i-th row of $L + U$, (L-part + U-part) is computed retain only the k largest elements in both parts.

➤ Advantages: controlled fill-in. Smaller memory overhead.

➤ Easy to implement and can be made quite inexpensive.

Other preconditioners

Many other techniques have been developed:

- Approximate inverse methods
- Polynomial preconditioners
- Multigrid - type methods
- Incomplete LU based on Crout factorization
- Multi-elimination and multilevel ILU (ARMS)