Linear Algebra

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MSIAM, 23–24 September 2015

Overview

1. Vectors and matrices
   - Elementary operations
   - Gram–Schmidt orthonormalization
   - Matrix norm
   - Conditioning
   - Specific matrices
   - Tridiagonalisation
   - LU and QR factorizations
2. Eigenvalues and eigenvectors
   - Power iteration algorithm
   - Deflation
   - Galerkin
   - Jacobi
   - QR
3. Numerical solution of linear systems
   - Direct methods
   - Iterative methods
   - Preconditioning
4. Storage
   - Band storage
   - Sparse storage
5. Bandwidth reduction

Elementary operations on vectors

$\mathbb{C}^n$ resp. $\mathbb{R}^n$: linear space of vectors with n entries in $\mathbb{C}$ resp. $\mathbb{R}$.
Generically: F^n, where F is a field.

Linear combination of vectors

$\vec{w} = \alpha\vec{u} + \beta\vec{v}$, $\alpha, \beta \in \mathbb{C}$ or $\mathbb{R}$.

```
for i = 1 to n
  w(i) = alpha * u(i) + beta * v(i)
end for
```

Scalar product of 2 vectors

$$\vec{u} \cdot \vec{v} = \sum_{i=1}^{n} u_i v_i$$

```
uv = 0
for i = 1 to n
  uv = uv + u(i) * v(i)
end for
```

ℓ^2 norm of a vector

$$\|\vec{u}\|_2 = \sqrt{\sum_{i=1}^{n} u_i^2}$$

```
uu = 0
for i = 1 to n
  uu = uu + u(i) * u(i)
end for
norm = sqrt(uu)
```

Elementary operations on matrices

$\mathcal{M}_{np}(F)$: linear space of matrices with $n \times p$ entries in F.

Linear combination of matrices

$C = \alpha A + \beta B$, $\alpha, \beta \in F$.

```
for i = 1 to n
  for j = 1 to p
    C(i,j) = alpha * A(i,j) + beta * B(i,j)
  end for
end for
```

Matrix–vector product

$$\vec{w} = A\vec{u},\ w_i = \sum_{j=1}^{p} A_{ij} u_j$$

```
for i = 1 to n
  wi = 0
  for j = 1 to p
    wi = wi + A(i,j) * u(j)
  end for
  w(i) = wi
end for
```

Matrix–matrix product

$$C = AB,\ C_{ij} = \sum_{k=1}^{p} A_{ik} B_{kj}$$

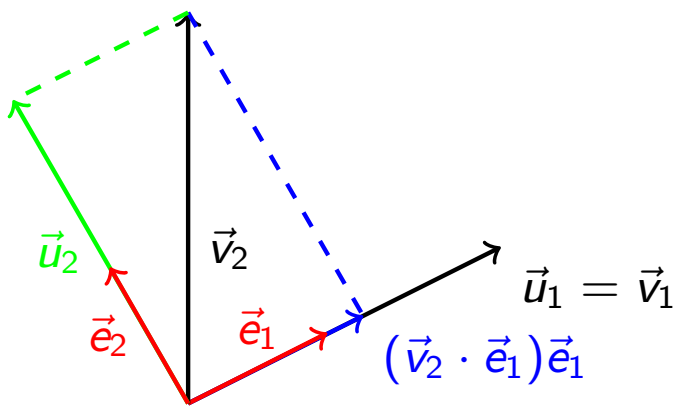
```
for i = 1 to n
  for j = 1 to q
    cij = 0
    for k = 1 to p
      cij = cij + A(i,k) * B(k,j)
    end for
    C(i,j) = cij
  end for
end for
```

Gram–Schmidt orthonormalization

Let $\{\vec{v}_1, \ldots, \vec{v}_p\}$ be a free family of vectors.
It generates the vector space E_p with dimension p.
We want to construct $\{\vec{e}_1, \ldots, \vec{e}_p\}$, an orthonormal basis of E_p.

Gram–Schmidt algorithm

$$
\begin{array}{lcllcl}
\vec{u}_1 & = & \vec{v}_1 & \vec{e}_1 & = & \dfrac{\vec{u}_1}{\|\vec{u}_1\|_2} \\
\vec{u}_2 & = & \vec{v}_2 - (\vec{v}_2 \cdot \vec{e}_1)\vec{e}_1 & \vec{e}_2 & = & \dfrac{\vec{u}_2}{\|\vec{u}_2\|_2} \\
 & \ldots & & & \ldots & \\
\vec{u}_p & = & \vec{v}_p - \displaystyle\sum_{k=1}^{p-1} (\vec{v}_p \cdot \vec{e}_k)\vec{e}_k & \vec{e}_p & = & \dfrac{\vec{u}_p}{\|\vec{u}_p\|_2}
\end{array}
$$



Matrix norms

Definition

$\|A\| \geq 0$, $\forall A \in \mathcal{M}_{nn}(F),\ F = \mathbb{C}$ or $\mathbb{R}$.

$\|A\| = 0 \Leftrightarrow A = 0$.

$\|\lambda A\| = |\lambda|\|A\|$, $\forall A \in \mathcal{M}_{nn}(F),\ \forall \lambda \in F$.

$\|A + B\| \leq \|A\| + \|B\|$, $\forall A, B \in \mathcal{M}_{nn}(F)$ (triangle inequality).

$\|AB\| \leq \|A\|\|B\|$, $\forall A, B \in \mathcal{M}_{nn}(F)$ (specific for matrix norms).

Subordinate matrix norms

$$\|A\|_p = \max_{\|x\|_p \neq 0} \frac{\|Ax\|_p}{\|x\|_p} = \max_{\|x\|_p = 1} \|Ax\|_p,\ \forall x \in F^n, \text{ where } \|\vec{x}\|_p = \sqrt[p]{\sum_{i=1}^{n} x_i^p}.$$

in particular: $\|A\|_1 = \max_j \sum_i |A_{ij}|$ and $\|A\|_\infty = \max_i \sum_j |A_{ij}|$.

Matrix-vector product estimate

$$\|A\|_p \geq \frac{\|Ax\|_p}{\|x\|_p} \text{ and hence } \|Ax\|_p \leq \|A\|_p \|x\|_p \text{ for all } x \in F^n.$$

Matrix conditioning

Definition

$$\mathrm{Cond}(A) = \|A^{-1}\|\|A\|.$$

Properties

$$\mathrm{Cond}(A) \geq 1,$$
$$\mathrm{Cond}(A^{-1}) = \mathrm{Cond}(A),$$
$$\mathrm{Cond}(\alpha A) = \mathrm{Cond}(A).$$

For the Euclidian norm

$$\mathrm{Cond}_2(A) = \frac{|\lambda_{\max}|}{|\lambda_{\min}|}.$$

Conditioning and linear systems

Problem

$(S_0)\ A\vec{x} = \vec{b}, \qquad (S_{\text{per}})\ (A+\delta A)(\vec{x}+\delta\vec{x}) = (\vec{b}+\delta\vec{b}).$

$(S_{\text{per}})-(S_0)$: $A\delta\vec{x} + \delta A(\vec{x}+\delta\vec{x}) = \delta\vec{b}$,

$$\delta\vec{x} = A^{-1}\left(\delta\vec{b} - \delta A(\vec{x}+\delta\vec{x})\right),$$

$$\|\delta\vec{x}\| \leq \|A^{-1}\| \left\|\delta\vec{b} - \delta A(\vec{x}+\delta\vec{x})\right\| \text{ (for a subordinate matrix norm)},$$

$$\|\delta\vec{x}\| \leq \|A^{-1}\| \left(\|\delta\vec{b}\| + \|\delta A\|\|\vec{x}+\delta\vec{x}\|\right),$$

$$\frac{\|\delta\vec{x}\|}{\|\vec{x}+\delta\vec{x}\|} \leq \|A^{-1}\| \left(\frac{\|\delta\vec{b}\|}{\|\vec{x}+\delta\vec{x}\|} + \|\delta A\|\right).$$

Result

$$\frac{\|\delta\vec{x}\|}{\|\vec{x}+\delta\vec{x}\|} \leq \text{Cond}(A) \left(\frac{\|\delta\vec{b}\|}{\|A\|\|\vec{x}+\delta\vec{x}\|} + \frac{\|\delta A\|}{\|A\|}\right).$$

relative error on x = Cond(A) (relative error on $\vec{b}$ + relative error on A).

Hermitian, orthogonal...

Transposed matrix: $({}^tA)_{ij} = A_{ji}$.
Adjoint matrix: $(A^*)_{ij} = \overline{A_{ji}}$.

Symmetric matrix

${}^tA = A$.

Hermitian matrix

$A^* = A$ and hence ${}^tA = \bar{A}$.

Orthogonal matrix (in $\mathcal{M}_{nn}(\mathbb{R})$)

${}^tAA = I$.

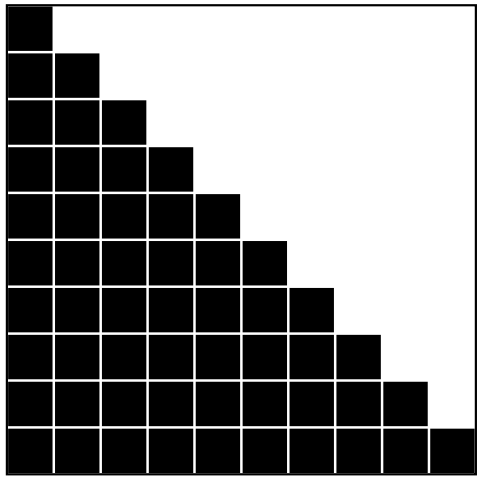
Unitary matrix (in $\mathcal{M}_{nn}(\mathbb{C})$)

$A^*A = I$.

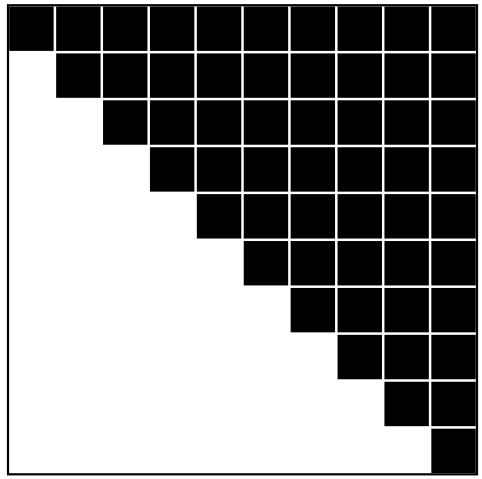
Similar matrices ("semblables" in French)

A and B are similar if $\exists P / B = P^{-1}AP$.

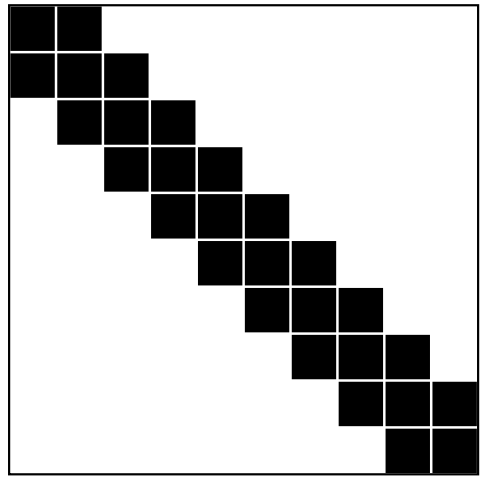
Profiles



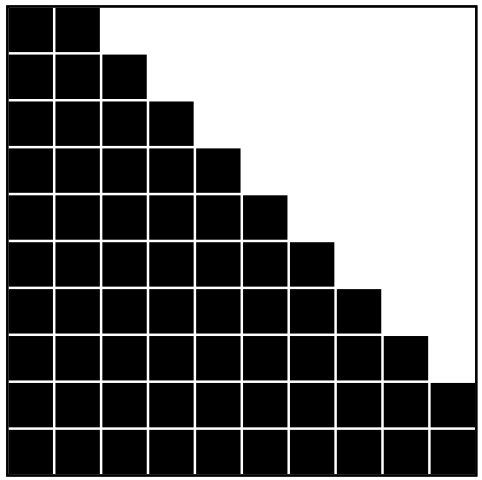
Lower triangular



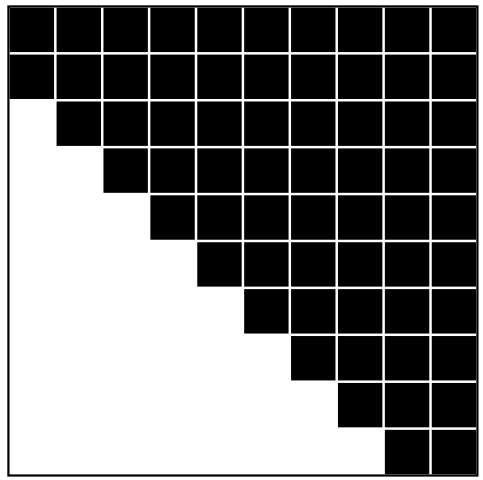
Upper triangular



Tridiagonal



Lower Hessenberg



Upper Hessenberg

Householder matrices

Definition

$$H_{\vec{v}} = I - 2\frac{\vec{v}^t\vec{v}}{\|\vec{v}\|_2^2}$$

Properties

1. $H_{\vec{v}}$ is orthogonal.
2. If $\vec{v} = \vec{a} - \vec{b} \neq \vec{0}$ and $\|\vec{a}\|_2 = \|\vec{b}\|_2$, then $H_{\vec{v}}\vec{a} = \vec{b}$.

${}^t\vec{v}\vec{v} = \|\vec{a}\|_2 - 2{}^t\vec{a}\vec{b} + \|\vec{b}\|_2 = 2\|\vec{a}\|_2 - 2{}^t\vec{a}\vec{b} = 2{}^t\vec{a}\vec{v} = 2{}^t\vec{v}\vec{a}$
$H_{\vec{v}}\vec{a} = \vec{a} - \frac{2\vec{v}^t\vec{v}\vec{a}}{\|\vec{v}\|_2} = \vec{a} - \vec{v} = \vec{b}.$

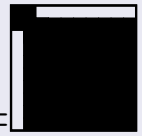
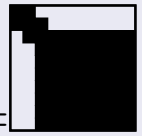
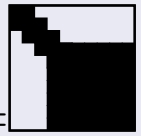
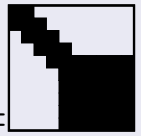
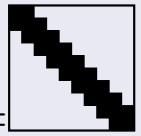
Application

Let $\vec{a} \in K^n$, we look for $H_{\vec{v}}$ such that $H_{\vec{v}}\vec{a} = {}^t(\alpha, 0, \ldots, 0)$.
Solution: take $\vec{b} = {}^t(\alpha, 0, \ldots, 0)$ with $\alpha = \|\vec{a}\|_2$, and $\vec{v} = \vec{a} - \vec{b}$. Then $H_{\vec{v}}\vec{a} = \vec{b}$.

Householder tridiagonalisation

Aim

A: symmetric matrix.
Construct a sequence $A^{(1)} = A, \ldots, A^{(n)}$ tridiagonal and $A^{(n)} n = HA^t H$.

$A^{(2)} =$  $A^{(3)} =$  $A^{(4)} =$  $A^{(5)} =$  $\ldots A^{(n)} =$ 

First step

$$A^{(1)} \equiv \begin{pmatrix} A_{11}^{(1)} & {}^t\vec{a}_{12}^{(1)} \\ \vec{a}_{21}^{(1)} & \tilde{A}^{(1)} \end{pmatrix} \quad H^{(1)} \equiv \begin{pmatrix} 1 & {}^t\vec{0} \\ \vec{0} & \tilde{H}^{(1)} \end{pmatrix} \quad A^{(2)} \equiv \begin{pmatrix} A_{11}^{(1)} & {}^t(\tilde{H}^{(1)}\vec{a}_{21}^{(1)}) \\ \tilde{H}^{(1)}\vec{a}_{21}^{(1)} & \tilde{H}^{(1)}\tilde{A}^{(1)\,t}\tilde{H}^{(1)} \end{pmatrix}.$$

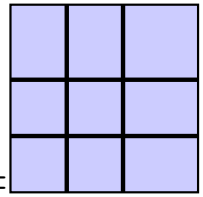
Choose $\tilde{H}^{(1)}$ such that $\tilde{H}^{(1)}\vec{a}_{21}^{(1)} = {}^t(\alpha, 0, \ldots, 0)_{n-1} = \alpha(\vec{e}_1)_{n-1}$.
$\alpha = \|\vec{a}_{21}^{(1)}\|_2$, $\vec{u}_1 = \vec{a}_{21}^{(1)} - \alpha(\vec{e}_1)_{n-1}$, $\tilde{H}^{(1)} = H_{\vec{u}_1}$.

Complexity

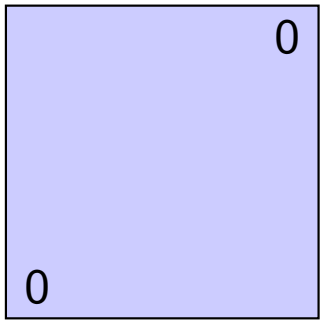
Order $\frac{2}{3}n^3$ products.

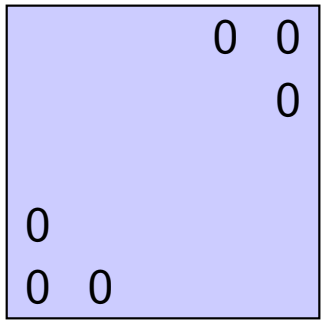
Givens tridiagonalization

Let $G_{pq}(c,s) = \begin{pmatrix} 1 & & & & & & 0 \\ & 1 & & & & & \\ & & c & & s & & \\ & & & 1 & & & \\ & & -s & & c & & \\ & & & & & 1 & \\ 0 & & & & & & 1 \end{pmatrix}$ with $c^2 + s^2 = 1$.

${}^tGAG =$ 

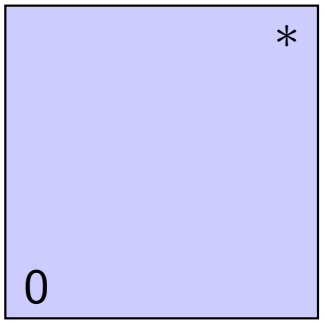
If A is symmetric:

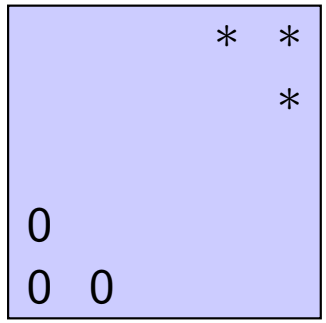




...

else: leads to Hessenberg matrix

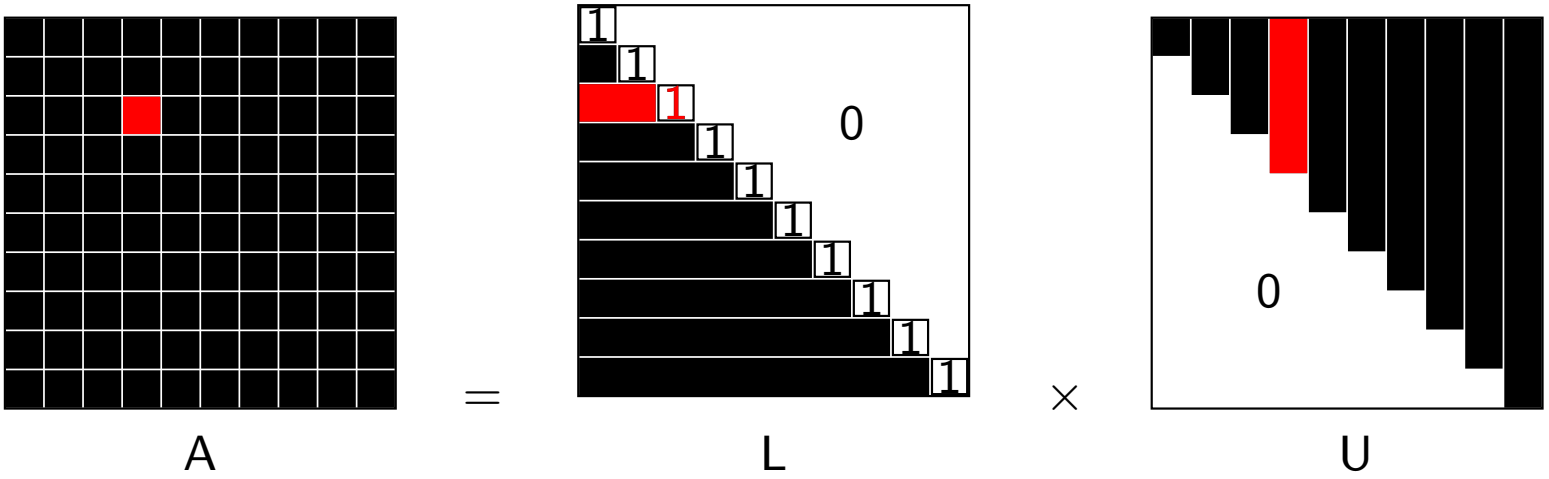




Complexity

Order $\frac{4}{3}n^3$ products.

Principles of LU factorization



- Some regular matrix (with non-zero determinant) are not LU-transformable, e.g. ([0 1; 1 1]) is not.
- If it exists, the LU decomposition of A is not unique.
  It is unique if A is non-singular.
- A is non-singular and LU-transformable
  $\Longleftrightarrow$ all the determinants of the fundamental principal minors are non zero (and in this case the decomposition is unique).

Doolittle LU factorization – principle

It proceeds line by line.

$$\begin{cases} A_{11} = L_{11}U_{11} & L_{11} = 1 \\ A_{12} = L_{11}U_{12} & \\ \cdots & \Rightarrow \{U_{1j}\}_{j=1,\ldots,n} \\ A_{1n} = L_{11}U_{1n} & \end{cases}$$

$$\begin{cases} A_{21} = L_{21}U_{11} & \Rightarrow L_{21} \\ A_{22} = L_{21}U_{12} + U_{22} & \\ \cdots & \Rightarrow \{U_{2j}\}_{j=2,\ldots,n} \\ A_{2n} = L_{21}U_{1n} + U_{2n} & \end{cases}$$

$$\begin{cases} A_{31} = L_{31}U_{11} & \Rightarrow L_{31} \\ A_{32} = L_{31}U_{12} + L_{32}U_{22} & \Rightarrow L_{32} \\ A_{33} = L_{31}U_{13} + L_{32}U_{23} + U_{33} & \\ \cdots & \Rightarrow \{U_{3j}\}_{j=3,\ldots,n} \\ A_{3n} = L_{31}U_{1n} + L_{32}U_{2n} + U_{3n} & \end{cases}$$

$$\ldots$$

Doolittle LU factorization – algorithm

Doolittle algorithm

$$L_{ij} = \frac{A_{ij} - \sum_{k=1}^{j-1} L_{ik} U_{kj}}{U_{jj}} \qquad U_{ij} = A_{ij} - \sum_{k=1}^{i-1} L_{ik} U_{kj}$$

```
for i = 1 to n
  for j = 1 to i-1
    sum = 0
    for k=1 to j-1
      sum = sum + L(i,k)*U(k,j)
    end for
    L(i,j) = (A(i,j)-sum)/U(j,j)
  end for
  L(i,i) = 1
  for j = i to n
    sum = 0
    for k = 1 to i-1
      sum = sum + L(i,k)*U(k,j)
    end for
    U(i,j) = A(i,j) - sum
  end for
end for
```

Complexity

Order n^3 products

Cholesky factorization for an Hermitian matrix

Principle

$A = C\ {}^t C$

Cholesky algorithm

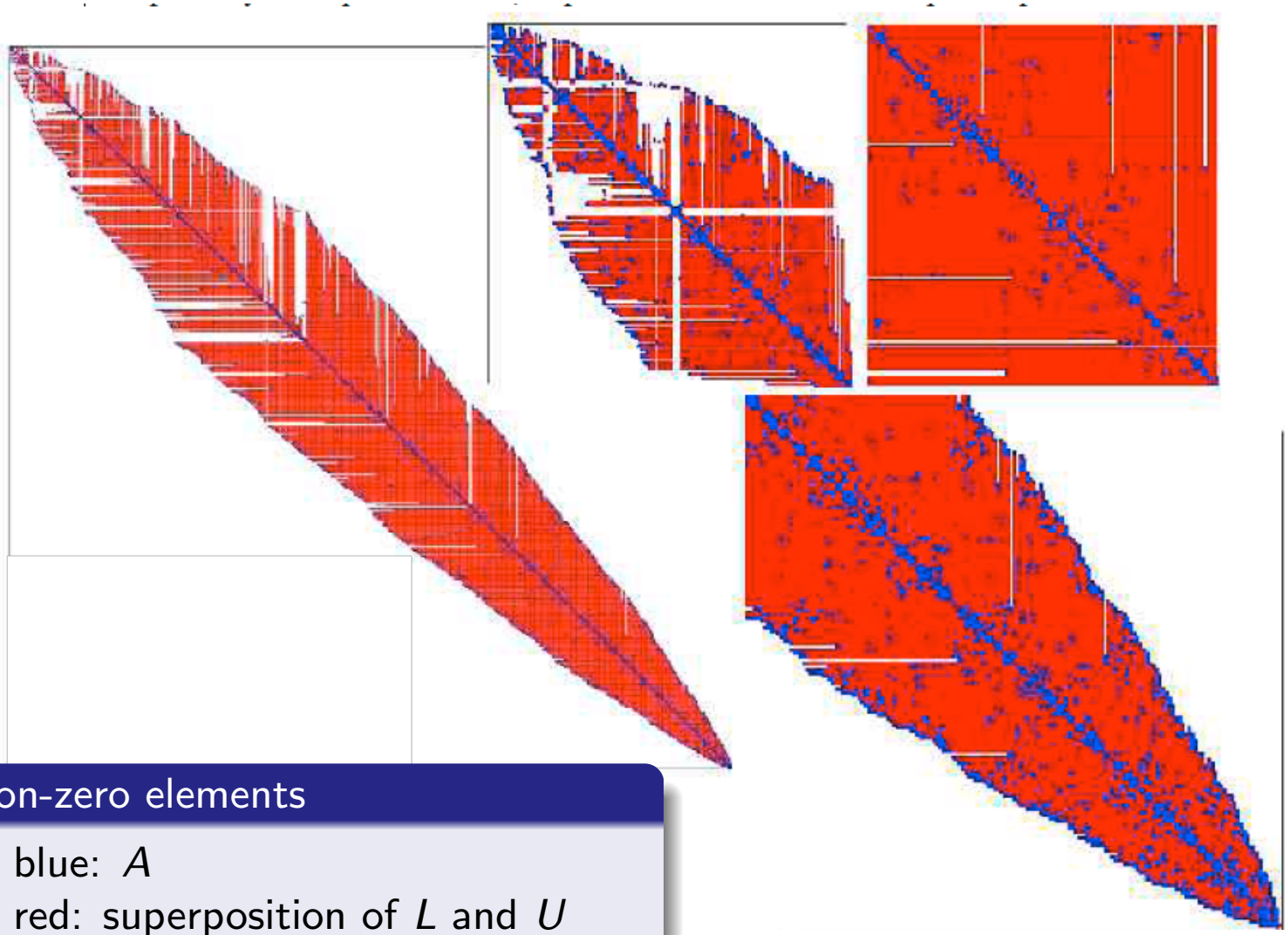
$$C_{ii} = \sqrt{A_{ii} - \sum_{k=1}^{i-1} C_{ik} C_{ik}} \qquad C_{ij} = \frac{A_{ij} - \sum_{k=1}^{j-1} C_{ik} C_{jk}}{C_{jj}}, \ j \neq i$$

```
C(1,1) = sqrt(A(1,1))
for i = 2 to n
  for j = 1 to i-1
    sum = 0
    for k = 1 to j-1
      sum = sum + C(i,k)*C(j,k)
    end for
    C(i,j) = (A(i,j)-sum)/C(j,j)
  end for
  sum=0
  for k = 1 to i-1
    sum = sum + C(i,k)*C(i,k)
  end for
  C(i,i) = sqrt(A(i,i) - sum)
end for
```

Complexity

Order n^3 products

LU factorization – profiles



Non-zero elements

In blue: A
In red: superposition of L and U

The interior of the profile is filled!

QR factorization – principle

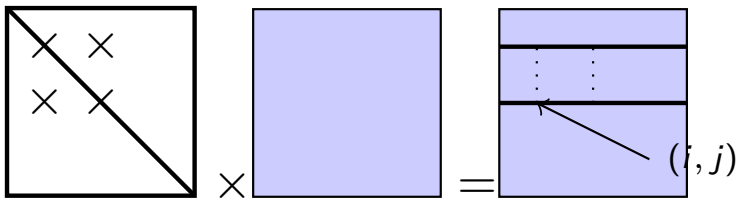
Principle

$A = QR$, where Q orthogonal and R right (upper) triangular.

$G_m \dots G_2 G_1 A = R$,

$A = \underbrace{{}^t G_1 \, {}^t G_2 \dots {}^t G_m}_{Q} R$

Let $G_{ij}(c,s) = \begin{pmatrix} 1 & & & & & & 0 \\ & 1 & & & & & \\ & & c & & s & & \\ & & & 1 & & & \\ & & -s & & c & & \\ & & & & & 1 & \\ 0 & & & & & & 1 \end{pmatrix}$ with $c^2 + s^2 = 1$.



$(GA)_{ij} = -sA_{jj} + cA_{ij}$

$c = \dfrac{A_{jj}}{\sqrt{A_{ij}^2 + A_{jj}^2}} \quad s = \dfrac{A_{ij}}{\sqrt{A_{ij}^2 + A_{jj}^2}}$

QR factorization – algorithm

Algorithm

```
R = A
Q = Id  // size of A
for i = 2 to n
  for j = 1 to i-1
    root = sqrt(R(i,j)*R(i,j)+R(j,j)*R(j,j))
    if root != 0
      c = R(j,j)/root
      s = R(i,j)/root
    else
      c = 1
      s = 0
    end if
    Construct Gji
    R = Gji*R                  // matrix product
    Q = Q*transpose(Gji)       // matrix product
  end for
end for
```

Complexity

Order n^3 products

QR factorization – Python example

$$A = \begin{pmatrix} 3 & 2 & 1 & 0 & 0 \\ 4 & 3 & 2 & 1 & 0 \\ 5 & 4 & 3 & 2 & 1 \\ 6 & 5 & 4 & 3 & 2 \\ 7 & 6 & 5 & 4 & 3 \end{pmatrix}$$

$$R = \begin{pmatrix} 11.619 & 9.467 & 7.316 & 5.164 & 3.271 \\ 3.437\ 10^{-16} & 6.086\ 10^{-01} & 1.217 & 1.826 & 1.704 \\ 4.476\ 10^{-17} & 1.989\ 10^{-18} & 2.324\ 10^{-15} & 3.768\ 10^{-15} & -3.775\ 10^{-01} \\ -6.488\ 10^{-16} & 1.082\ 10^{-17} & 0.000 & 1.618\ 10^{-16} & -6.764\ 10^{-02} \\ -6.671\ 10^{-16} & -2.548\ 10^{-17} & 0.000 & -3.082\ 10^{-33} & -5.029\ 10^{-01} \end{pmatrix}$$

$$Q = \begin{pmatrix} 0.2582 & -0.7303 & -0.3775 & -0.0676 & -0.5029 \\ 0.3443 & -0.4260 & -0.0062 & -0.1589 & 0.821 \\ 0.4303 & -0.1217 & 0.5407 & 0.7050 & -0.1030 \\ 0.5164 & 0.1826 & 0.4472 & -0.6627 & -0.2466 \\ 0.6025 & 0.4869 & -0.6042 & 0.1842 & 0.0311 \end{pmatrix}$$

Power iteration algorithm – Python experiment

$$A = \begin{pmatrix} 10 & 0 \\ -9 & 1 \end{pmatrix}$$

Eigenvalues and eigenvectors:

$$\lambda_1 = 1, \lambda_2 = 10, \vec{v}_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Construct the series

$$\vec{x}^k = A\vec{x}^{k-1}$$

$$\vec{x}^0 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \vec{x}^1 = \begin{pmatrix} 20 \\ -17 \end{pmatrix}, \vec{x}^2 = \begin{pmatrix} 200 \\ -197 \end{pmatrix}, \vec{x}^3 = \begin{pmatrix} 2000 \\ -1997 \end{pmatrix} \cdots$$

$\vec{x}$ tends to the direction of the eigenvector associated to the higher modulus eigenvalue.

"$\vec{x}^k / \vec{x}^{k-1}$" tends to the higher modulus eigenvalue.

Power iteration algorithm – Algorithm

Computation of the eigenvalue with higher modulus.
A may be diagonalizable or not, the dominant eigenvalue can be unique or not.

Algorithm

```
choose q(0)
for k = 1 to convergence
  x(k) = A * q(k-1)
  q(k) = x(k) / norm(x(k))
end for
lambdamax = x(k)(j)/q(k-1)(j)
```

Attention: good choice of component j.

Power iteration algorithm – Python example

$$A = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Rotations:

$$R_1 = \begin{pmatrix} \cos(1) & 0 & \sin(1) \\ 0 & 1 & 0 \\ -\sin(1) & 0 & \cos(1) \end{pmatrix}, R_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(2) & \sin(2) \\ 0 & -\sin(2) & \cos(2) \end{pmatrix}$$

$$B = R_2 R_1 A^t {R_1}^t {R_2} = \begin{pmatrix} 4.33541265 & -3.30728724 & 1.51360499 \\ -3.30728724 & 7.20313893 & -1.00828318 \\ 1.51360499 & -1.00828318 & 5.46144841 \end{pmatrix}$$

Eigenvalues and eigenvectors:

$$\lambda_1 = 2, \lambda_2 = 5, \lambda_3 = 10,$$

$$\vec{v}_1 = \begin{pmatrix} -0.8415 \\ -0.4913 \\ 0.2248 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} 1.365\ 10^{-16} \\ 0.4161 \\ 0.9093 \end{pmatrix}, \vec{v}_3 = \begin{pmatrix} -0.5403 \\ 0.7651 \\ -0.3502 \end{pmatrix}.$$

Power iteration algorithm – Remarks

1. Convergence results depend on the fact that
   - the matrix is diagonalizable or not
   - the dominant eigenvalue is multiple or not
2. The choice of the norm is not explicit: usually max norm or euclidian norm
3. $\vec{q}_0$ should not be orthogonal to the eigen-subspace associated to the dominant eigenvalue.

Inverse iteration algorithm – Algorithm

Computation of the eigenvalue with smallest modulus.
A may be diagonalizable or not, the dominant eigenvalue can be unique or not.
Based on the fact that

$$\lambda_{\min}(A) = \left(\lambda_{\max}(A^{-1})\right)^{-1}.$$

Algorithm

```
choose q(0)
for k = 1 to convergence
   solve A * x(k) = q(k-1)
   q(k) = x(k) / norm(x(k))
end for
lambdamin = q(k-1)(j) / x(k)(j)
```

Inverse iteration algorithm – Python example

$$A = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Rotations:

$$R_1 = \begin{pmatrix} \cos(1) & 0 & \sin(1) \\ 0 & 1 & 0 \\ -\sin(1) & 0 & \cos(1) \end{pmatrix}, R_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(2) & \sin(2) \\ 0 & -\sin(2) & \cos(2) \end{pmatrix}$$

$$B = R_2 R_1 A^t {R_1}^t {R_2} = \begin{pmatrix} 4.33541265 & -3.30728724 & 1.51360499 \\ -3.30728724 & 7.20313893 & -1.00828318 \\ 1.51360499 & -1.00828318 & 5.46144841 \end{pmatrix}$$

Eigenvalues and eigenvectors:

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Generalized inverse iteration algorithm – Algorithm

Computation of the closest eigenvalue to a given μ.
The eigenvalues of $A - \mu I$ are the $\lambda_i - \mu$,
where λ_i are the eigenvalues of A.
$\Rightarrow$ apply the inverse iteration algorithm to $A - \mu I$.

Algorithm

```
choose q(0)
for k = 1 to convergence
   solve (A-mu*I) * x(k) = q(k-1)
   q(k) = x(k) / norm(x(k))
end for
lambda = q(k-1)(j) / x(k)(j) + mu
```

Generalized inverse iteration algorithm – Python example

$$A = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \mu = 4.$$

Rotations:

$$R_1 = \begin{pmatrix} \cos(1) & 0 & \sin(1) \\ 0 & 1 & 0 \\ -\sin(1) & 0 & \cos(1) \end{pmatrix}, R_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(2) & \sin(2) \\ 0 & -\sin(2) & \cos(2) \end{pmatrix}$$

$$B = R_2 R_1 A^t {R_1}^t {R_2} = \begin{pmatrix} 4.33541265 & -3.30728724 & 1.51360499 \\ -3.30728724 & 7.20313893 & -1.00828318 \\ 1.51360499 & -1.00828318 & 5.46144841 \end{pmatrix}$$

Eigenvalues and eigenvectors:

$$\lambda_1 = 2, \lambda_2 = 5, \lambda_3 = 10,$$

$$\vec{v}_1 = \begin{pmatrix} -0.8415 \\ -0.4913 \\ 0.2248 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} 1.365\ 10^{-16} \\ 0.4161 \\ 0.9093 \end{pmatrix}, \vec{v}_3 = \begin{pmatrix} -0.5403 \\ 0.7651 \\ -0.3502 \end{pmatrix}.$$

Deflation – Algorithm and Python example

Computation of all the eigenvalues in modulus decreasing order.

When an eigenelement (λ, q) is found, it is removed from further computation by replacing $A \leftarrow A - \lambda \vec{q}^t \vec{q}$.

Algorithm

```
  for i = 1 to n
    choose q(0)
    for k = 1 to convergence
      x(k) = A * q(k-1)
      q(k) = x(k) / norm(x(k))
    end for
    lambda = x(k)(j) / q(k-1)(j)
    A = A - lambda * q * transpose(q)
// eliminates direction q
  end for
```

Galerkin method – Algorithm

Let H be a subspace of dimension m, generated by the orthonormal basis $(\vec{q}_1, \ldots, \vec{q}_m)$.
Construct the rectangular matrix $Q = (\vec{q}_1, \ldots, \vec{q}_m)$.
Remark: $Q^* Q = Id_m$

Goal

Look for eigenvectors in H.

If $\vec{u} \in H$, $\vec{u} = \sum_{i=1}^{m} \alpha_i \vec{q}_i$ (unique).
$\vec{u} = Q\vec{U}$, where $\vec{U} = {}^t(\alpha_1, \ldots, \alpha_m)$.

$A\vec{u} = \lambda\vec{u} \Leftrightarrow AQ\vec{U} = \lambda Q\vec{U}$.
Project on H: $Q^*AQ\vec{U} = \lambda Q^*Q\vec{U} = \lambda\vec{U}$.

$\Rightarrow$ We look for eigenelements of $B = Q^*AQ$.

Vocabulary:
- $\{\lambda_i, \vec{u}_i\}$ are the Ritz elements,
- B is the Rayleigh matrix.

Jacobi method – Algorithm

Goal

Diagonalize the (real symmetric) matrix.

Until a "reasonably diagonal" matrix is obtained:

- Choose the largest off-diagonal element (largest modulus)
- Construct a rotation matrix that annihilates this term

In the end, the eigenvalues are the diagonal elements.

QR method – Algorithm

Algorithm

```
A(1) = A
for k = 1 to convergence
   [Q(k),R(k)] = QR_factor(A(k))
   A(k+1) = R(k)*Q(k)
end for
```

The eigenvalues are the diagonal elements of the last matrix A_{k+1}.

Properties

- $A_{k+1} = R_k Q_k = Q_k^* Q_k R_k Q_k = Q_k^* A_k Q_k$
  $\Rightarrow A_{k+1}$ and A_k are similar.
- If A_k is tridiagonal or Hessenberg, A_{k+1} also is
  $\Rightarrow$ First restrict to this case keeping similar matrices.

QR method – Convergence and Python example

Theorem

Let V^* be the matrix of left eigenvectors of A ($A^* \vec{u}^* = \lambda \vec{u}^*$).
If

- the principal minors of V are non-zero.
- the eigen-values of A are such that $|\lambda_1| > \cdots > |\lambda_n|$.

Then the QR method converges A_{k+1} tends to an upper triangular form and $(A_k)_{ii}$ tends to λ_i.

Eigenvalues – Summary

We want to know all the eigenvalues

- QR method — better than Jacobi
  Preprocessing: find a similar tridiagonal or Heisenberg matrix (Householder or Givens algorithm).

We only want one eigenvector whose eigenvalue is known (or an approximation)

- Power iteration algorithm and variants...

We only want a sub-set of eigenelements

- We know the eigenvalues and look for eigenvectors: deflation and variants
- We know the subspace for eigenvectors: Galerkin and variants

Principles

$$A\vec{x} = \vec{b}$$

Elimination methods

The solution to the system remains unchanged if

- lines are permuted,
- line i is replaced by a linear combination $\ell_i \leftarrow \sum_{k=1}^{n} \mu_k \ell_k$, with $\mu_i \neq 0$.

Factorisation methods

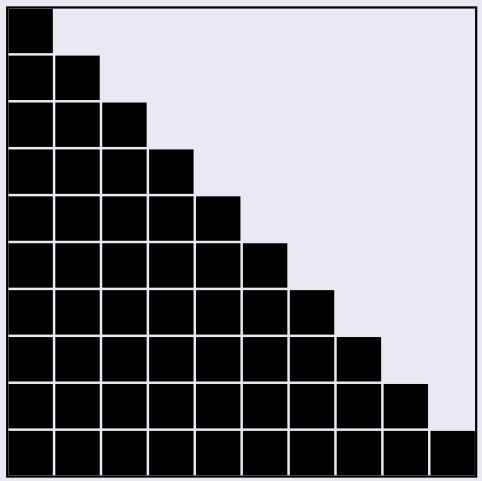
$A = LU$
$LU\vec{x} = \vec{b}$
We solve two triangular systems
$L\vec{y} = \vec{b}$
$U\vec{x} = \vec{y}$.

Lower triangular matrix

$$x_i = \frac{b_i - \sum_{k=1}^{i-1} A_{ik} x_k}{A_{ii}}$$

Algorithm

```
if A(1,1)==0 then stop
x(1) = b(1)/A(1,1)
for i = 2 to n
   if A(i,i)==0 then stop
   ax = 0
   for k = 1 to i-1
      ax = ax + A(i,k)*x(k)
   end for
   x(i) = (b(i)-ax)/A(i,i)
end for
```



Complexity

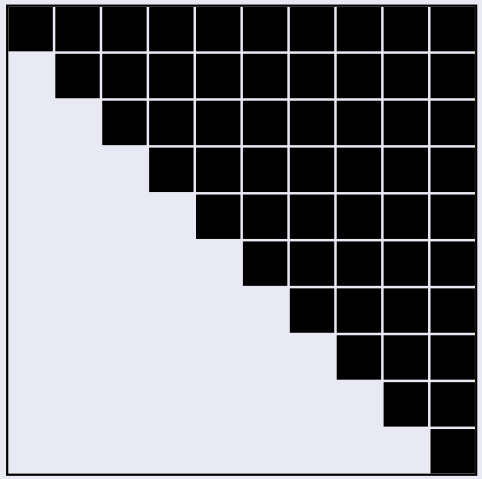
Order $n^2/2$ products.

Upper triangular matrix

$$x_i = \frac{b_i - \sum_{k=i+1}^{n} A_{ik} x_k}{A_{ii}}$$

Algorithm

```
if A(n,n)==0 then stop
x(n) = b(n)/A(n,n)
for i = n-1 to 1
   if A(i,i)==0 then stop
   ax = 0
   for k = i+1 to n
      ax = ax + A(i,k)*x(k)
   end for
   x(i) = (b(i)-ax)/A(i,i)
end for
```



Complexity

Order $n^2/2$ products.

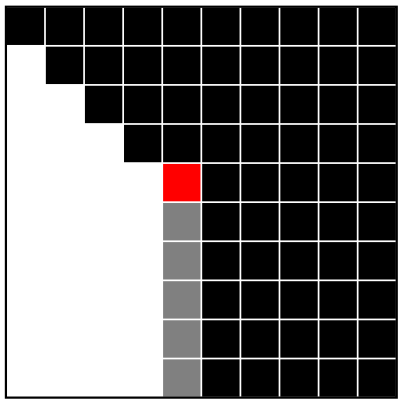
Gauss elimination – Principle

Aim

Transform A to upper triangular matrix.

At rank $p-1$:

$$A_{ij} = 0 \qquad \text{if } i > j,\ j < p.$$



$$\ell_i \leftarrow \ell_i - A_{ip}\frac{\ell_p}{A_{pp}}$$

```
for p = 1 to n
  pivot = A(p,p)
  if pivot == 0 stop
  line(p) = line(p)/pivot
  for i = p+1 to n
    Aip = A(i,p)
    line(i) = line(i) - Aip * line(p)
  end for
end for
x = solve(A,b) // upper triangular
```

Complexity

Still order n^3 products.

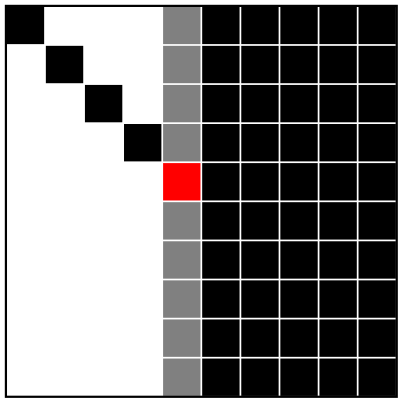
Gauss–Jordan elimination – Principle

Aim

Transform A to identity.

At rank $p-1$:

$$A_{ii} = 1 \qquad \text{if } i < p,$$
$$A_{ij} = 0 \qquad \text{if } i \neq j,\ j < p.$$



$$\ell_i \leftarrow \ell_i - A_{ip}\frac{\ell_p}{A_{pp}}$$

```
for p = 1 to n
  pivot = A(p,p)
  if pivot == 0 stop
  line(p) = line(p)/pivot
  for i = 1 to n, i!=p
    Aip = A(i,p)
    line(i) = line(i) - Aip * line(p)
  end for
end for
x = b
```

Attention

- take into account le right-hand side in the "line".
- what if $A_{pp} = 0$?

Gauss–Jordan elimination – Algorithm


```
// unknown entries numbering
for i = 1 to n
  num(i) = i
end for

for p=1 to n
  // maximal pivot
  pmax = abs(A(p,p))
  imax = p
  jmax = p
  for i = p to n
    for j = p to n
      if abs(A(i,j)) > pmax then
        pmax = abs(A(i,j))
        imax = i
        jmax = j
      end if
    end for
  end for
  // line permutation
  for j = p to n
    permute(A(p,j),A(imax,j))
  end for
  permute(b(p),b(imax))
  // column permutation
  for i = p to n
    permute(A(i,p),A(i,jmax))
  end for
  permute(num(p),num(jmax))
  pivot = A(p,p)
  if pivot == 0 stop, rank(A) = p-1
  for j = p to n
    A(p,j) = A(p,j)/pivot
  end for
  b(p) = b(p)/pivot
  for i = 1 to n, i!=p
    Aip = A(i,p)
    for j = p to n
      A(i,j) = A(i,j) - Aip * A(p,j)
    end for
    b(i) = b(i) - Aip*b(p)
  end for
end for  // loop on p

for i = 1 to n
  x(num(i)) = b(i)
end for
```

Complexity

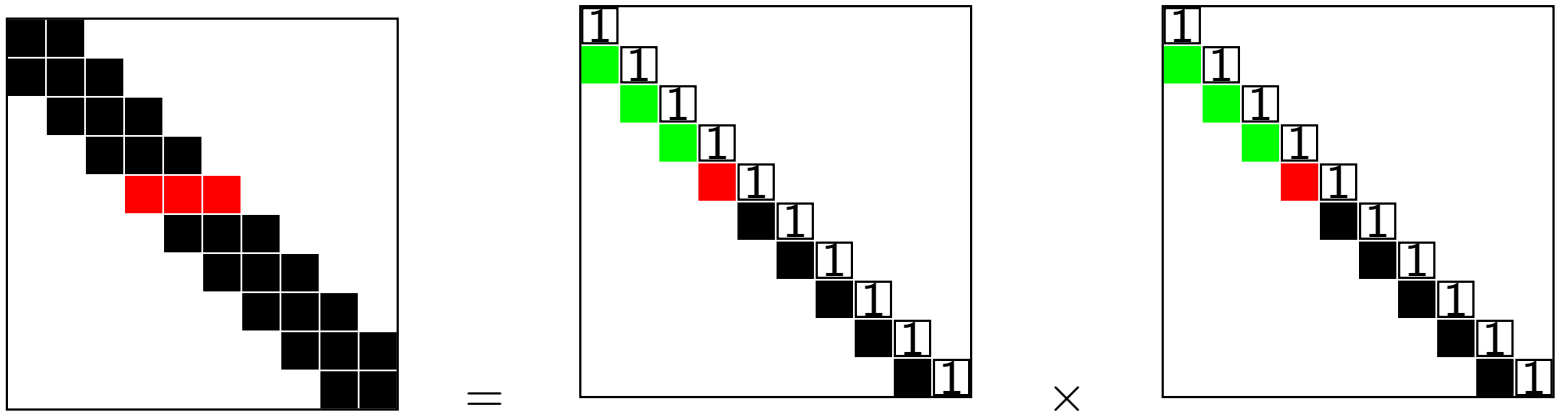
Order n^3 products.

Remark

Also computes the rank of the matrix.

Factorization methods — Thomas algorithm — principle

LU decomposition for tridiagonal matrices.



We suppose that L_{ij} and U_{ij} are known for $i < p$. Then

$$\begin{aligned} A_{p,p-1} &= L_{p,p-1} U_{p-1,p-1}, \\ A_{p,p} &= L_{p,p-1} U_{p-1,p} + U_{p,p}, \\ A_{p,p+1} &= U_{p,p+1}. \end{aligned}$$

$\Rightarrow$

$$\begin{aligned} L_{p,p-1} &= A_{p,p-1} / U_{p-1,p-1}, \\ U_{p,p} &= A_{p,p} - L_{p,p-1} U_{p-1,p} = A_{p,p} - A_{p,p-1} U_{p-1,p} / U_{p-1,p-1}, \\ U_{p,p+1} &= A_{p,p+1}. \end{aligned}$$

Factorization methods — Thomas algorithm — algorithm

Algorithmm

```
// factorization
U(1,1) = A(1,1)
U(1,2) = A(1,2)
for i = 2 to n
   if U(i-1,i-1) = 0 then stop
   L(i,i-1) = A(i,i-1)/U(i-1,i-1)
   U(i,i) = A(i,i) - L(i,i-1)*U(i-1,i)
   U(i,i+1) = A(i,i+1)
end for
// construction of the solution
y = solve(L,b) // lower triangular
x = solve(U,y) // upper triangular
```

Complexity

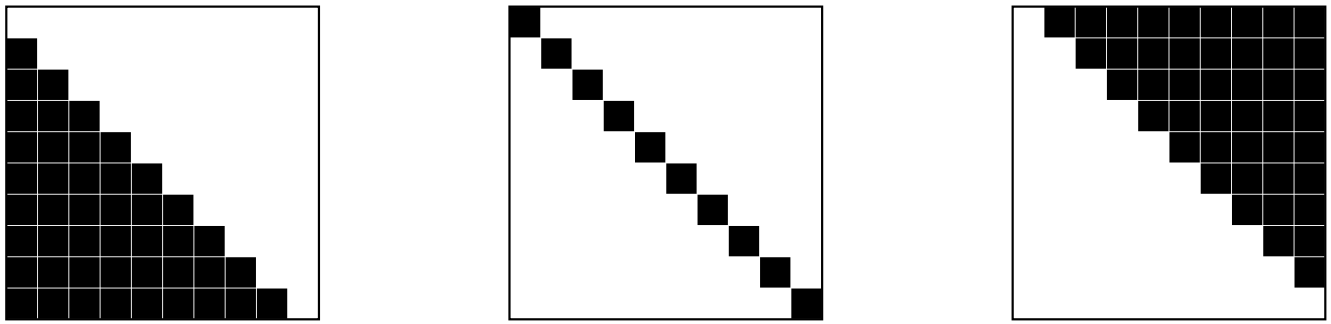
Order $5n$ products.

Factorization methods — general matrices

For general matrices:

- Factorize the matrix
  - LU algorithm
  - Choleski algorithm
- Solve upper triangular system
- Solve lower triangular system.

Iterative methods — Principle



To solve $A\vec{x} = \vec{b}$, write $A = M - N$
and iterate $M\vec{x}^{k+1} - N\vec{x}^{k} = \vec{b}$, i.e. $\vec{x}^{k+1} = M^{-1}N\vec{x}^{k} + M^{-1}\vec{b}$.

Attention

- M should be easy to invert.
- $M^{-1}N$ should lead to a stable algorithm.

Jacobi $M = D,\ N = -(E + F)$,

Gauss–Seidel $M = D + E,\ N = -F$,

Successive Over Relaxation $M = \dfrac{D}{\omega} + E,\ N = \left(\dfrac{1}{\omega} - 1\right) D - F.$

Jacobi method

Algorithm

```
choose x(k=0)
for k = 0 to convergence
  for i = 1 to n
    rhs = b(i)
    for j = 1 to n, j!=i
      rhs = rhs - A(i,j)*x(j,k)
    end for
    x(i,k+1) = rhs / A(i,i)
  end for
  test = norm(x(k+1)-x(k))<epsilon
end for (while not test)
```

$$
\begin{aligned}
x_i^{k+1} &= \frac{1}{A_{ii}} \left(b_i - \sum_{j=1, j\neq i}^{n} A_{ij} x_j^k \right) \\
\vec{x}^{k+1} &= D^{-1}(\vec{b} - (E+F)\vec{x}^k) \\
&= D^{-1}(\vec{b} + (D-A)\vec{x}^k) \\
&= D^{-1}\vec{b} + (I - D^{-1}A)\vec{x}^k.
\end{aligned}
$$

Remarks

- simple,
- two copies of the variable $\vec{x}^{k+1}$ and $\vec{x}^k$,
- insensible to permutations,
- converges if the diagonal is strictly dominant.

Gauss–Seidel method

$$x_i^{k+1} = \frac{1}{A_{ii}} \left(b_i - \sum_{j=1}^{i-1} A_{ij} x_j^{k+1} - \sum_{j=i+1}^{n} A_{ij} x_j^k \right)$$

Algorithm

```
choose x(k=0)
for k = 0 to convergence
  for i = 1 to n
    rhs = b(i)
    for j = 1 to i-1
      rhs = rhs - A(i,j)*x(j,k+1)
    end for
    for j = i+1 to n
      rhs = rhs - A(i,j)*x(j,k)
    end for
    x(i,k+1) = rhs / A(i,i)
  end for
  test = norm(x(k+1)-x(k))<epsilon
end for (while not test)
```

Remarks

- still simple,
- one copy of the variable $\vec{x}$,
- sensible to permutations,
- often converges better than Jacobi.

SOR method

$$x_i^{k+1} = \frac{\omega}{A_{ii}} \left(b_i - \sum_{j=1}^{i-1} A_{ij} x_j^{k+1} - \sum_{j=i+1}^{n} A_{ij} x_j^k \right) + (1-\omega) x_i^k$$

$$\vec{x}^{k+1} = \left(\frac{D}{\omega} + E \right)^{-1} \vec{b} + \left(\frac{D}{\omega} + E \right)^{-1} \left[\left(\frac{1}{\omega} - 1 \right) D - F \right] \vec{x}^k$$

Remarks

- still simple,
- one copy of the variable $\vec{x}$,
- Necessary condition for convergence: $0 < \omega < 2$.

Descent method — general principle

For A symmetric definite positive!!

Principle

Construct a series of approximations of the solution to the system

$$\vec{x}^{k+1} = \vec{x}^{k} + \alpha^{k}\vec{p}^{k},$$

where $\vec{p}^{k}$ descent direction and α^{k} to be determined.

The solution $\underline{\vec{x}}$ minimizes the functional $J(\vec{x}) = {}^{t}\vec{x}A\vec{x} - 2{}^{t}\vec{b}\vec{x}$.

$$\begin{aligned}
\frac{\partial J}{\partial x_i}(\vec{x}) &= \frac{\partial}{\partial x_i}\left(\sum_{j,k} x_j A_{jk} x_k - 2\sum_j b_j x_j\right) \\
&= \sum_k A_{ik}x_k + \sum_j x_j A_{ji} - 2b_i \\
&= 2\left(A\vec{x} - \vec{b}\right)_i, \\
\frac{\partial J}{\partial x_i}(\underline{\vec{x}}) &= 0.
\end{aligned}$$

Descent method — determining α_k

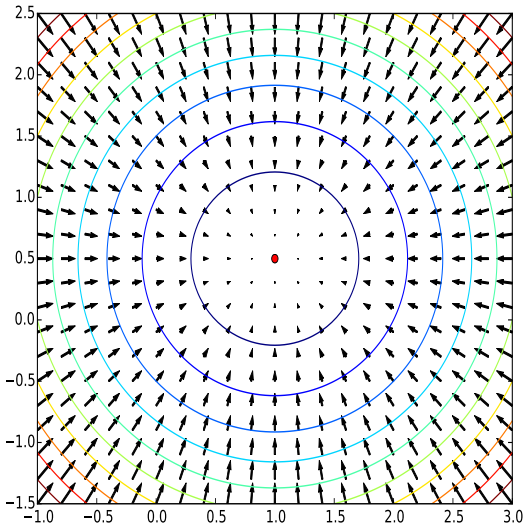
$\underline{\vec{x}}$ also minimizes the functional $E(\vec{x}) = {}^t(\vec{x} - \underline{\vec{x}})A(\vec{x} - \underline{\vec{x}})$, and $E(\underline{\vec{x}}) = 0$.
For a given $\vec{p}^k$, which α minimizes $E(\vec{x}^{k+1})$?

$$\begin{aligned} E(\vec{x}^k + \alpha\vec{p}^k) &= {}^t(\vec{x}^k + \alpha\vec{p}^k - \underline{\vec{x}})A(\vec{x}^k + \alpha\vec{p}^k - \underline{\vec{x}}), \\ \frac{\partial}{\partial\alpha}E(\vec{x}^k + \alpha\vec{p}^k) &= {}^t\vec{p}^k A(\vec{x}^k + \alpha\vec{p}^k - \underline{\vec{x}}) + {}^t(\vec{x}^k + \alpha\vec{p}^k - \underline{\vec{x}})A\vec{p}^k \\ &= 2{}^t(\vec{x}^k + \alpha\vec{p}^k - \underline{\vec{x}})A\vec{p}^k. \end{aligned}$$

$$\begin{aligned} &{}^t(\vec{x}^k + \alpha^k\vec{p}^k - \underline{\vec{x}})A\vec{p}^k = 0 \\ &{}^t\vec{x}_k A\vec{p}_k + \alpha_k {}^t\vec{p}_k A\vec{p}^k - {}^t\underline{\vec{x}}A\vec{p}^k = 0 \\ &{}^t\vec{p}^k A\vec{x}^k + \alpha^k {}^t\vec{p}_k A\vec{p}^k - {}^t\vec{p}^k A\underline{\vec{x}} = 0. \end{aligned}$$

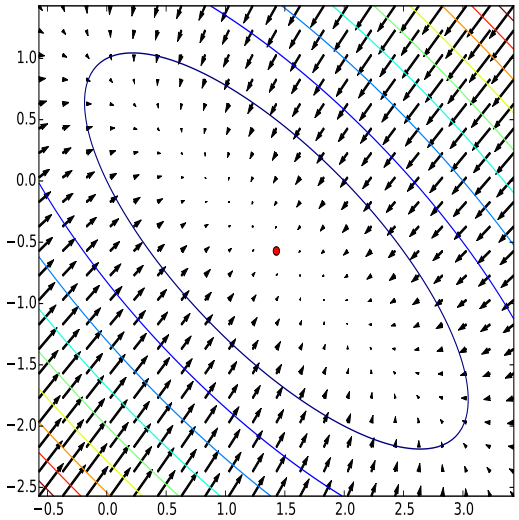
$$\alpha^k = \frac{{}^t\vec{p}^k A\vec{x}^k - {}^t\vec{p}^k A\underline{\vec{x}}}{{}^t\vec{p}^k A\vec{p}^k}$$

Descent method — functional profiles (good cases)

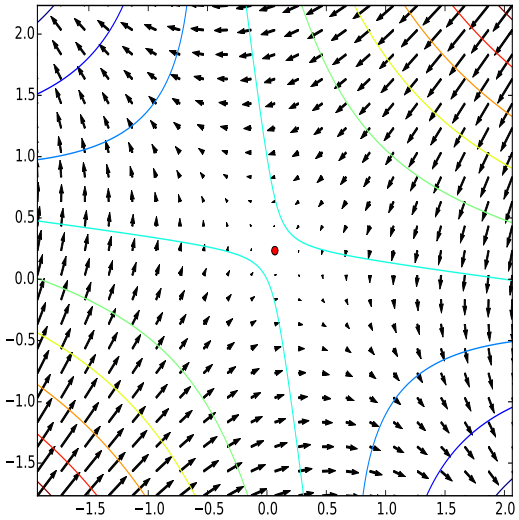


$$A = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \quad \vec{b} = A \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$
$$\text{Cond}(A) = 1$$

$$A = \begin{pmatrix} 2 & 1.5 \\ 1.5 & 2 \end{pmatrix}, \quad \vec{b} = A \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$
$$\text{Cond}(A) = 7$$



Descent method — functional profiles (bad cases)

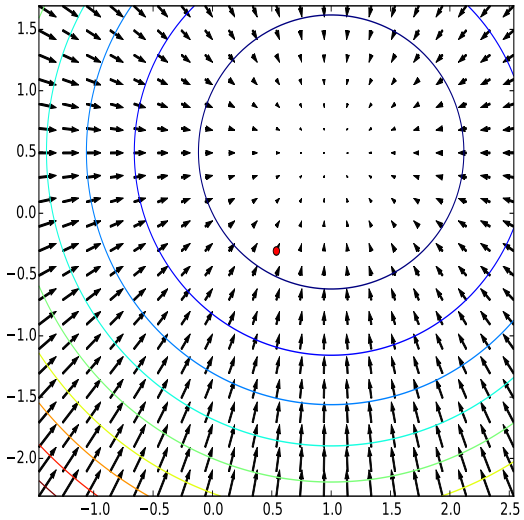


Nonpositive case

$$A = \begin{pmatrix} 2 & 8 \\ 8 & 2 \end{pmatrix}, \quad \vec{b} = A \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

Nonsymmetric case

$$A = \begin{pmatrix} 2 & -3 \\ 3 & 2 \end{pmatrix}, \quad \vec{b} = A \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$



Descent method — optimal parameter (principle)

Principle

- Choose $\vec{p}^k = \vec{r}^k \equiv \vec{b} - A\vec{x}^k$.
- Choose α^k is such that $\vec{r}^{k+1}$ is orthogonal to $\vec{p}^k$.

$$\begin{aligned} \vec{r}^{k+1} &= \vec{b} - A\vec{x}^{k+1} = \vec{b} - A(\vec{x}^k + \alpha\vec{p}^k) = \vec{r}^k - \alpha^k A\vec{p}^k, \\ 0 &= {}^t\vec{p}^k\vec{r}^{k+1} = {}^t\vec{p}^k\vec{r}^k - \alpha^k {}^t\vec{p}^k A\vec{p}^k. \end{aligned}$$

$$\alpha^k = \frac{{}^t\vec{p}^k\vec{r}^k}{{}^t\vec{p}^k A\vec{p}^k}.$$

$$E(\vec{x}^{k+1}) = (1-\gamma^k)E(\vec{x}^k)$$

$$\text{with } \gamma^k = \frac{({}^t\vec{p}^k\vec{r}^k)^2}{({}^t\vec{p}^k A\vec{p}^k)({}^t\vec{r}^k A^{-1}\vec{r}^k)} \geq \frac{1}{\text{Cond}(A)} \frac{|{}^t\vec{p}^k\vec{r}^k|}{\|\vec{p}^k\|\|\vec{r}^k\|}.$$

Descent method — optimal parameter (algorithm)

Algorithm

```
choose x(k=1)
for k = 1 to convergence
  r(k) = b - A * x(k)
  p(k) = r(k)
  alpha(k) = r(k) . p(k) / p(k) . A * p(k)
  x(k+1) = x(k) + alpha(k) * p(k)
end for  //r(k) small
```

Descent method — conjugate gradient (principle)

Principle

- Choose $\vec{p}^k = \vec{r}^k + \beta^k \vec{p}^{k-1}$.
- Choose β^k to minimize the error, i.e. maximize the factor γ^k

Properties

- ${}^t\vec{r}^k \vec{p}^j = 0 \ \forall j < k$,
- $\text{Span}(\vec{r}^1, \vec{r}^2, \ldots, \vec{r}^k) = \text{Span}(\vec{r}^1, A\vec{r}^1, \ldots, A^{k-1}\vec{r}^1)$
- $\text{Span}(\vec{p}^1, \vec{p}^2, \ldots, \vec{p}^k) = \text{Span}(\vec{r}^1, A\vec{r}^1, \ldots, A^{k-1}\vec{r}^1)$
- ${}^t\vec{p}^k A\vec{p}^j = 0 \ \forall j < k$
- ${}^t\vec{r}^k A\vec{p}^j = 0 \ \forall j < k$
- The algorithm converges in at most n iterations.

Descent method — conjugate gradient (algorithm)

Algorithm

```
choose x(k=1)
p(1) = r(1) = b - A*x(1)
for k = 1 to convergence
   alpha(k) = r(k) . p(k) / p(k) . A * p(k)
   x(k+1) = x(k) + alpha(k) * p(k)
   r(k+1) = r(k) - alpha(k) * A * p(k)
   beta(k+1) = r(k+1) . r(k+1) / r(k) . r(k)
   p(k+1) = r(k+1) + beta(k+1) * p(k)
end for  //r(k) small
```

Descent method — GMRES

For generic matrices A

GMRES: General Minimal RESidual method

- Take a "fair" approximation $\vec{x}^k$ of the solution
- Construct the m-dimensional set of free vectors

$$\{\vec{r}^k, A\vec{r}^k, \ldots, A^{m-1}\vec{r}^k\}$$

  This spans the Krylov space H_m^k.
- Construct an orthonormal basis for H_m^k – e.g. via Gram-Schmidt

$$\{\vec{v}_1, \ldots, \vec{v}_m\}$$

- Look for a new approximation $\vec{x}^{k+1} \in H_m^k$:

$$\vec{x}^{k+1} = \sum_{j=1}^{m} X_j \vec{v}_j = [V]\vec{X}$$

- We obtain a system of n equations with m unknowns

$$A\vec{x}^{k+1} = A[V]\vec{X} = \vec{b}.$$

Descent method — GMRES (cont'd)

- Project on H_m^k
$$[{}^tV]A[V]\vec{X} = [{}^tV]\vec{b}.$$
- Solve this system of m equations with m unknowns
- $\vec{x}^{k+1} = [V]\vec{X}$.
- and so on...

To work well GMRES should be preconditioned!

Preconditioning – principle

Principle

Replace system $A\vec{x} = \vec{b}$ by $C^{-1}A\vec{x} = C^{-1}\vec{b}$
where $\mathrm{Cond}(C^{-1}A) \ll \mathrm{Cond}(A)$.

Which matrix C?

C should be easily invertible, typically the product of two triangular matrices.

- $C = \mathrm{diag}(A)$, simplest but well...
- incomplete Cholesky or LU factorization
- ...

Preconditioning – symmetry issues

Symmetry

Even if A and C are symmetric, $C^{-1}A$ may not be symmetric.
What if symmetry is needed?

Let $C^{-1/2}$ such that $C^{-1/2}C^{-1/2} = C^{-1}$.
Then $C^{-1/2}AC^{-1/2}$ is similar to $C^{-1}A$.

We consider the system

$$C^{+1/2}(C^{-1}A)C^{-1/2}C^{+1/2}\vec{x} = C^{+1/2}C^{-1}\vec{b}$$

$$(C^{-1/2}AC^{-1/2})C^{+1/2}\vec{x} = C^{-1/2}\vec{b}$$

Solve

$$(C^{-1/2}AC^{-1/2})\vec{y} = C^{-1/2}\vec{b}$$

and then

$$\vec{y} = C^{+1/2}\vec{x}.$$

Preconditioning – preconditioned conjugate gradient

Algorithm

```
choose x(k=1)
r(1) = b - A*x(1)
solve Cz(1) = r(1)
p(1) = r(1)
for k = 1 to convergence
   alpha(k) = r(k) . z(k) / p(k) . A * p(k)
   x(k+1) = x(k) + alpha(k) * p(k)
   r(k+1) = r(k) - alpha(k) * A * p(k)
   solve C z(k+1) = r(k+1)
   beta(k+1) = r(k+1) . z(k+1) / r(k) . z(k)
   p(k+1) = z(k+1) + beta(k+1) * p(k)
end for
```

At each iteration a system $C\vec{z} = \vec{r}$ is solved.

Storage – main issues

- Problems involve often a large number of variables, of degrees of freedom, say 10^6.
- To store a full matrix for a 10^6-order system, 10^{12} real numbers (if real) are needed... In simple precision this necessitates 4 To of memory.
- But high order problems are often very sparse.
- We therefore use a storage structure which consists in only storing relevant, non-zero, data.
- Access to one element A_{ij} should be very efficient.

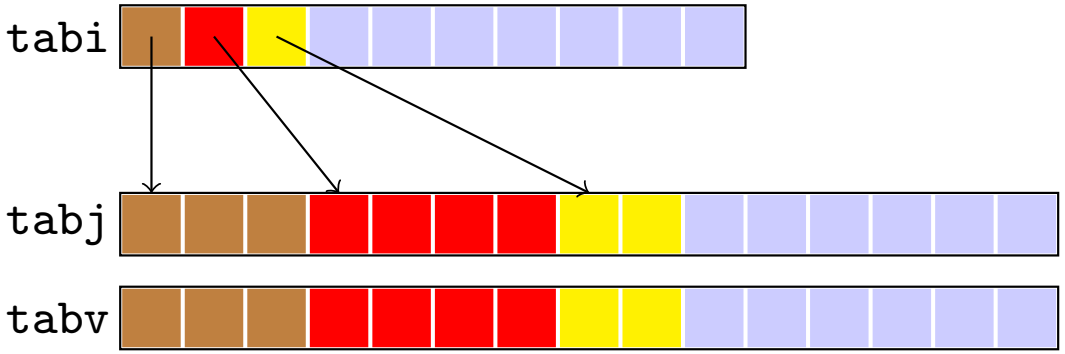
CDS: Compressed Diagonal Storage

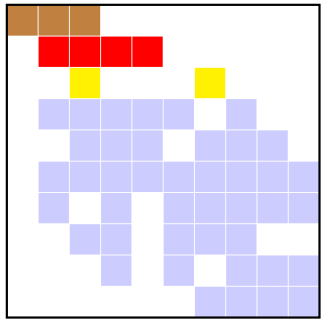
$$L(A) = \max_i L_i(A)$$

where

$$L_i(A) = \max_{j/A_{ij} \neq 0} |i - j|$$

CRS: Compressed Row Storage





- All the non-zero values of the matrix are stored in a table `tab`; they are stored line by line in the increasing order of columns.
- A table `tabj`, with same size than `tab` stores the column number of the values in `tabv`.
- A table `tabi` with size $n+1$ stores the indices in `tabj` of the first element of each line. The last entry is the size of `tabv`.

CCS: Compressed Column Storage = Harwell Boeing

Generalization to symmetric matrices

CRS: Compressed Row Storage – exercise

Question

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

CRS storage?

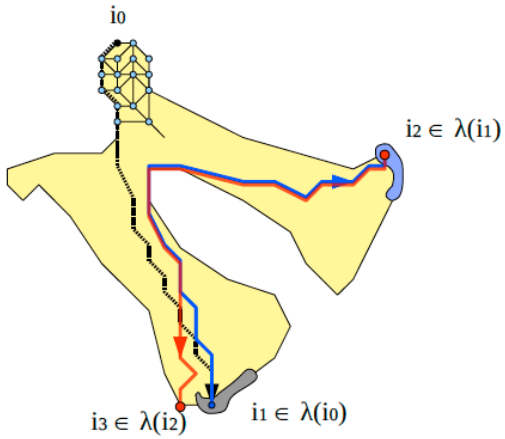
Solution

$$\begin{aligned} \texttt{tabi} &= \{1, 4, 6, 8, 10\} \\ \texttt{tabj} &= \{2, 3, 4, 1, 3, 2, 3, 3, 4\} \\ \texttt{tabv} &= \{4, 1, 6, 2, 5, 9, 7, 3, 8\} \end{aligned}$$

Cuthill–McKee algorithm – construction of a graph

Goal

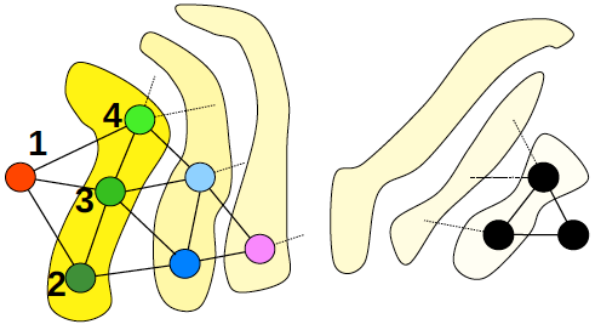
Reduce the bandwidth of a large sparse matrix by renumbering the unknowns.



Construction

- The nodes of the graph are the unknowns of the system. They are labelled with a number from 1 to n.
- The edges are the relations between the unknowns. Two unknowns i and j are linked if $A_{ij} \neq 0$.
- The distance $d(i, j)$ between two nodes is the minimal number of edges to follow to join both nodes.
- The excentricity $E(i) = \max_j d(i, j)$
- Far neighbors are $\lambda(i) = \{j / d(i, j) = E(i)\}$
- Graph diameter $D = \max_i E(i)$
- Peripheral nodes $P = \{j / E(j) = D\}$.

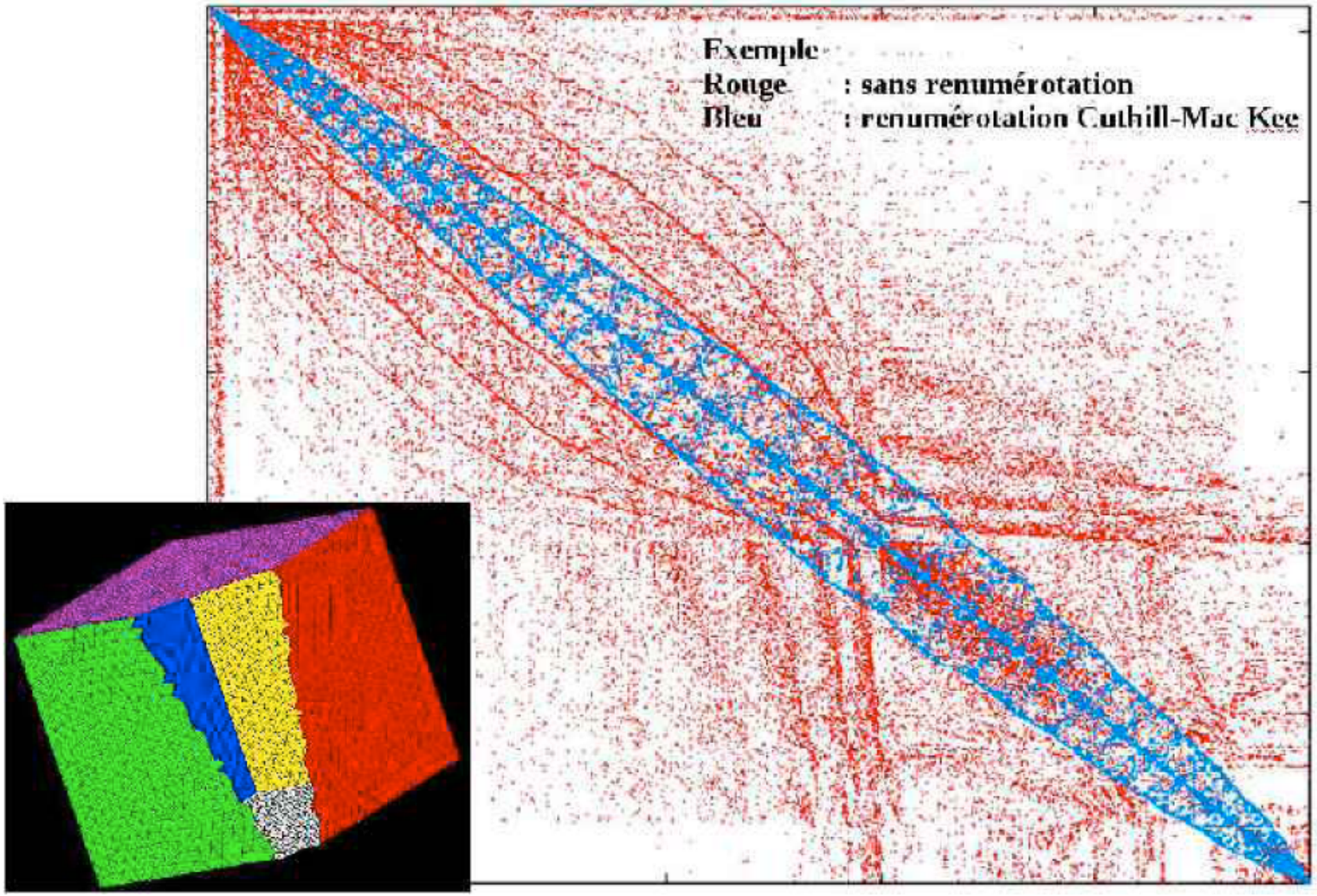
Cuthill–McKee algorithm – bandwidth reduction



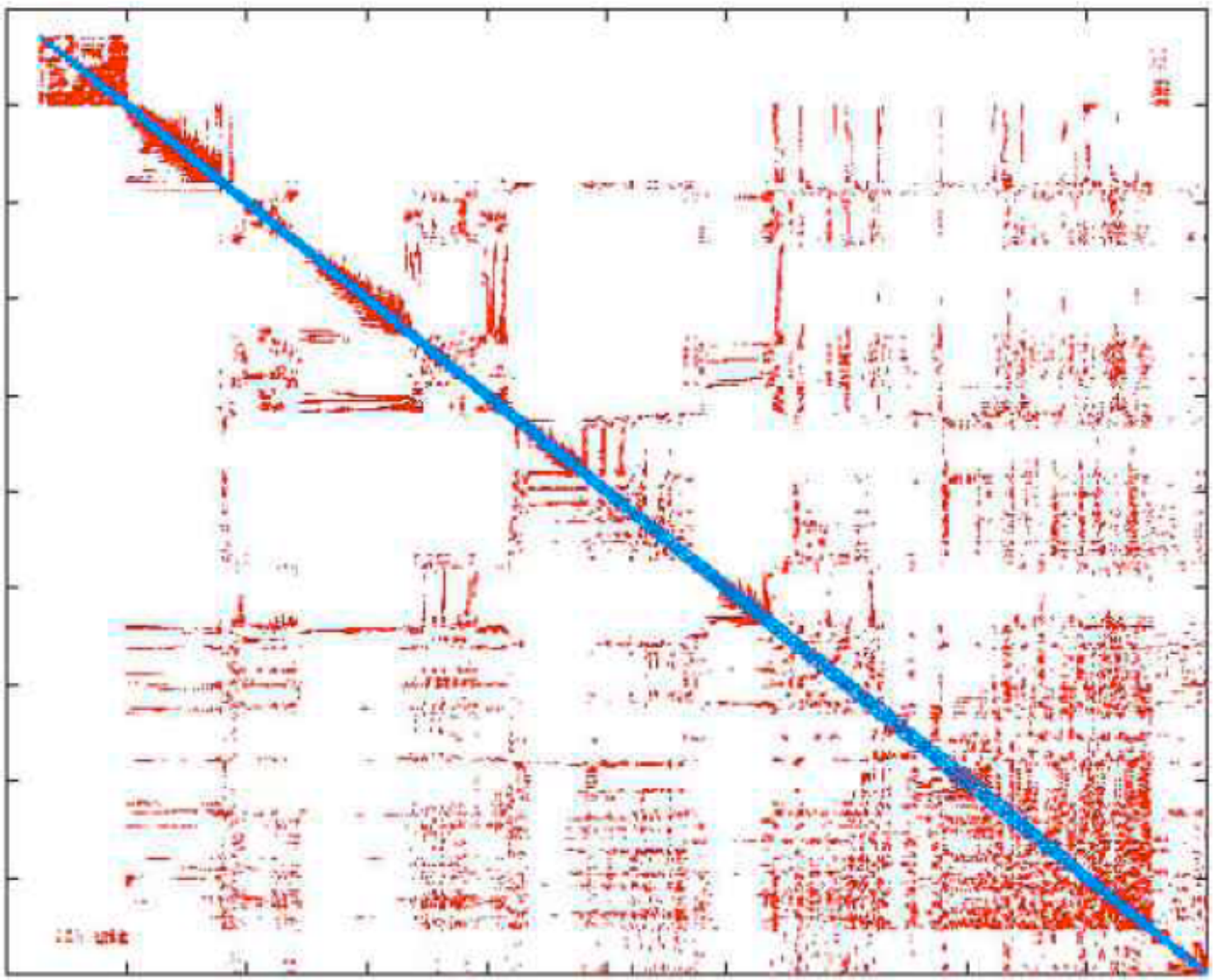
This graph is used to renumber the unknonws.

- Choose a first node and label it with 1.
- Attribute the new numbers (2,3,...) to the neighbors of node 1 with have the less non-labelled neighbors.
- Label the neighbors of node 2
- and so on...
- until all nodes are labelled.
- once this is done the numbering is reversed: the first become the last.

Cuthill–McKee algorithm – example 1



Cuthill–McKee algorithm – example 2



Bibliography

P. Lascaux, R. Théodor, *Analyse numérique matricielle appliquée à l'art de l'ingénieur* Volumes 1 and 2, 2ème édition, Masson (1997).

Gene H. Golub, Charles F. van Loan, *Matrix Computations*, 3rd edition, Johns Hopkins University Press (1996).