# Matrix Form of Arnoldi ONB

$$U_m = \text{span}(b, Ab, \ldots, A^{m-1}b) = \text{span}(u_1, u_2, \ldots, u_m) \quad \text{(ONB)}$$

Write this orthogonalization method in matrix form

$$Au_{j-1} = \sum_{k=1}^{j-1} h_{k,j-1} u_k + \widetilde{u}_j = \sum_{k=1}^{j} h_{k,j-1} u_k$$

$$AU_m = A(u_1 \quad \ldots \quad u_m) = (u_1 \quad \ldots \quad u_{m+1})\widetilde{H}_{m+1,m} = U_{m+1}\widetilde{H}_{m+1,m}$$

$$\widetilde{H}_{m+1,m} = \begin{pmatrix} h_{11} & \cdots & \cdots & h_{1m} \\ h_{21} & \ddots & & \vdots \\ 0 & \ddots & \ddots & \vdots \\ & & \ddots & h_{mm} \\ 0 & & 0 & h_{m+1,m} \end{pmatrix}$$

# GMRES: Minimization

This leads to minimization problem

$$\begin{aligned}
\min_{x \in U_m} \|Ax - b\| &= \min_{y} \|AU_m y - b\| \\
&= \min_{y} \left\| U_{m+1} \widetilde{H}_{m+1,m} y - \|b\| u_1 \right\| \\
&= \min_{y} \left\| U_{m+1} (\widetilde{H}_{m+1,m} y - \|b\| e_1) \right\| \\
&= \min_{y} \left\| \widetilde{H}_{m+1,m} y - \|b\| e_1 \right\|
\end{aligned}$$

Because $U_{m+1}$ is part of an orthogonal matrix.

# GMRES: QR

Use Givens matrices to compute a QR-factorization of the upper Hessenberg matrix $\widetilde{H}_{m+1,m}$.

$$G_1 \cdot \begin{pmatrix} * & \cdots & * \\ * & \ddots & \vdots \\ & \ddots & * \\ & & * \end{pmatrix} = \begin{pmatrix} * & \cdots & * \\ 0 & \ddots & \vdots \\ & \ddots & * \\ & & * \end{pmatrix} =$$

$$G_m \cdots G_2 G_1 \cdot \widetilde{H}_{m+1,m} = Q \cdot \widetilde{H}_{m+1,m} = \begin{pmatrix} R_m \\ 0 \end{pmatrix}$$

QR via Givens matrices is a simplified version of QR via Householder matrices.

# GMRES

$$
\begin{aligned}
\min_{x \in K_m} \|Ax - b\| &= \min_y \left\| \widetilde{H}_{m+1,m} y - \|b\| e_1 \right\| \\
&= \min_y \left\| Q^T R y - \|b\| e_1 \right\| = \min_y \|Ry - \|b\| Q e_1\| \\
&= \min_y \left\| \begin{pmatrix} R_m \\ 0 \end{pmatrix} y - \widetilde{b} \right\| = \min_y \left\| \begin{pmatrix} R_m y - \widetilde{b}_m \\ -\widetilde{\beta}_m \end{pmatrix} \right\|
\end{aligned}
$$

Solution:

$$R_m y = \widetilde{b}_m, \quad x_m = U_m y$$

# GMRES Algorithm

- GMRES is a clever implementation of this sequence of least squares problems.
- Computing step by step for increasing $m$
  - next $Au_m$
  - enlarged $H_{m+1,m}$ by Arnoldi orthogonalization (gives new $u_{m+1}$)
  - next Givens matrix $G_m$
  - update triangular solves to get next $y_m$ and $x_m$.

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  - next Givens matrix $G_m$
  - update triangular solves to get next $y_m$ and $x_m$.
- Disadvantage: large Hessenberg matrices!
- Therefore, use restarted GMRES, e.g. GMRES(20).

# GMRES Algorithm: First Step

Start: $b,\ u_1 := \frac{b}{\|b\|}$

$$h_{2,1}u_2 = Au_1 - h_{1,1}u_1, \quad H_{2,1} = \begin{pmatrix} h_{1,1} \\ h_{2,1} \end{pmatrix}, \quad G_1 H_{2,1} = \begin{pmatrix} \nu_{1,1} \\ 0 \end{pmatrix},$$

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$$\begin{aligned} \|Ax - b\| &= \|AU_1 y_1 - b\| = \|H_{2,1} y_1 - \|b\| e_1\| \\ &= \left\| G_1^T \begin{pmatrix} \nu_{1,1} \\ 0 \end{pmatrix} y_1 - \|b\| e_1 \right\| = \left\| \begin{pmatrix} \nu_{1,1} \\ 0 \end{pmatrix} y_1 - \|b\| G_1 e_1 \right\| \end{aligned}$$

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$$y_1 = \frac{(G_1 e_1 \|b\|)_1}{\nu_{1,1}}, \qquad x_1 = u_1 y_1 = U_1 y_1$$

# GMRES Algorithm: Second Step

$$h_{3,2}u_3 = Au_2 - h_{2,2}u_2 - h_{1,2}u_1, \qquad H_{3,2} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \\ 0 & h_{32} \end{pmatrix},$$

$$G_1 H_{3,2} = \begin{pmatrix} \nu_1 & * \\ 0 & * \\ 0 & * \end{pmatrix}, \qquad G_2 G_1 H_{3,2} = \begin{pmatrix} \nu_{1,1} & \nu_{1,2} \\ 0 & \nu_{2,2} \\ 0 & 0 \end{pmatrix}$$

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$$\|Ax - b\| = \|AU_2 y_2 - b\| = \|H_{3,2} y_2 - \|b\| e_1\|$$

$$= \left\| G_1^T G_2^T \begin{pmatrix} \nu_{1,1} & \nu_{1,2} \\ 0 & \nu_{2,2} \\ 0 & 0 \end{pmatrix} y_2 - \|b\| e_1 \right\| = \left\| \begin{pmatrix} \nu_{1,1} & \nu_{1,2} \\ 0 & \nu_{2,2} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_{2,1} \\ y_{2,2} \end{pmatrix} - \|b\| G_2 G_1 e_1 \right\|$$

$$y_{2,2} = \frac{(G_2 G_1 e_1 \|b\|)_2}{\nu_{2,2}}, \qquad y_{2,1} = \frac{(G_2 G_1 e_1 \|b\|)_1 - \nu_{1,2} y_{2,2}}{\nu_{1,1}}$$

$x_2 = U_2 y_2 = u_1 y_{2,1} + u_2 y_{2,2}$ and so forth...

# GMRES Error ($A$ diagonalisable)

$$
\begin{aligned}
\|r_m\| &= \|Ax_m - b\| = \min_{x \in U_m} \|Ax - b\| \\
&= \min_{\alpha_1,\ldots,\alpha_m} \left\| A\left(\sum_{j=0}^{m-1} \alpha_j A^j b\right) - b \right\| = \min_{\mathcal{P}^{(m-1)}} \left\| A\mathcal{P}^{(m-1)}(A)b - b \right\| \\
&= \min_{\mathcal{Q}^{(m)}(0)=1} \left\| \mathcal{Q}^{(m)}(A)b \right\| = \min_{\mathcal{Q}^{(m)}(0)=1} \left\| V\mathcal{Q}^{(m)}(\Lambda)V^{-1}b \right\| \\
&= \min_{\mathcal{Q}^{(m)}(0)=1} \left\| V \operatorname{diag}(\mathcal{Q}^{(m)}(\lambda_j))V^{-1}b \right\| \leq \\
&\leq \kappa_2(V) \cdot \min_{\mathcal{Q}^{(m)}(0)=1} \left[ \max_{j=1,\ldots,n} \left| \mathcal{Q}^{(m)}(\lambda_j) \right| \right] \|r_0\|
\end{aligned}
$$

# Iterative Methods: Survey

- Basic iterative methods (not considering multigrid!)
- SPD $A$: PCG (preconditioned conjugate gradient method)
- symmetric indefinite $A$: MINRES, SYMMLQ, (PCG on normal equations)
- general $A$:

  GMRES (optimal like CG, but expensive)

  BiCG, BiCGSTAB, CGS (not optimal, but cheap, instable?)

  QMR (quasi optimal, cheap)

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- Basic iterative methods (not considering multigrid!)
- SPD *A*: PCG (preconditioned conjugate gradient method)
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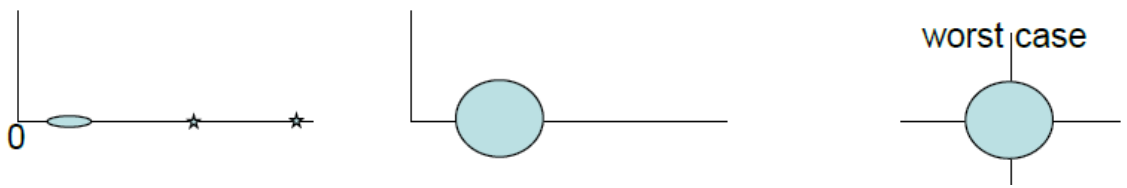
- general *A*:
  - GMRES (optimal like CG, but expensive)
  - BiCG, BiCGSTAB, CGS (not optimal, but cheap, instable?)
  - QMR (quasi optimal, cheap)
- Essential for convergence is position of eigenvalues (singular values)
- Fast convergence for well conditioned problems or matrices with clustered spectrum



# 5.4. Preconditioning

- Direct solvers: sequential, loosing sparsity
- Iterative solvers: easy parallel and sparse, but possibly slowly convergent

# 5.5. Preconditioning

- Direct solvers: sequential, loosing sparsity
- Iterative solvers: easy parallel and sparse, but possibly slowly convergent
- Combination of both methods (2 variants):
  1. Include preconditioner $M \approx A$ in the form $M^{-1}Ax = M^{-1}b$, such that
     - $M$ is easy to deal with in parallel (reduced approximate direct solver)
     - spectrum of $M^{-1}A$ is much better clustered
  2. Or include preconditioner $M \approx A^{-1}$ in the form $MAx = Mb$, such that
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- General both-sided preconditioning:

$$Ax = b \Leftrightarrow MA(Ky) = Mb \text{ and } Ky = x$$

# Overview of Following Preconditioners

- Stationary preconditioners
- ILU preconditioner

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- Stationary preconditioners
- ILU preconditioner
- Polynomial preconditioners
- Sparse approximate inverse preconditioners:
  - SPAI for the general nonsymmetric case
  - FSPAI for the SPD case
  - MSPAI using SPAI with probing

# 5.6.1. Stationary Preconditioners

Consider preconditioner $M \approx A$ in the form $M^{-1}Ax = M^{-1}b$.

- Stationary iteration to splitting $A = M - N$. Convergence depends on
$$\|I - M^{-1}A\| < 1$$
- That is exactly a condition for a good preconditioner: spectrum clustered around 1, $M^{-1}A \approx I$

# 5.6.2. Stationary Preconditioners

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$$\|I - M^{-1}A\| < 1$$
- That is exactly a condition for a good preconditioner: spectrum clustered around 1, $M^{-1}A \approx I$
- If splitting leads to fast convergence, than $M$ is also a good preconditioner.
- In this sense, PCG with stationary preconditioner $M$ can be seen as an accelaration of the stationary method with splitting $M - N$.

# Stationary Preconditioners (cont.)

- Jacobi splitting with $D = \text{diag}(A)$ gives Jacobi preconditioner $M := D$.
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$$x^{(k,\text{new})} := (1 - \omega)x^{(k-1)} + \omega x^{(k)}$$

  As convex combination of old and new iterate (Jacobi or GS)

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- Symmetrization: first iteration with preconditioner $M$, second iteration with $M^T$.

$$M_{\text{new}} := M + M^T - M^T A M$$

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- Symmetrization: first iteration with preconditioner $M$, second iteration with $M^T$.

$$M_{\text{new}} := M + M^T - M^T A M$$

- Special case: damped GS $\rightarrow$ SSOR:

$$M_{\text{new}} = \frac{1}{2-\omega}\left(\frac{1}{\omega}D - L\right)\left(\frac{1}{\omega}D\right)^{-1}\left(\frac{1}{\omega}D - L\right)^T$$

# 5.6.3. ILU Preconditioner, Sequentially

# ILU Preconditioner, Sequentially

- Apply Gaussian elimination algorithm, but only on allowed pattern $\Rightarrow$ incomplete LU factorization called ILU.
- Reduce in the `for`-loops the indices to the indices with
  - allowed pattern, e.g. ILU(0) for pattern of $A$
  - values that are not too small, ILUT for ILU with treshold

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$$A = LU + R, \quad \text{preconditioner} \quad M = LU$$

with all ignored fill-in entries collected in $R$.

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  with all ignored fill-in entries collected in $R$.
- MILU (modified ILU): collect all ignored fill-in entries on the related main diagonal elements $\rightarrow$ maintains the row sum or the action on $(1, 1, \ldots, 1)^T$.

# 5.6.4. Parallel ILU

Consider iterative solution of the system $A = LU$ on given pattern $\mathcal{S}$. So $L$ and $U$ are sparse with pattern $\mathcal{S}$, and the equations have to be satisfied only on the pattern $\mathcal{S}$:

$$A_{i,j} = \sum_{k,(i,k)\in\mathcal{S},(k,j)\in\mathcal{S}} L_{i,k}U_{k,j} \quad \text{for} \quad (i,j) \in \mathcal{S}$$

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Use $A = LU$ as fixed point iteration in the form:

- freeze $L$, compute new $U$
- freeze $U$, compute new $L$
- repeat until convergence

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Use $A = LU$ as fixed point iteration in the form:

- freeze $L$, compute new $U$
- freeze $U$, compute new $L$
- repeat until convergence

$$l_{i,j} = \frac{1}{u_{j,j}}(a_{i,j} - \sum_{k=1}^{j-1} l_{i,k}u_{k,j}) \tag{1}$$

$$u_{i,j} = \frac{1}{l_{i,i}}(a_{i,j} - \sum_{k=1}^{i-1} l_{i,k}u_{k,j}) \; . \tag{2}$$

# 5.6.7. Iterative ILU Algorithm

Set unknowns $l_{i,j}$ and $u_{i,j}$ to initial values

FOR sweep = 1,2,... until convergence

  WHILE $(i,j) \in S$

    IF $i > j$

      $l_{i,j} = \frac{1}{u_{j,j}}(a_{i,j} - \sum_{k=1}^{j-1} l_{i,k} u_{k,j})$

    ELSE

      $u_{i,j} = a_{i,j} - \sum_{k=1}^{i-1} l_{i,k} u_{k,j}$

    END

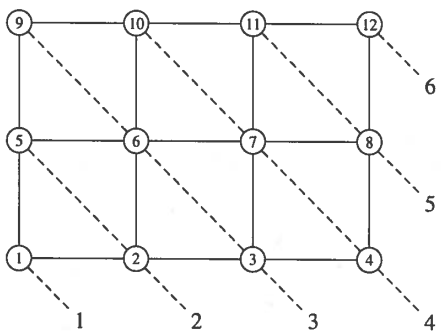
  END

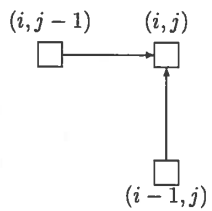
END

# 5.6.8. Direct Triangular Solves

Remaining problem: Solve $Lx = b$ in parallel!

- There exist parallel direct solvers based on graph coloring, but with restricted parallelism.
- Using data dependency graph:




Stencil

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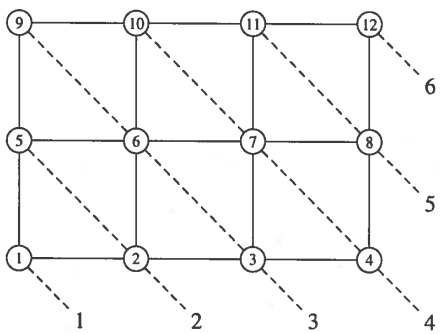


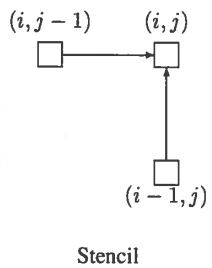


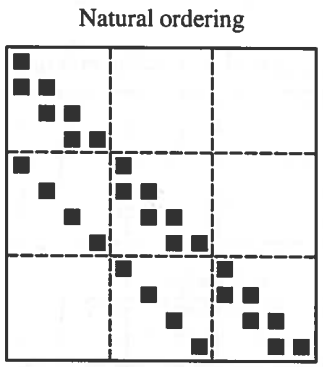


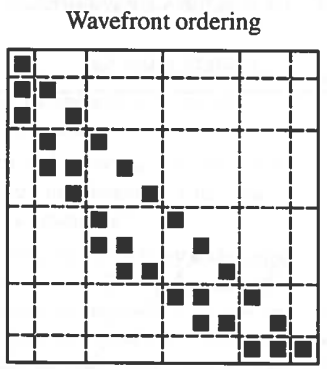


- Collect indices that can be directly derived: LEVEL 1
- From data dependency graph collect indices depending only on the first level: LEVEL 2
- and so on.

Unknowns in the same level can be updated in parallel. Compare colored GS, Cuthill-McKee and multifrontal solvers!

# 5.6.10. Iterative Triangular Solves

Resort: Jacobi iteration for $b = Lx = (D + L_0)x$ resulting in the iteration

$$Dx^{k+1} = b - L_0 x^k \ , k = 0, 1, 2, ...$$

# 5.6.11. Iterative Triangular Solves

Resort: Jacobi iteration for $b = Lx = (D + L_0)x$ resulting in the iteration

$$Dx^{k+1} = b - L_0 x^k \ , k = 0, 1, 2, ...$$

Nice feature: Iteration matrix $L_0$ has zero eigenvalues. Therefore

convergence guaranteed via special norm:

$$\|e_k\| \leq \|L_0\|^k \|e_0\|$$

and there exists a norm with $\|L_0\| < 1$. But often slow convergence!

Improvement: Block-Jacobi.

Search for iterative fast converging and fully parallel methods! Later on more!

# Overview Explicit Preconditioners

- ILU and stationary methods use approximations on $A$ itself.
- The resulting preconditioners are given by triangular matrices $L$, that have to be solved in each iteration step: $L^{-1}x^{(k)}$!
- Jacobi easy to parallelize, but slow convergence.

# Overview Explicit Preconditioners

- ILU and stationary methods use approximations on $A$ itself.
- The resulting preconditioners are given by triangular matrices $L$, that have to be solved in each iteration step: $L^{-1}x^{(k)}$!
- Jacobi easy to parallelize, but slow convergence.
- Question: How to derive preconditioners that lead to fast convergence and are easy to parallelize?
- Until now considered variant 1.; In the following variant 2.:

  Find approximations on $M \approx A^{-1}$. Then the solution of the linear system given by the preconditioner, is only $Mx^{(k)}$, a matrix vector product!

# Parallel Preconditioning

- Find preconditioner $M$, that satisfies three conditions:
  - **(i)** The computation of $M$ is fast in parallel
  - **(ii)** The application $Mx$ in each iteration step is easy in parallel
  - **(iii)** The spectrum $AM$ or $MA$ is clustered $\rightarrow$ fast convergence

# Parallel Preconditioning

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- Examples:

  For GS is (i) ok, but not (ii)

  For Jacobi (i) and (ii) ok, but not (iii)

  For ILU (iii) ok, (i) also iteratively, but not (ii)

- Note that preconditioners also have to be well defined! Zero on diagonals?

# 5.6.12. Polynomial Preconditioners

- Characteristic polynomial for $A$:

$$0 = q(A) = \gamma_n A^n + \gamma_{n-1} A^{n-1} + \ldots + \gamma_1 A + \gamma_0 I$$

  Gives polynomial representation for $A^{-1}$ ($\gamma_0 \neq 0$):

$$A^{-1} = \frac{1}{\gamma_0} \left( -\gamma_n A^{n-1} - \gamma_{n-1} A^{n-2} - \ldots - \gamma_1 I \right) = p(A)$$

- Therefore, it makes sense to approximate $A^{-1}$ by a polynomial.

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- Therefore, it makes sense to approximate $A^{-1}$ by a polynomial.
- Better approximation by finding region $S \in \mathbb{R}$ or $\mathbb{C}$ that contains nearly all eigenvalues, and then find polynomial $p$ that is near the inverse in $S$:

$$\min_{p_n} \|P(A)A - I\|, \quad \min_{p_n(x)} \left( \max_{\lambda \text{ eigenvalue}} |p(\lambda)\lambda - 1| \right)$$

- Solution: Normalized Chebyshev polynomials.

# 5.6.14. Polynomial Preconditioners

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$$A^{-1} = \frac{1}{\gamma_0}\left(-\gamma_n A^{n-1} - \gamma_{n-1} A^{n-2} - \ldots - \gamma_1 I\right) = p(A)$$

- Therefore, it makes sense to approximate $A^{-1}$ by a polynomial.
- Better approximation by finding region $S \in \mathbb{R}$ or $\mathbb{C}$ that contains nearly all eigenvalues, and then find polynomial $p$ that is near the inverse in $S$:

$$\min_{p_n} \|P(A)A - I\|, \quad \min_{p_n(x)} \left( \max_{\lambda \text{ eigenvalue}} |p(\lambda)\lambda - 1| \right)$$

- Solution: Normalized Chebyshev polynomials.

\+ Advant. of pol. prec.: better in parallel (mtx-vec product, BLAS 2)

\- Disadvantage: non-optimal approximation in Krylov subspace

# 5.6.15. Sparse Approximate Inverses

- Other approach for approximating $A^{-1}$ by norm minimization

$$\min_{M \in \mathcal{P}} \|AM - I\| \qquad \text{over some sparsity pattern } \mathcal{P}.$$

# 5.6.16. Sparse Approximate Inverses

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  - analytic (to allow the explicit solution of this problem)
  - easy to compute (in parallel)

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  - easy to compute (in parallel)

- Optimal norm is Frobenius norm:

$$\|A\|_F^2 := \sum_{i,j=1}^{n} a_{i,j}^2 = \sum_{j=1}^{n} \|A_{\bullet,j}\|^2 = \text{trace}(A^T A)$$

# SPAI in Parallel

- First, we choose pattern $\mathcal{P}$ in a static way a priori, e.g. as the pattern of $A$

$$\min_{M \in \mathcal{P}} \|AM - I\|_F^2 = \min_{M \in \mathcal{P}} \sum_{k=1}^{n} \|(AM - I)e_k\|_2^2 = \sum_{k=1}^{n} \min_{M_k \in \mathcal{P}_k} \|AM_k - e_k\|_2^2$$

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- Hence, to minimize the Frobenius norm, we have to solve $n$ least squares problems in the sparse columns of $M$!
- This can be done fully in parallel!
- But costs for least squares problems?

# SPAI and Least Squares

$$\min_{M_k \in \mathcal{P}_k} \|AM_k - e_k\|_2^2 = \min_{M_k \in \mathcal{P}_k} \left\| A \begin{pmatrix} 0 \\ * \\ 0 \\ * \\ 0 \\ 0 \end{pmatrix} - e_k \right\|_2^2 = \min_{M_k \in \mathcal{P}_k} \|A(:, \mathcal{J}_k) M_k(\mathcal{J}_k) - e_k\|_2^2$$

# SPAI and Least Squares

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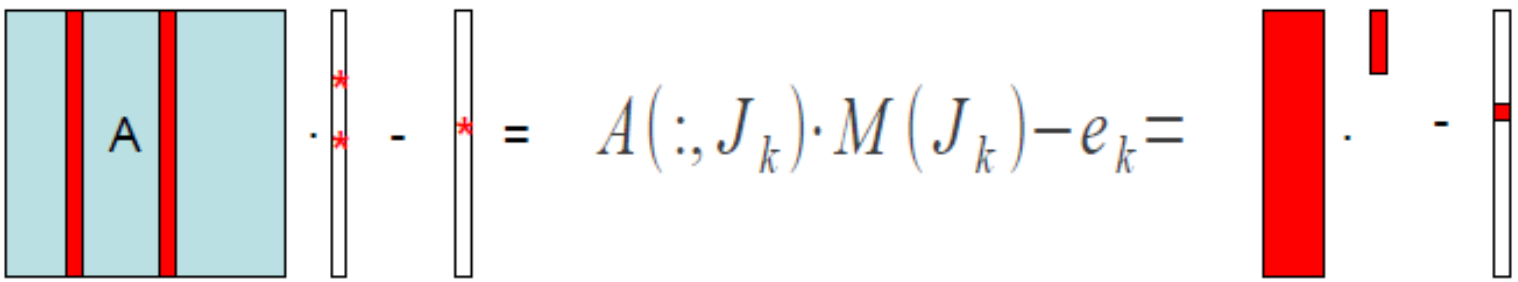
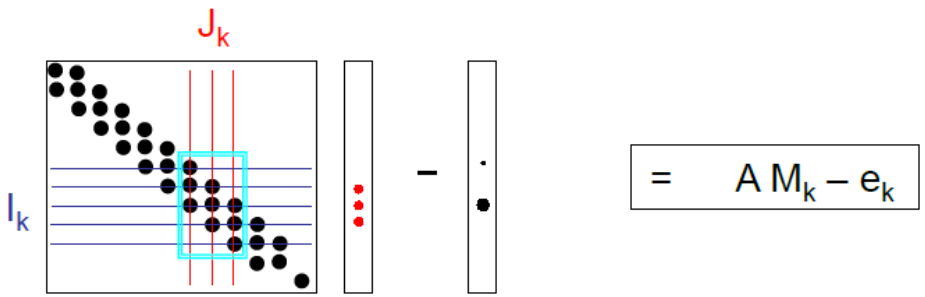
Denote by $\mathcal{J}_k$ the set of allowed indices in the $k$th column of $M$.



# SPAI and Sparse Least Squares

- $A(:, \mathcal{J}_k)$ is a sparse rectangular matrix. $\mathcal{I}_k$ is index set called *shadow* of $\mathcal{J}_k$.
- Delete superfluous zeros in least squares problem:
  - For index set $\mathcal{J}_k$ in $M_k$ keep only $A(:, \mathcal{J}_k)$
  - In $A(:, \mathcal{J}_k)$ keep only nonzero rows $A(\mathcal{I}_k, \mathcal{J}_k)$



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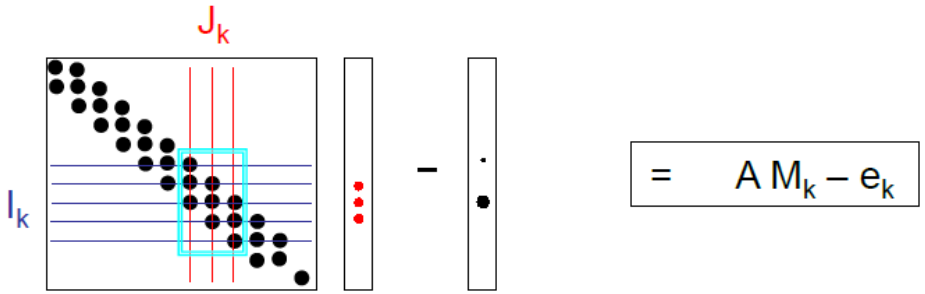


- Hence, reduction of sparse LS to $A(\mathcal{I}_k, \mathcal{J}_k)$:

$$\min_{M_k \in \mathcal{P}_k} \|A(\mathcal{I}_k, \mathcal{J}_k)M(\mathcal{J}_k) - e(\mathcal{I}_k)\|_2^2 = \min_{M_k \in \mathcal{P}_k} \left\|\widetilde{A}\widetilde{M}_k - \widetilde{e}_k\right\|_2^2$$

- Solve small LS problem by Householder *QR* for

$$A(\mathcal{I}_k, \mathcal{J}_k) \to \widetilde{M}_k \to M_k$$

# Sparsity Pattern: Static A Priori Choice

- $A^{-1}$ will be no more sparse!
- As a priori choice of a good approximate sparsity pattern for $M$ we can choose the pattern of
  - $A^k$ or $(A^T)^k$
  - $(A^T A)^k A^T$ for some $k = 1, 2$
  - $A_\epsilon$ with sparsified $A$
  - a combination of above
- $A_\epsilon$ by sparsification of $A$: delete all entries with $|A_{ij}| < \epsilon$

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- Start with thin approximate pattern $\mathcal{J}_k$ for $M_k$
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$$\begin{aligned}\min_{M_k \in \mathcal{P}_k} \left\| A(M_k + \lambda e_j) - e_k \right\|_2^2 &= \min_{M_k \in \mathcal{P}_k} \left\| (AM_k - e_k) + \lambda A e_j \right\|_2^2 = \\ &= \min \left( \|r_k\|_2^2 + 2\lambda (r_k^T A_j) + \lambda^2 \|A_j\|_2^2 \right)\end{aligned}$$

For each possible index candidate $j$ compute

$$\lambda_j = -\frac{r_k^T A_j}{\|A_j\|_2^2}$$

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Choose index $j$ with $r_k^T A_j \neq 0$ and $j = \arg\min(\lambda_j)$ since

$$\min = \|r_k\|_2^2 - \frac{(r_k^T A_j)^2}{\|A_j\|_2^2}.$$

# Error Estimates

- Assume that for all columns holds

$$\|r_k\| = \|AM_k - e_k\| < \epsilon$$

- Then

$$\begin{aligned} \|AM - I\|_F &\leq \sqrt{n}\epsilon \\ \|AM - I\|_2 &\leq \sqrt{n}\epsilon \\ \|AM - I\|_1 &\leq \sqrt{p}\epsilon \end{aligned}$$

with $p$ being the maximum number of nonzero entries in $r_k$, $k = 1, \ldots, n$.