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Iterative Methods for Solving Linear Systems

Preconditioning Methods

Supported by Intel

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Problem statement

- Let us consider a system of n linear equations that looks as follows:

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$$

...

$$a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n = b_n$$

- This system can be represented as a matrix

$$Ax=b$$

- $A=(a_{ij})$ is a $n \times n$ real matrix; A is a sparse matrix; b and x are vectors consisting of n elements; the exact system solution is x^* .
- *An iterative method* generates a sequence of vectors $x^{(s)} \in R^n$, $s=0,1,2,\dots$, where $x^{(s)}$ is an approximate system solution.

Convergence of Iterative Methods

- Iterative method is convergent if

$$\forall x^{(0)} \in R^m \quad \lim_{s \rightarrow \infty} \|x^{(s)} - x^*\| = 0$$

- For iterative methods, the following is true

$$\|z^{(s+1)}\| \leq (\varphi(\mu_A))^s \|z^{(0)}\|$$

where $z^{(s)} = x^{(s)} - x^*$ is the next approximation error,

φ is a function, $\varphi \rightarrow 0$ when $\sigma \rightarrow \infty$.

$\mu_A = \lambda_{\max} / \lambda_{\min}$ is the condition number.

Example for the conjugate gradient method

$$\varphi(\mu_A) = \frac{\sqrt{\mu_A} - 1}{\sqrt{\mu_A} + 1}$$



Idea of Preconditioning

- ❑ $\mu_A \approx 1$ – the convergence rate is high (A is well-conditioned)
- ❑ $\mu_A \gg 1$ – the convergence rate is low (A is ill-conditioned)
- ❑ The idea of preconditioning lies in converting an ill-conditioned system

$$Ax=b$$

to a well-conditioned one

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

Here, M is a preconditioner.

- ❑ $M^{-1}A$ is not computed explicitly as $M^{-1}A$ is very likely to be a dense matrix
- ❑ Corrective steps allowing for preconditioning are added to the iterative method.

Requirements to the Preconditioner

1. M must be close to A ($M^{-1}A$ is well-conditioned)
2. M must be easy to compute;
3. M must allow for fast solution of systems such as

$$Mz = r$$

in relation to an unknown vector z .

Example 1.

Let $M=A$. Then requirements 1 and 2 are satisfied.

Requirement 3 is not satisfied. $Az=r$ is the same problem as the initial one.

Example 2.

Let $M=\text{diag}(A)$. Then requirements 2 and 3 are satisfied.

Requirement 1 may not be satisfied



Preconditioning Types

$Ax=b$ is the initial system

1. Left preconditioning

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

2. Right preconditioning

$$AM^{-1}u=b, \text{ where } x=M^{-1}u.$$

3. Split preconditioning

Let us present the preconditioner as $M = M_L M_R$

4. Then

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

Basic Preconditioners

- ❑ Let us remember the basic iterative methods that include Jacobi, Seidel and over relaxation (SOR and SSOR) methods.
- ❑ All the methods above are particular cases of the simple iteration method.

$$x^{(s+1)} = Gx^{(s)} + c$$

where $A=M-N$ and $G = M^{-1}N = M^{-1}(M - A) = E - M^{-1}A$

- ❑ Simple iteration method (*) for the system

$$(E - G)x = c$$

that may be formulated as follows

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

- ❑ As a result, the Jacobi, Seidel, SOR and SSOR methods are equivalent to the simple iteration method with a preconditioner.



Basic Preconditioners

Therefore, the following preconditioners are obtained:

1. $M_J = D$ (Jacobi)

may be explicitly applied to the system - multiply by D^{-1} .

2. $M_{GS} = D + L$ (Gauss-Seidel)

3. $M_{SOR} = \frac{1}{\omega}(D + \omega L)$

4. $M_{SSOR} = \frac{1}{\omega(2 - \omega)}(D + \omega L)D^{-1}(D + \omega R)$

$$A = \begin{pmatrix} & & R \\ & D & \\ L & & \end{pmatrix}$$

SSOR-preconditioning

- ❑ How to select ω ?
- ❑ Parameter selection for the preconditioner is not as critical as for the SSOR method: $\omega=1$
- ❑ Symmetric Gauss-Seidel preconditioner

$$M_{SGS} = (D + L)D^{-1}(D + R)$$

- ❑ Use of preconditioner, i.e. system solution

$$M_{SGS} z = r$$

is as complex as multiplying a matrix by vector.

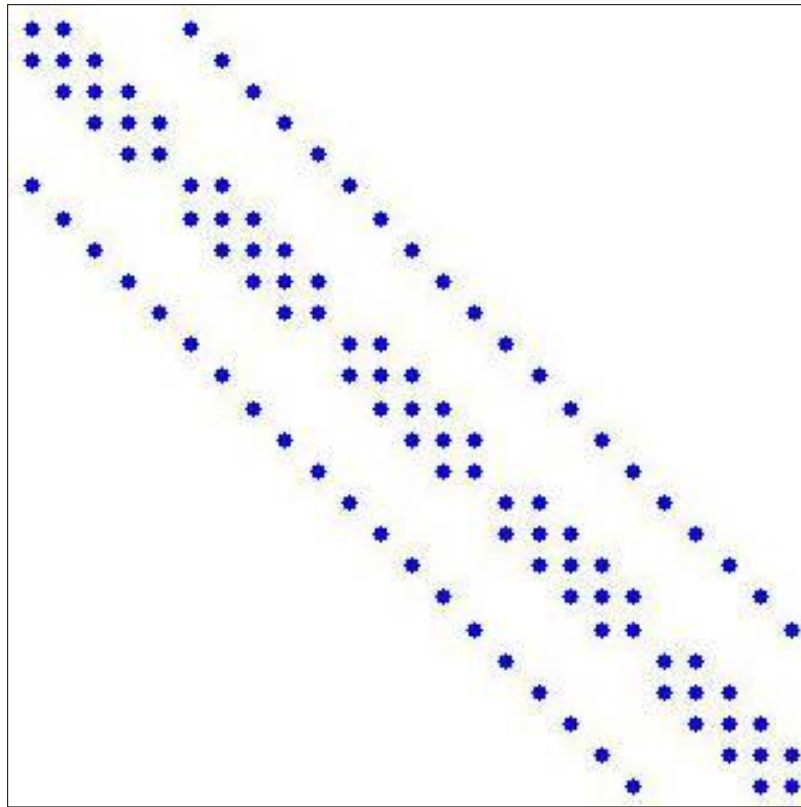
- ❑ Upon the whole, M_{SGS} is better than M_J , but is still insufficient.

SGS-Preconditioning – Example

Numerical solution of Poisson Equation for a 5×5 grid

Matrix A: size $n=25$ ($n^2 = 625$), number of non-zeroes $nz = 105$,

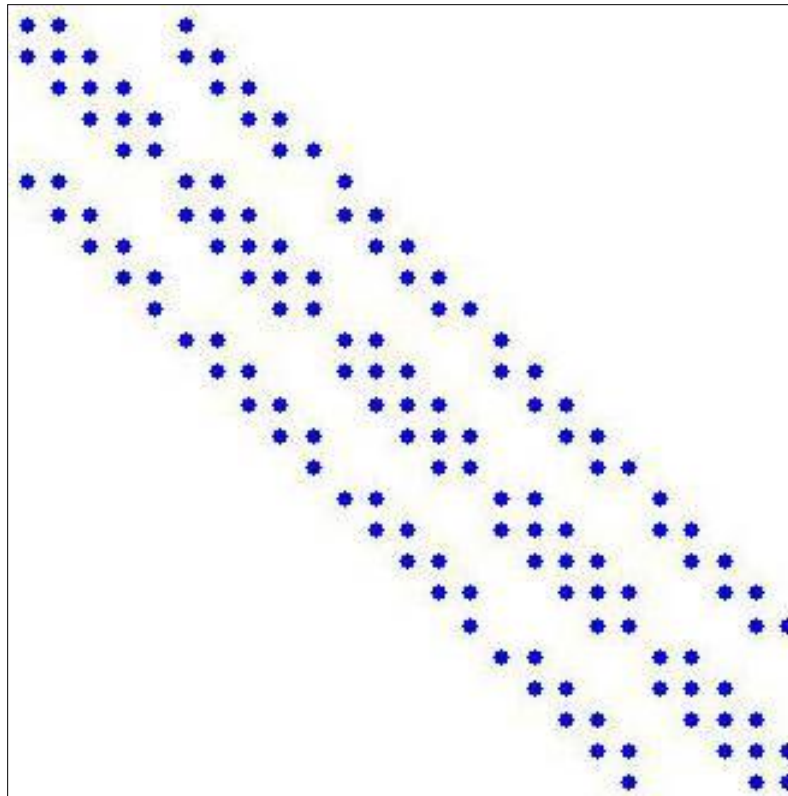
Condition number $\text{cond}(A) = 20.7$



SGS-Preconditioning – Example

Symmetric Gauss-Seidel preconditioner

$$M_{SGS} = (D + L)D^{-1}(D + R)$$



Initial system: $\text{cond}(A)=20.7$;
 M_{SGS} : $\text{cond}(M^{-1}A)=5.1$.

Poisson equation for a 40×40 grid
Matrix size 1600×1600 .

Initial system: $\text{cond}(A)=989$;
 M_{SGS} : $\text{cond}(M^{-1}A)=210$.

ILU(0)-Preconditioning

- Let A be a sparse matrix
 $NZ(A) = \{(i,j): a_{ij} \neq 0\}$
- Let A factorization has been found in the form of

$$A = LU - R$$

L and U are lower (with a single diagonal) and upper triangular matrices;

$$NZ(L) \cup NZ(U) = NZ(A);$$

$$r_{ij} = 0 \text{ for all } (i,j) \in NZ(A).$$

Then ILU(0) is a preconditioner for $M = LU \approx A$.

- The requirements above do not provide for a unique determination of ILU(0).



ILU(0)-Preconditioning

- ❑ Constructive definition of ILU(0) : Perform LU -factorization of A zeroing all filling elements in L and U outside $NZ(A)$ at the same time.

- ❑ LU -factorization (method of Gaussian elimination)

for $i=2, \dots, n$ do

 for $k=1, \dots, i-1$ do

$$a_{ik} = a_{ik}/a_{kk}$$

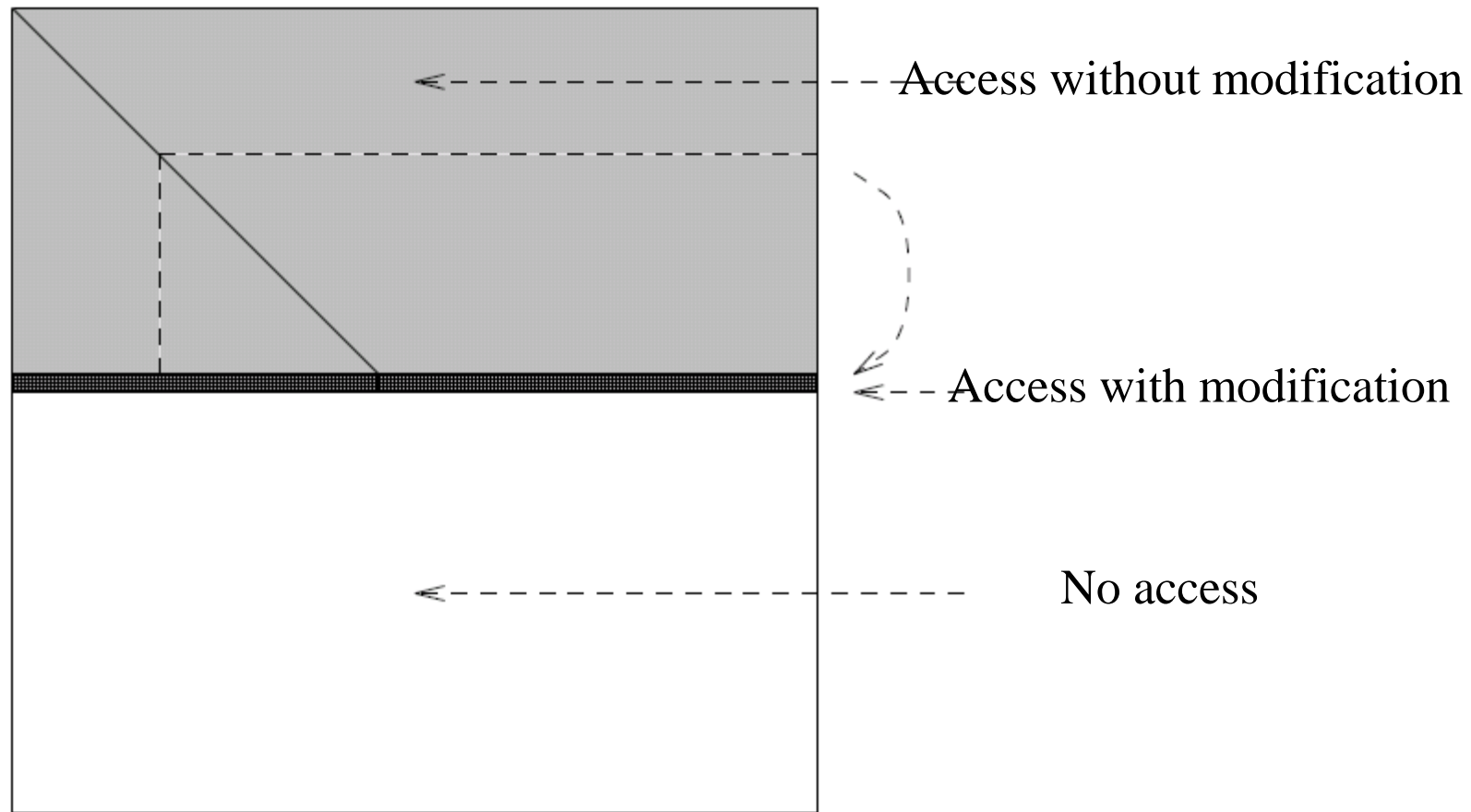
 for $j=k+1, \dots, n$ do

$$a_{ij} = a_{ij} - a_{ik} * a_{kj}$$

 end i

end k

Memory State



Access to the matrix lines: effective for sparse matrices in CRS format

ILU(0)-Factorization - Algorithm

```
for  $i=2, \dots, n$  do
  for  $k=1, \dots, i-1$  and if  $(i,k) \in NZ(A)$  do
     $a_{ik} = a_{ik}/a_{kk}$ 
    for  $j=k+1, \dots, n$  and if  $(i,j) \in NZ(A)$  do
       $a_{ij} = a_{ij} - a_{ik} * a_{kj}$ 
    end  $j$ 
  end  $k$ 
end  $i$ 
```

- If the matrix A is symmetric positive definite, then $ILU(0)$ transforms to $IC(0)$: this is incomplete Cholesky factorization.

ILU(0)-Factorization – Example 1

Let us consider factorization of the matrix A

$$A = \begin{bmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{bmatrix}$$

and perform a complete LU -factorization

$$A = LU = \begin{bmatrix} 1 & & & \\ -0.25 & 1 & & \\ -0.25 & -0.067 & 1 & \\ 0 & -0.0267 & -0.286 & 1 \end{bmatrix} \begin{bmatrix} 4 & -1 & -1 & 0 \\ 3.75 & -0.25 & -1 & \\ 3.733 & -1.067 & & \\ 3.429 & & & \end{bmatrix}$$

ILU(0)-Factorization – Example 1

Incomplete factorization $A \approx IL * IU$

$$IL = \begin{bmatrix} 1 & & & \\ -0.25 & 1 & & \\ -0.25 & 0 & 1 & \\ 0 & -0.267 & -0.267 & 1 \end{bmatrix} \quad IU = \begin{bmatrix} 4 & -1 & -1 & 0 \\ & 3.75 & 0 & -1 \\ & & 3.75 & -1 \\ & & & 3.467 \end{bmatrix}$$

Incomplete factorization residue

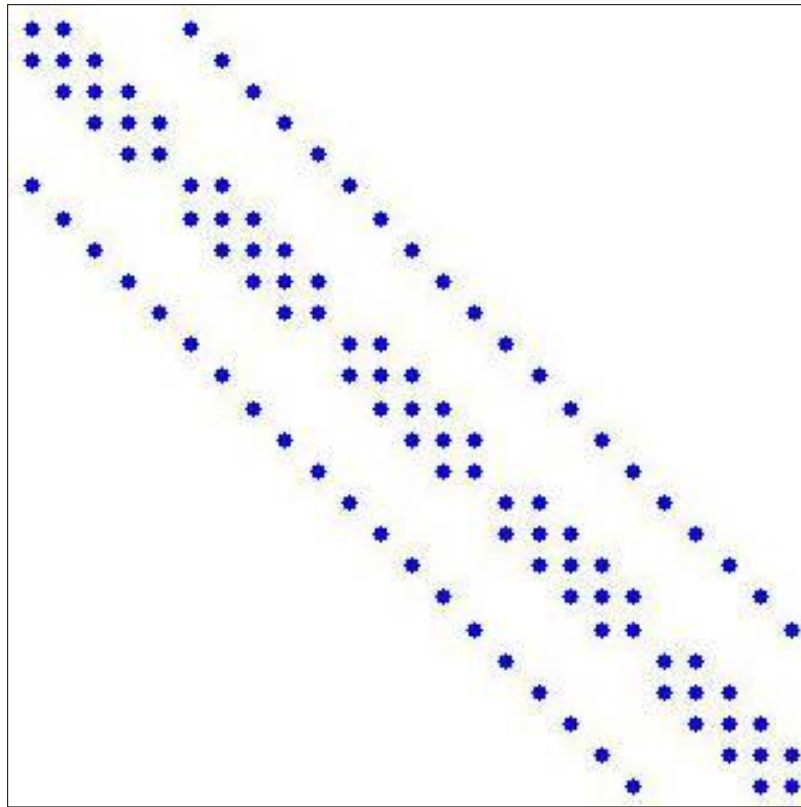
$$A - IL * IU = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -0.25 & 0 \\ 0 & -0.25 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

ILU(0)-factorization – Example 2

Numerical solution of Poisson equation for a 5×5 grid

Matrix A: size $n=25$ ($n^2 = 625$), number of nonzeros $n_z = 105$,

Condition number $\text{cond}(A) = 20.7$

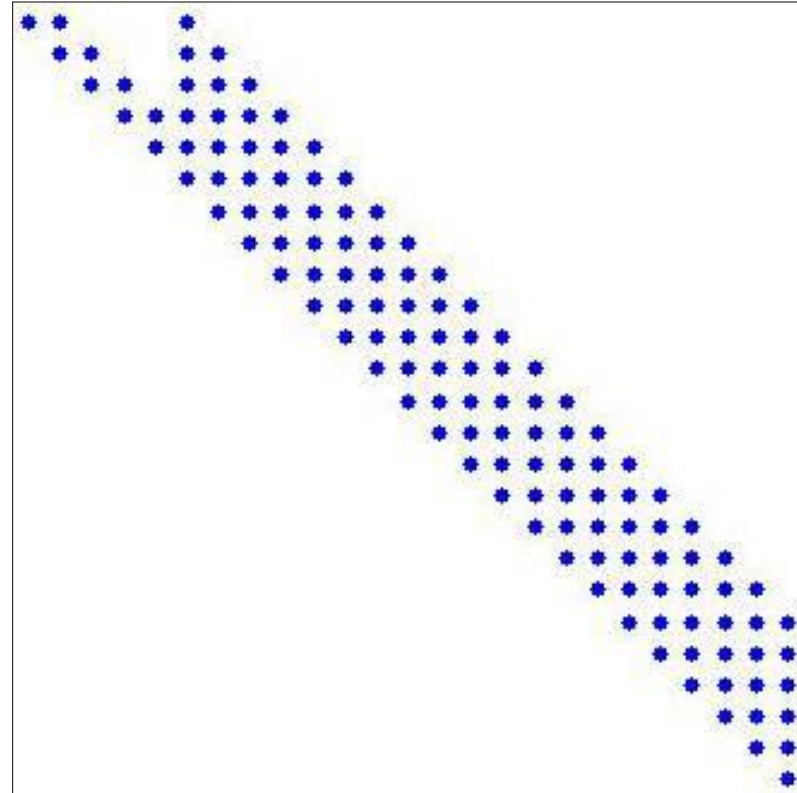
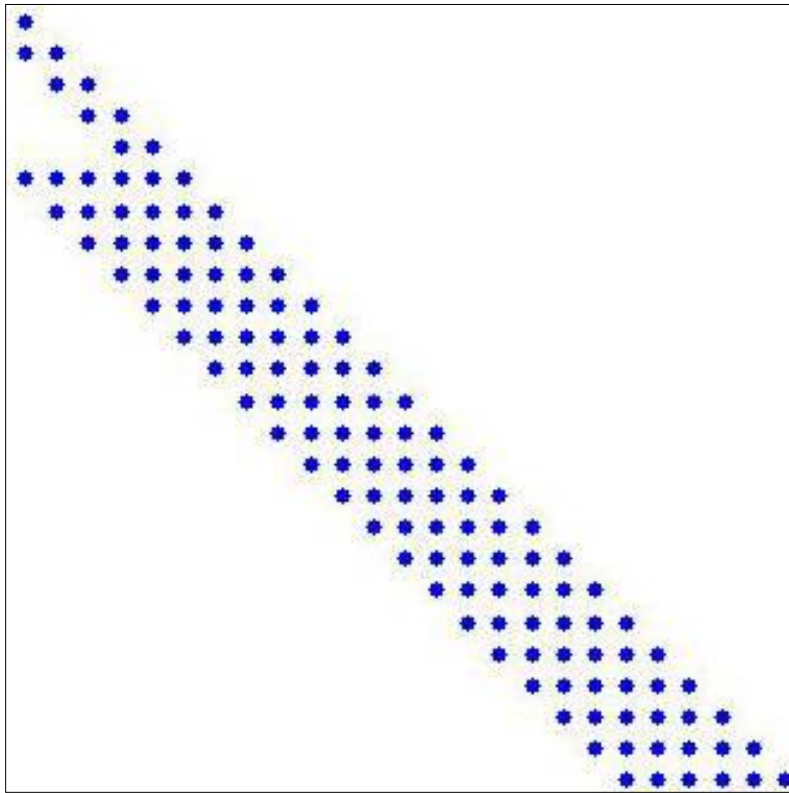


ILU(0)-Factorization – Example 2

Perform a complete LU -factorization

L

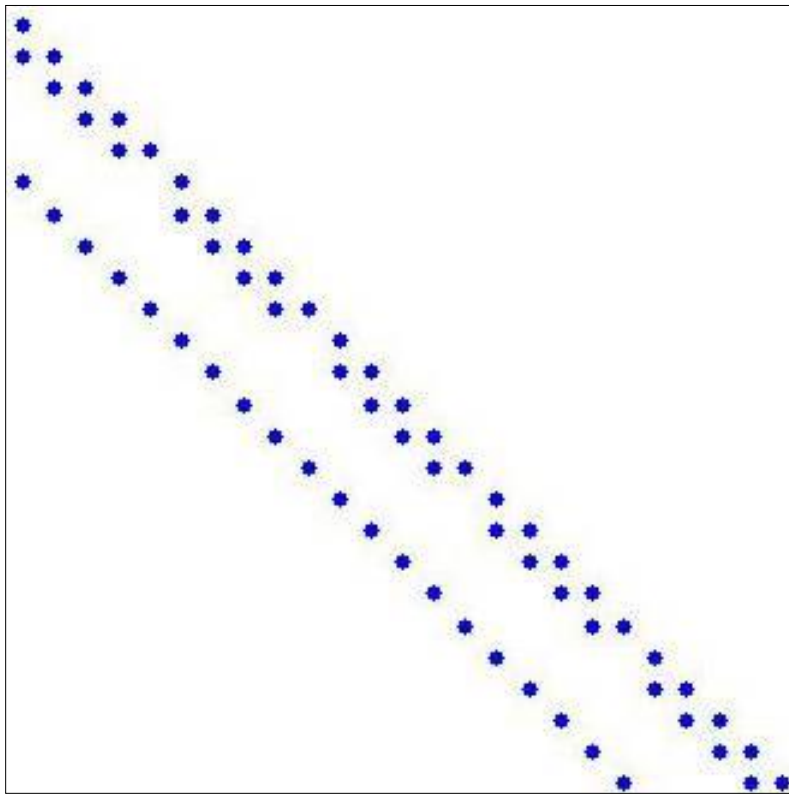
U



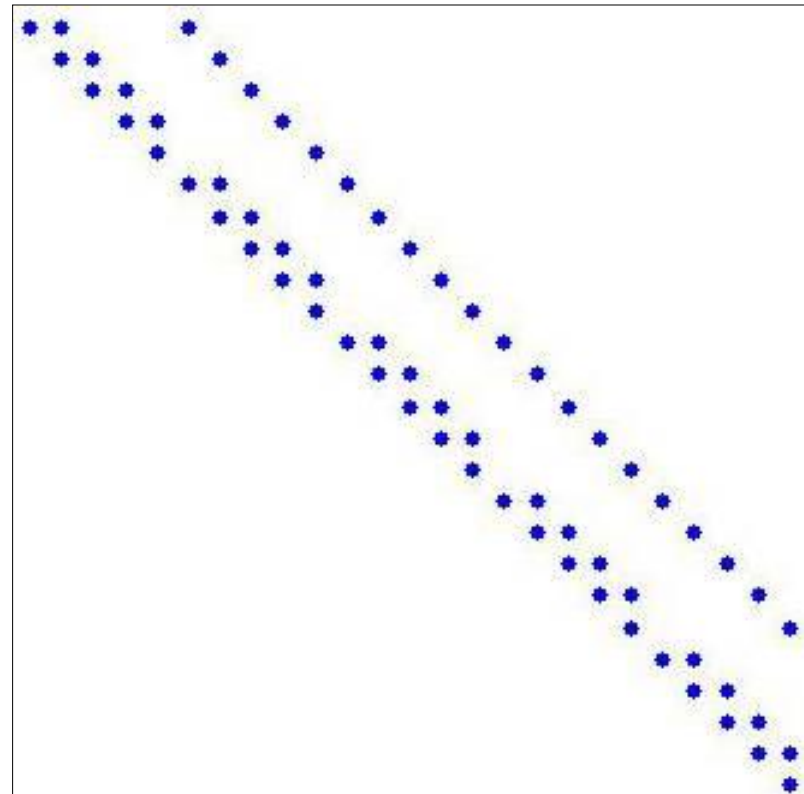
ILU(0)-Factorization – Example 2

Perform $ILU(0)$ -factorization of $A \approx IL * IU$

IL



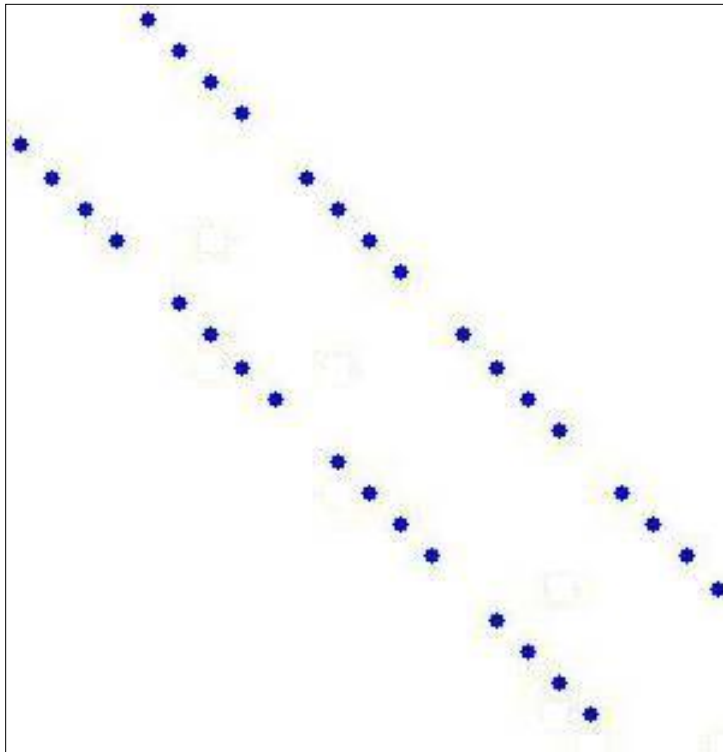
IU



ILU(0)-Factorization – Example 2

ILU(0)-factorization residual

$$A - IL * IU$$



Initial system: $\text{cond}(A)=20.7$;

M_{SGS} : $\text{cond}(M^{-1}A)=5.1$.

$M_{ILU(0)}$: $\text{cond}(M^{-1}A)=3.6$.

Poisson equation for a 40×40 grid

Matrix size 1600×1600 .

Initial system: $\text{cond}(A)=989$;

M_{SGS} : $\text{cond}(M^{-1}A)=210$.

$M_{ILU(0)}$: $\text{cond}(M^{-1}A)=143$.

Filling Control. ILU(p)-Factorization

- ❑ A more exact ILU-factorization can be obtained by allowing a certain degree of factor filling
 - for matrices with a regular structure p additional diagonals may be filled;
 - generalization for matrices with an irregular structure via the *filling level* concept.
- ❑ Initial l_{ij} filling level value

$$l_{ij} = \begin{cases} 0, & \text{если } a_{ij} \neq 0 \text{ или } i = j, \\ \infty, & \text{иначе.} \end{cases}$$

- ❑ At the i -th step of Gaussian elimination

$$l_{ij} = \min\{ l_{ij}, l_{ik} + l_{kj} + 1 \}$$

ILU(p)-Factorization - Algorithm

□ ILU(p) strategy is to zero all elements whose filling level exceeds p .

for $i = 2, \dots, n$ do

for $k = 1, \dots, i - 1$ and if $a_{ik} \neq 0$ do

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

$$a_{i*} = a_{i*} - a_{ik} * a_{i*}$$

update filling levels for a_{i*} :

for i -th line: if $l_{ij} > p$ then $a_{ij} = 0$

$$l_{ij} = \min\{ l_{ij}, l_{ik} + l_{kj} + 1 \}$$

end k

end i

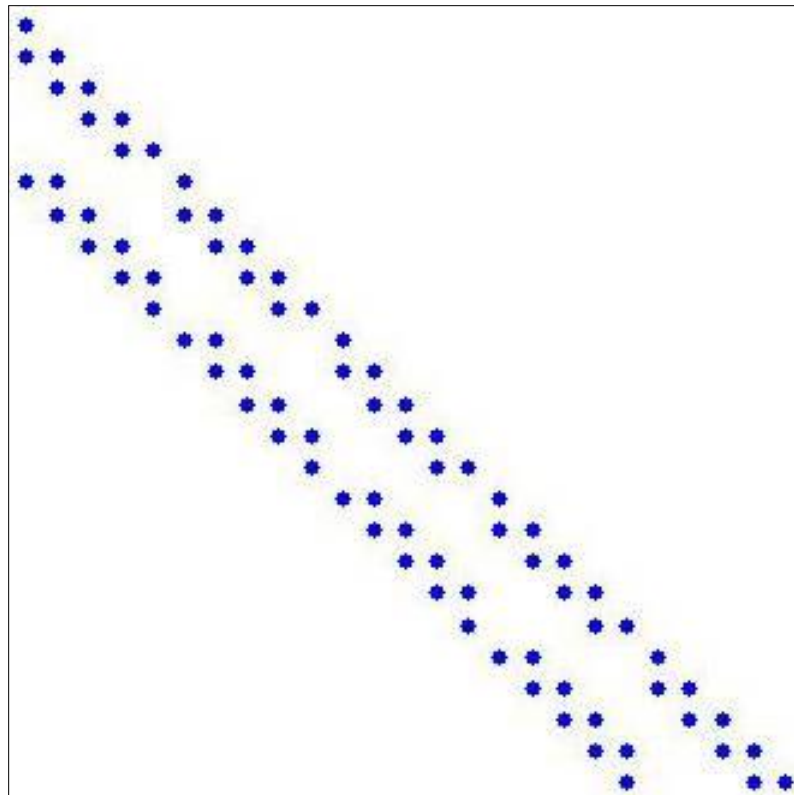
□ The algorithm may be divided into two parts: symbolic (L and U patterns) and numeric (L and U values)

ILU(p)-Factorization - Example

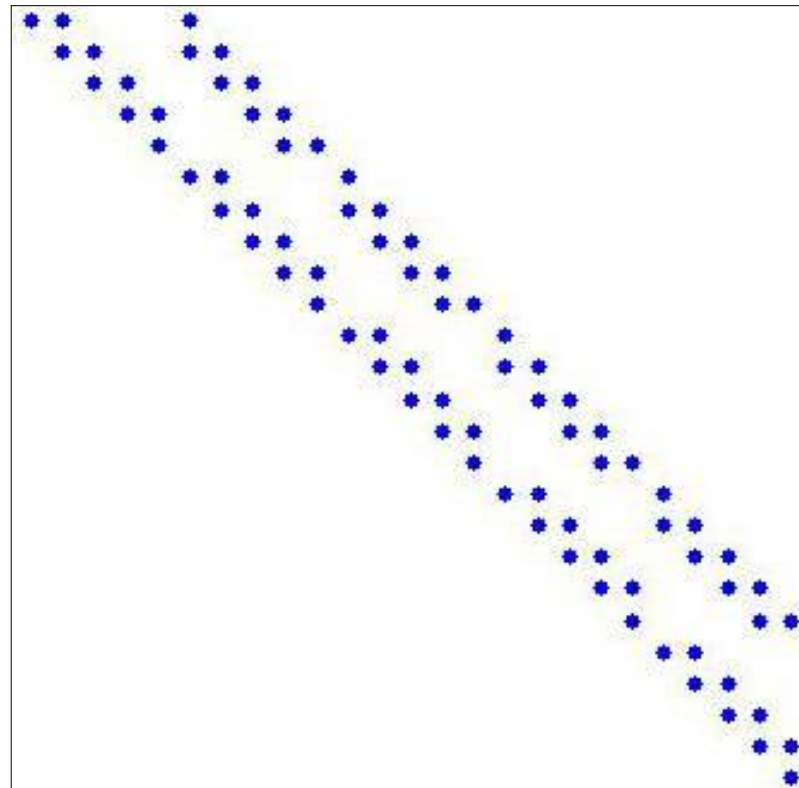
Numerical solution of Poisson equation for a 5×5 grid

Perform $ILU(1)$ -factorization of $A \approx IL * IU$

IL



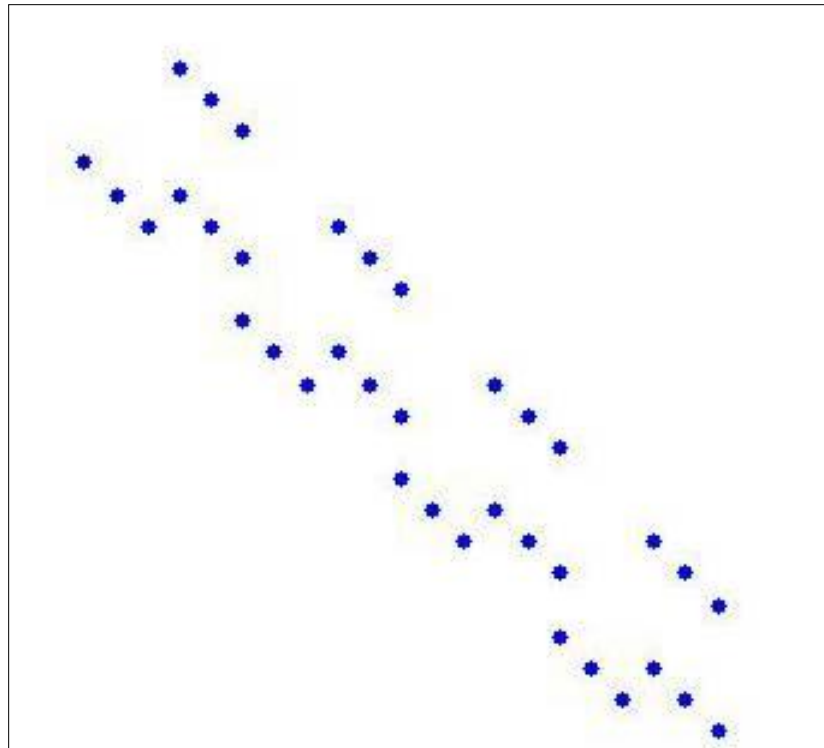
IU



ILU(p)-Factorization - Example

ILU(1)-factorization residual

$$A - IL * IU$$



Initial system: $\text{cond}(A)=20.7$;

M_{SGS} : $\text{cond}(M^{-1}A)=5.1$.

$M_{ILU(0)}$: $\text{cond}(M^{-1}A)=3.6$.

$M_{ILU(1)}$: $\text{cond}(M^{-1}A)=1.5$.

Poisson Equation for a 40×40 grid

Matrix size 1600×1600 .

Initial system: $\text{cond}(A)=989$;

M_{SGS} : $\text{cond}(M^{-1}A)=210$.

$M_{ILU(0)}$: $\text{cond}(M^{-1}A)=143$.

$M_{ILU(0)}$: $\text{cond}(M^{-1}A)=54$.

Conclusion

- As part of this lecture, we have reviewed the following:
 - Concept of preconditioning
 - Requirements to preconditioners
 - Preconditioning types
 - Basic preconditioners
 - Jacobi (J), Gauss-Seidel (GS)
 - SOR, SSOR, SGS
 - Partial LU-factorization
 - General Pattern
 - ILU(0), factorization without filling
 - ILU(0), factorization with filling control
 - Experimental results

References

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3. J. Dongarra et al. Templates for the solution of linear systems: building blocks for iterative methods. SIAM, 1994.
4. Y. Saad. Iterative Methods for Sparse Linear Systems. SIAM, 2003.



Internet Resources

5. Intel Math Kernel Library Reference Manual.

[<http://software.intel.com/sites/products/documentation/hpc/mkl/mklman.pdf>].



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