# 3.3. *QR*-Decomposition with Householder Matrices

## 3.3.1. QR-decomposition

- Gaussian elimination $\rightarrow$ *LU*-decomposition: sometimes numerically not stable, over/underdetermined systems
- Improvement:

  *QR*-decomposition $A = QR$ with $Q$ orthogonal, $R$ triangular,
  Solve linear system Ax=b numerically stable via

  $$b = Ax = QRx \Leftrightarrow Rx = Q^T b$$

  by cheap matrix-vector multiplication and triangular solve.

# Overdetermined Systems

- $Ax = b$ with

  $A$ being $m \times n$ matrix, $n \ll m$

  $x$ vector of length $n$

  $b$ vector of length $m$

- Best **approximate** solution by solving minimization

$$\min_x \|Ax - b\|_2^2 = \min_x (x^T A^T Ax - 2x^T A^T b + b^T b)$$

- Gradient equal zero $\Leftrightarrow A^T Ax = A^T b$ (normal equations)

- Solution by considering linear system $A^T A$, but condition number worse:

$$\text{cond}(A^T A) = \text{cond}(A)^2$$

# Advantage of QR-Decomposition

$$A = QR, \quad R = \begin{pmatrix} R_1 \\ 0 \end{pmatrix}, \quad \text{cond}(R_1) = \text{cond}(A), \quad \hat{b} = Q^T b = \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \end{pmatrix}$$

$$A^T A x = A^T b \Leftrightarrow (QR)^T (QR) x = (QR)^T b \Leftrightarrow$$

$$R^T R x = R^T (Q^T b) \Leftrightarrow (R_1^T \ 0) \begin{pmatrix} R_1 \\ 0 \end{pmatrix} x = (R_1^T \ 0) \hat{b} \Leftrightarrow$$

$$R_1^T R_1 x = (R_1^T \ 0) \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \end{pmatrix} \Leftrightarrow R_1^T R_1 x = R_1^T \hat{b}_1 \Leftrightarrow R_1 x = \hat{b}_1$$

- Instead of solving the normal equations we only have to consider the triangular system in $R_1$ .
- Cheap and better condition number.

# 3.3.2. Householder Method

- Define special orthogonal and simple matrices $H$ called Householder matrices (compare Givens):

$$u \in \mathbb{R}^n, \ \|u\|_2 = 1 : \quad H = I - 2uu^T$$

- $H$ as rank-1 perturbation of the identity is symmetric, idempotent and orthogonal:

$$H^T = I - 2uu^T = H$$

$$H^T H = H^2 = (I-2uu^T)(I-2uu^T) = I-2uu^T-2uu^T+4u\underbrace{u^T u}_{=1}u^T = I$$

- For complex problems:
orthogonal $\rightarrow$ unitary, symmetric $\rightarrow$ hermitian

# Householder Method (cont.)

- Use $H_1$ with appropriate vector $u_1$ to eliminate first column of $A$

$$H_1 A = (I - 2u_1 u_1^T)(a_1 \ \cdots \ a_m) = (a_1 - 2(u_1^T a_1)u_1 \ \cdots \ *) = \begin{pmatrix} \alpha & * \\ 0 & * \\ \vdots & \vdots \\ 0 & * \end{pmatrix}$$

- To satisfy this equation we have to find a vector $u_1$ of length 1 with

$$a_1 - 2(u_1^T a_1)u_1 = \alpha e_1$$

- Because $H_1$ is orthogonal it holds:

$$\|H_1 a_1\|_2 = \|a_1\|_2 = \|\alpha e_1\|_2 = |\alpha| \Rightarrow \alpha = \pm\|a_1\|_2, \text{ e.g. } \alpha = \|a_1\|_2$$

$$u_1 = \frac{a_1 - \|a_1\|_2 e_1}{2(u_1^T a_1)} = \frac{a_1 - \|a_1\|_2 e_1}{\|a_1 - \|a_1\|_2 e_1\|_2}$$

# Householder Method (cont. 2)

- Repeat for all columns of $A$

$$H_1 A = H_1 A_1 = (I - 2u_1 u_1^T)A = \left(\begin{array}{c|ccc} \|a_1\|_2 & * & \cdots & * \\ \hline 0 & & & \\ \vdots & & A_2 & \\ 0 & & & \end{array}\right)$$

- Apply the same procedure on $A_2$, $(n-1) \times (m-1)$ matrix.

$$\tilde{H}_2 A_2 = (I - 2\tilde{u}_2 \tilde{u}_2^T)A_2 = \left(\begin{array}{c|ccc} \alpha_2 & * & \cdots & * \\ \hline 0 & & & \\ \vdots & & A_3 & \\ 0 & & & \end{array}\right)$$

- Extend

$$u_2 := \begin{pmatrix} 0 \\ \tilde{u}_2 \end{pmatrix}, \qquad H_2 := I - 2u_2 u_2^T = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \tilde{H}_2 & \\ 0 & & & \end{pmatrix}$$

# Householder Method (cont. 3)

- For column $1, 2, \ldots, m$ this gives Householder matrices $H_1, \ldots, H_m$ with

$$\underbrace{H_m \cdots H_2 H_1}_{= Q^T} \cdot A = H_m \cdots H_3 \cdot \left(\begin{array}{cc|ccc} \alpha_1 & * & * & \cdots & * \\ 0 & \alpha_2 & * & \cdots & * \\ \hline 0 & 0 & & & \\ \vdots & \vdots & & A_3 & \\ 0 & 0 & & & \end{array}\right) = \begin{pmatrix} R_1 \\ 0 \end{pmatrix} =: R$$

- Hence:

$$A = QR, \qquad Q := (H_m \cdots H_2 H_1)^T = H_1 H_2 \cdots H_m$$

- Remark: for $m = n$: $H_1, \ldots, H_{m-1}$ is enough, because last column is scalar.

# 3.3.3. Householder Method in Parallel - Blockwise

Idea: work again blockwise.

- In a first step compute $u_1$ and the application of $H_1$ on the first $k$ columns of $A$. Do not compute $H_1 A$ fully!
- Then compute $u_2, \ldots, u_k$ and the application of $H_1 \ldots H_k$ on the first columns of $A$.

$$H_k \cdots H_1 (A_1 \quad A_2) = (H_k \cdots H_1 A_1 \quad (H_k \cdots H_1) A_2) = (A_1^{(k)} \quad VA_2)$$

- Still to compute: $VA_2$.
- How can we take advantage of parallelism in this computation? $\rightarrow$ represent $V$ in special form that allows fast and parallel evaluation of $VA_2$.

# Property of Householder matrices

Theorem 3: For Householder matrices $H_k, \ldots, H_i$ it holds

$$H_k \cdots H_i = (I - 2u_k u_k^T) \cdots (I - 2u_i u_i^T) = I - \underbrace{(u_k \quad \cdots \quad u_i)}_{=: Y} T_i \begin{pmatrix} u_k^T \\ \vdots \\ u_i^T \end{pmatrix}$$

with $T_i$ being upper triangular.

**Proof by induction**:

Representation obviously fulfilled for one Householder mtx $i = k$.

Assume, representation holds for $H_k, \ldots, H_i$. Then ... (next slide)

# Property of Householder matrices (cont.)

$$\left[(I - 2u_k u_k^T) \cdots (I - 2u_i u_i^T)\right](I - 2u_{i-1} u_{i-1}^T) =$$

$$= \left[I - (u_k \quad \cdots \quad u_i) T_i \begin{pmatrix} u_k^T \\ \vdots \\ u_i^T \end{pmatrix}\right] \cdot (I - 2u_{i-1} u_{i-1}^T) =$$

$$= I - 2u_{i-1} u_{i-1}^T - (u_k \quad \cdots \quad u_i) T_i \begin{pmatrix} u_k^T \\ \vdots \\ u_i^T \end{pmatrix} + 2(u_k \quad \cdots \quad u_i) \underbrace{T_i \begin{pmatrix} u_k^T u_{i-1} \\ \vdots \\ u_i^T u_{i-1} \end{pmatrix}}_{=: y} u_{i-1}^T =$$

$$= I - (u_k \quad \cdots \quad u_i \quad u_{i-1}) \cdot \begin{pmatrix} T_i & -2y \\ 0 & 2 \end{pmatrix} \cdot \begin{pmatrix} u_k^T \\ \vdots \\ u_i^T \\ u_{i-1}^T \end{pmatrix}$$

# Algorithm for parallel Householder

Computation of $H_k \cdots H_i A = V_{ki} A = (I - YTY^T)A$ in the form

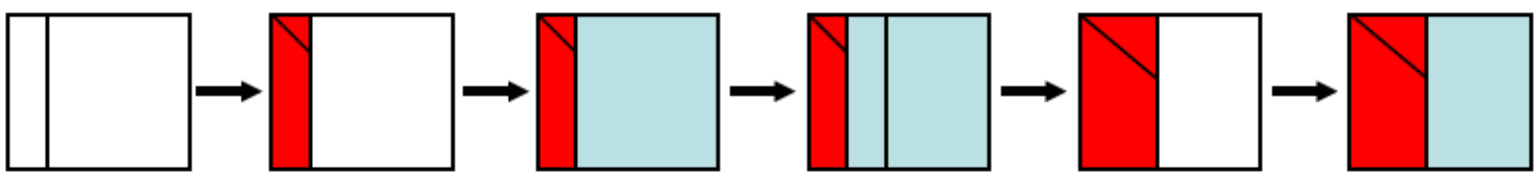
$$V_{ki} A = V_{ki}(A_1 \quad A_2) = (* \quad V_{ki} A_2)$$

and

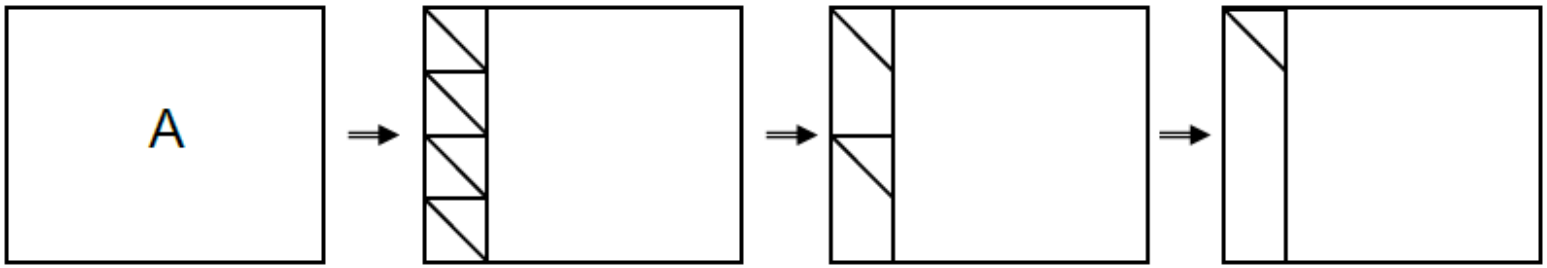
$$V_{ki} A_2 = (I - YTY^T)A_2 = A_2 - Y[T(Y^T A_2)]$$

Algorithm:

- Compute $u_1$ and $H_1 A_1$; $u_2$ and $H_2 A_1$; ...; $u_k$ and $H_k A_1$ (sequential)
- Compute $Y$ and $VA_2$ (parallel)
- Repeat with indices $k+1, \ldots, 2k$; $2k+1, \ldots, 3k$; ...



# Communication Avoiding QR




- Four independent QR-factorisations

↓

- Two independent reduced QR-factorisations

↓

- One reduced QR-factorisation

# Tall Skinny QR

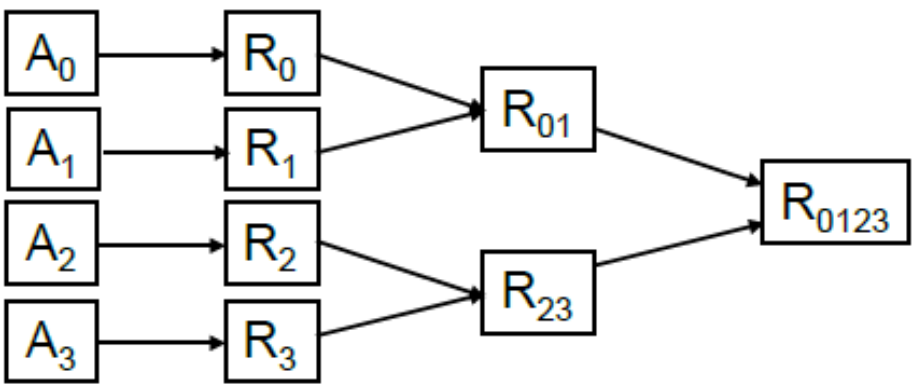
$$A = \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} Q_0 R_0 \\ Q_1 R_1 \\ Q_2 R_2 \\ Q_3 R_3 \end{pmatrix} = \begin{pmatrix} Q_0 & & & \\ & Q_1 & & \\ & & Q_2 & \\ & & & Q_3 \end{pmatrix} \begin{pmatrix} R_0 \\ R_1 \\ R_2 \\ R_3 \end{pmatrix}$$

$$\begin{pmatrix} R_0 \\ R_1 \\ R_2 \\ R_3 \end{pmatrix} = \left( \begin{pmatrix} R_0 \\ R_1 \end{pmatrix} \begin{pmatrix} R_2 \\ R_3 \end{pmatrix} \right) = \begin{pmatrix} Q_{01} R_{01} \\ Q_{23} R_{23} \end{pmatrix} = \begin{pmatrix} Q_{01} & \\ & Q_{23} \end{pmatrix} \begin{pmatrix} R_{01} \\ R_{23} \end{pmatrix}$$

$$\begin{pmatrix} R_{01} \\ R_{23} \end{pmatrix} = Q_{0123} R_{0123}$$

# Tall Skinny QR (cont.)

$$A = \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{pmatrix} = \left\{ \begin{pmatrix} Q_0 & & & \\ & Q_1 & & \\ & & Q_2 & \\ & & & Q_3 \end{pmatrix} \cdot \begin{pmatrix} Q_{01} & \\ & Q_{23} \end{pmatrix} \cdot Q_{0123} \right\} \cdot R_{0123}$$




Advantage:
Messages in $\mathcal{O}(\log(P))$ compared to $\mathcal{O}(2n\log(P))$ for ScaLAPACK.

# Cholesky QR Decomp. for Tall Skinny A

$$A^T A = L^T L$$

$$Q := L^{-T} A^T$$

$$QQ^T = L^{-T} A^T A L^{-1} = I$$

Advantage:
$A^T A$ fully parallel and needs only small Cholesky decomposition L.

Disadvantage:
Numerical stability.

Compromise:
Use Cholesky-QR only for well-conditioned A.

# Parallel Numerics, WT 2013/2014

## *4 Sparse Matrices*

# Contents

# 4.1. General Properties of Sparse Matrices

- Full $n \times n$-matrix: storage $\mathcal{O}(n^2)$, solution $\mathcal{O}(n^3) \rightarrow$ too costly for most applications, esp. for fine discretization (large $n$)
- Formulate given problem in clever way that leads to a linear system that is sparse: $\mathcal{O}(n)$, solution $\mathcal{O}(n)$?
  - (that is structured: storage $\mathcal{O}(n)$, solution $O(n\log(n))$, e.g., FFT)
  - (that is dense, but reduced from, e.g., 3D to 2D)
  - (based on sparse grids)
  - (based on tensor approximations)
- Examples:
  - tridiagonal matrix
  - banded matrix
  - block band matrix

# Sparse Matrix Example

$$\begin{pmatrix} 1 & 0 & 0 & 2 & 0 \\ 3 & 4 & 0 & 5 & 0 \\ 6 & 0 & 7 & 8 & 9 \\ 0 & 0 & 10 & 11 & 0 \\ 0 & 0 & 0 & 0 & 12 \end{pmatrix}$$

Additionally we need to store:

- the size of the matrix $n = 5$
- the number of nonzero entries $\text{nnz} = 12$

# 4.1.1. Storage in Coordinate Form

| values | AA | 12 | 9 | 7 | 5 | 1 | 2 | 11 | 3 | 6 | 4 | 8 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| row | JR | 5 | 3 | 3 | 2 | 1 | 1 | 4 | 2 | 3 | 2 | 3 | 4 |
| column | JC | 5 | 5 | 3 | 4 | 1 | 4 | 4 | 1 | 1 | 2 | 4 | 3 |

To store:

- $n$
- nnz
- $2 \cdot$ nnz integer for row and column indices in JR and JC
- nnz float in AA

No sorting included. Redundant information.

# Storage in Coordinate Form (cont.)

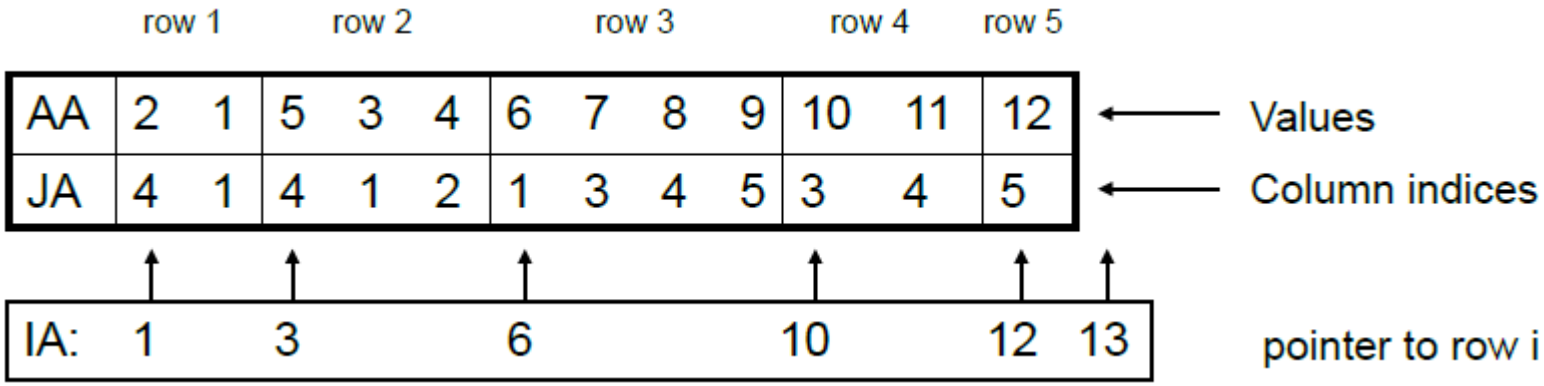
| values | AA | 12 | 9 | 7 | 5 | 1 | 2 | 11 | 3 | 6 | 4 | 8 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| row | JR | 5 | 3 | 3 | 2 | 1 | 1 | 4 | 2 | 3 | 2 | 3 | 4 |
| column | JC | 5 | 5 | 3 | 4 | 1 | 4 | 4 | 1 | 1 | 2 | 4 | 3 |

Pseudocode for computing $c = A \cdot b$:

$c = 0;$
`for` $j = 1 \ : \ \text{nnz}(A)$
$\quad c_{JR(j)} = c_{JR(j)} + \underbrace{AA(j)}_{A_{JR(j),JC(j)}} * b_{JC(j)};$
`end`

- Disadvantage: Indirect addressing (indexing) in vector $c$ and $b \rightarrow$ jumps in memory
- Advantage: No difference between columns and rows ($A$ and $A^T$), simple.

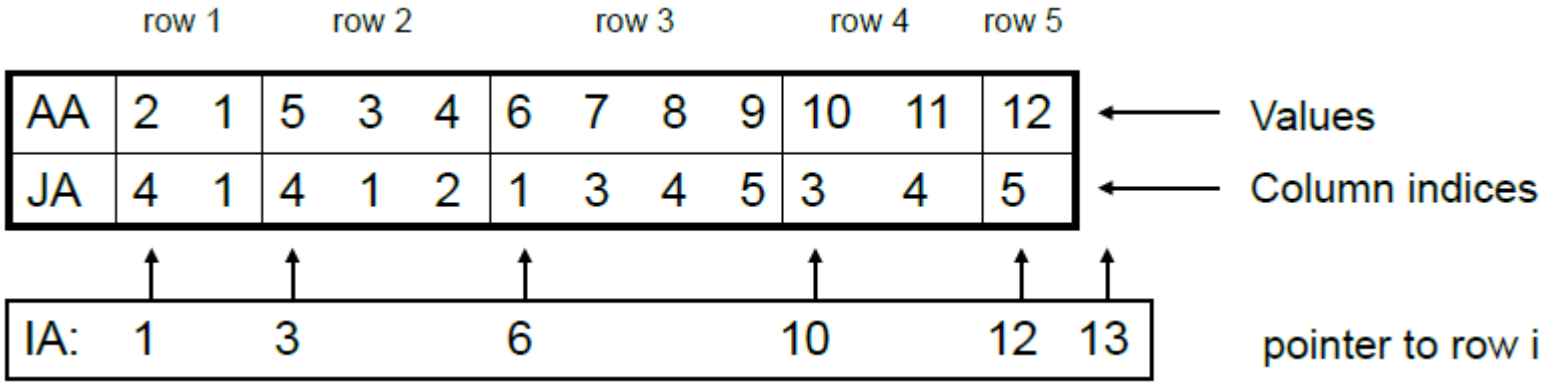
# 4.1.2. Compressed Sparse Row Format: CSR




Storage:

- $n$ and nnz
- $n + \text{nnz} + 1$ integer
- nnz float

# Compressed Sparse Row: CSR (cont.)

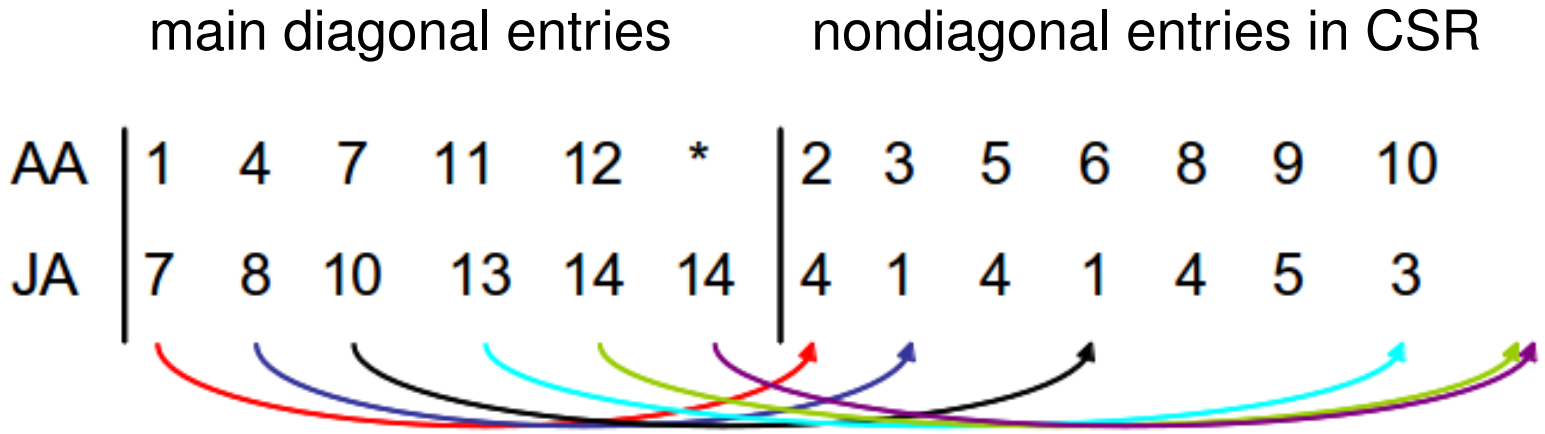



Pseudocode for computing $c = A \cdot b$:

```
c = 0;
for i = 1 : n
   for j = IA(i) : IA(i+1) - 1
      c_i = c_i + AA(j) * b_JA(j);
   end
end
```

- Indirect addressing only in $b$.
- Columnwise $\rightarrow$ compressed sparse column format.

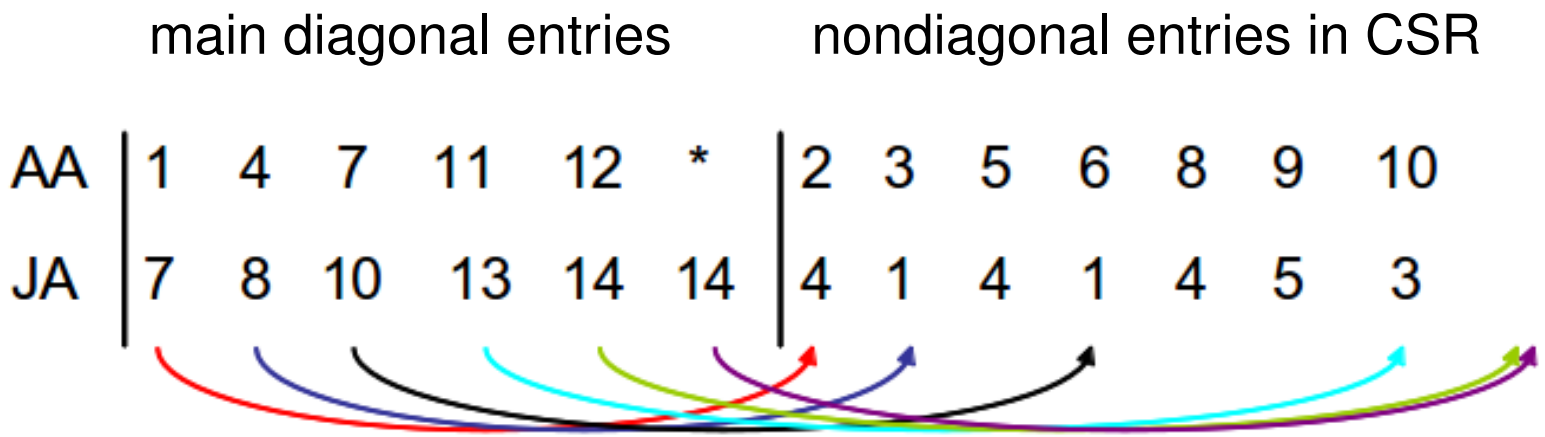
# 4.1.3. CSR with Extracted Main Diagonal




Storage:

- $n$ and nnz
- nnz $+1$ integer
- nnz $+1$ float

# CSR with Extracted Main Diagonal (cont.)




Pseudocode for computing $c = A \cdot b$:

```
c = 0;
for i = 1 : n
   c_i = AA_i * b_i;
   for j = JA(i) : JA(i+1) - 1
      c_i = c_i + AA_j * b_JA(j);
   end
end
```

# 4.1.4. Diagonalwise Storage

$$\begin{pmatrix} 1 & 0 & 2 & 0 & 0 \\ 3 & 4 & 0 & 5 & 0 \\ 0 & 6 & 7 & 0 & 8 \\ 0 & 0 & 9 & 10 & 0 \\ 0 & 0 & 0 & 11 & 12 \end{pmatrix}$$

New matrix $A$!
Different matrix to slides before!

Diagonal numbers: $-1 \;\; 0 \;\; 2$

Values in:

$$\text{DIAG} = \begin{pmatrix} * & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \\ 9 & 10 & * \\ 11 & 12 & * \end{pmatrix}, \quad \text{IOFF} = (-1 \;\; 0 \;\; 2)$$

Storage: $n$, $nd :=$ #diagonals, $nd$ integers for IOFF and $n \cdot nd$ float

# 4.1.5. Rectangular Storage Scheme by Pressing from the Right

$$\left(\begin{array}{ccccc|} 1 & 0 & 2 & 0 & 0 \\ 3 & 4 & 0 & 5 & 0 \\ 0 & 6 & 7 & 0 & 8 \\ 0 & 0 & 9 & 10 & 0 \\ 0 & 0 & 0 & 11 & 12 \end{array}\right) \leftarrow \text{pressing from right}$$

gives

$$\text{COEF} = \begin{pmatrix} 1 & 2 & 0 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \\ 9 & 10 & 0 \\ 11 & 12 & 0 \end{pmatrix} \qquad \text{JCOEF} = \begin{pmatrix} 1 & 3 & * \\ 1 & 2 & 4 \\ 2 & 3 & 5 \\ 3 & 4 & * \\ 4 & 5 & * \end{pmatrix}$$

Storage: $n$, $n \cdot nl$ integer and float ($nl :=$ nnz of longest row)

# Rectangular Storage Scheme by Pressing from the Right (cont.)

Pseudocode for computing $c = A \cdot b$:

```
c = 0;
for i = 1 : n
   for j = 1 : nl
      c_i = c_i + COEF(i,j) * b(JCOEF(i,j));
   end
end
```

This format was used in ELLPACK (package of subroutines for elliptic PDEs).

# 4.1.6. Jagged Diagonal Form

Prestep: Sort rows after their length. Long rows first.

$$A = \begin{pmatrix} 1 & 0 & 2 & 0 & 0 \\ 3 & 4 & 0 & 5 & 0 \\ 0 & 6 & 7 & 0 & 8 \\ 0 & 0 & 9 & 10 & 0 \\ 0 & 0 & 0 & 11 & 12 \end{pmatrix} \Rightarrow PA = \begin{pmatrix} 3 & 4 & 0 & 5 & 0 \\ 0 & 6 & 7 & 0 & 8 \\ 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 9 & 10 & 0 \\ 0 & 0 & 0 & 11 & 12 \end{pmatrix}$$

Length 3

Length 2

- Values of PA: DJ = (3 6 1 9 11 | 4 7 2 10 12 | 5 8|)
- Column indices: JDIAG = (1 2 1 3 4 | 2 3 3 4 5 | 4 5|)
- Pointer to beginning of jth diagonal: IDIAG = (1 6 11 13)

# Jagged Diagonal Form (cont.)

NDIAG := number of jagged diagonals

Storage: $n$, NDIAG, nnz float, nnz + NDIAG integer

Pseudocode for computing $c = A \cdot b$:

$c = 0;$
`for` $j = 1 \ : \ NDIAG$
  `for` $i = 1 \ : \ IDIAG(j+1) - IDIAG(j)$
    $k = IDIAG(j) + i - 1;$
    $c_i = c_i + DJ(k) \ * \ b(JDIAG(k));$
  `end`
`end`

- Always start with row 1.
- More operations on neighboring data.
- Less indirect addressing.
- Pre-permutation changes only rows. Can be done implicitly.

# Survey on Sparse Storage Formats

Coordinate form and CSR traditional way to specify sparse matrix in MATLAB.

| | global int | idx int | value floats |
|---|---|---|---|
| Coordiante | 2 | $2 \cdot \text{nnz}$ | nnz |
| CSR | 2 | $n + \text{nnz} + 1$ | nnz |
| CSR with Extract. Diag. | 2 | $\text{nnz} + 1$ | $\text{nnz} + 1$ |
| Diagonalwise | 2 | $nd$ | $n \cdot nd$ |
| Rectang. with Pressing | 1 | $n \cdot nl$ | $n \cdot nl$ |
| Jagged Diagonal | 2 | $\text{nnz} + nd$ | nnz |