USN-HCMV PARIS 13

JOINT MASTER 2

# High Performance Computing

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**Purpose** : This is all about solving $Ax = b$, where $A$ is a square matrix and $b$ is a given righthand side, or a family of given righthand sides, and the size of the system is huge.

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# Chapitre 1

# Classical methods

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## 1.1 Direct methods

### 1.1.1 Gauss method

**Example**

$$\underbrace{\begin{pmatrix} 1 & 3 & 1 \\ 1 & 1 & -1 \\ 3 & 11 & 6 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} 9 \\ 1 \\ 36 \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} 9 \\ 1 \\ 36 \end{pmatrix}}_{b}$$

Take the $3 \times 4$ matrix $\bar{A} = [A \,|\, b]$. Define

$$M_1 = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix}$$

and multiply on the left by $M_1$ to put zeros under the diagonal in the first column :

$$M_1[A\,|\,b] = \left(\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 0 & -2 & -2 & -8 \\ 0 & 2 & 3 & 9 \end{array}\right).$$

Multiply now on the left by $M_2$ to put zeros under the diagonal in the second column :

$$M_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

$$M_2\,M_1[A\,|\,b] = \left(\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 0 & -2 & -2 & -8 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

Define $M = M_2 M_1$. Then the column $j$ of $M$ is the column $j$ of $M_j$ :

$$M = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 1 & 1 \end{pmatrix}.$$

$$M[A\,|\,b] = [MA\,|\,Mb].$$

$$Ax = b \iff MAx = Mb : M \text{ is a } \textbf{preconditioner}.$$

The matrix $U = MA$ is upper triangular, and solving $Ux = Mb$ is simpler than solving $Ax = b$. Define $L = M^{-1}$. In the column $j$, the entries below the diagonal are those of $M$ with a change of signe.

$$L := M^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & -1 & 1 \end{pmatrix}.$$

$$U = MA \iff A = LU, Ax = b \iff LUx = b \iff \begin{cases} Ly = b \\ Ux = y \end{cases}$$

Solving $Ax = b$ is then equivalent to performing the $LU$ decomposition, and solving two triangular systems. Counting of operations :

1. $LU$ decomposition $\mathcal{O}(\frac{2n^3}{3})$ elementary operations.
2. Solve $Ly = b$ $\quad \mathcal{O}(n^2)$ elementary operations.
3. Solve $Ux = y$ $\quad \mathcal{O}(n^2)$ elementary operations.

For $P$ values of the righthand side, $N_{op} \sim \frac{2n^3}{3} + P \times 2n^2$.

### 1.1.2 Codes

```
function x=BackSubstitution(U,b)
% BACKSUBSTITUTION solves by backsubstitution a linear system
% x=BackSubstitution(U,b) solves Ux=b, U upper triangular by
% backsubstitution
n=length(b);
```

```
for k=n:-1:1
s=b(k);
for j=k+1:n
s=s-U(k,j)*x(j);
end
x(k)=s/U(k,k);
end
x=x(:);
```

```
function x=Elimination(A,b)
% ELIMINATION solves a linear system by Gaussian elimination
% x=Elimination(A,b) solves the linear system Ax=b using Gaussian
% Elimination with partial pivoting. Uses the function
% BackSubstitution
n=length(b);
norma=norm(A,1);
A=[A,b]; % augmented matrix
for i=1:n
[maximum,kmax]=max(abs(A(i:n,i))); % look for Pivot A(kmax,i)
kmax=kmax+i-1;
if maximum < 1e-14*norma; % only small pivots
error('matrix is singular')
end
if i ~= kmax % interchange rows
h=A(kmax,:); A(kmax,:)=A(i,:); A(i,:)=h;
end
A(i+1:n,i)=A(i+1:n,i)/A(i,i); % elimination step
A(i+1:n,i+1:n+1)=A(i+1:n,i+1:n+1)-A(i+1:n,i)*A(i,i+1:n+1);
end
x=BackSubstitution(A,A(:,n+1));
```

### 1.1.3 Theoretical results

**Theorem 1.1 (Regular case)** *Let $A$ be an invertible matrix, with all principal minors $\neq 0$. Then there exists a unique matrix $L$ lower triangular with $l_{ii} = 1$ for all $i$, and a unique matrix $U$ upper triangular, such that $A = LU$. Furthermore $\det(A) = \prod_{i=1}^{n} u_{ii}$.*

**Theorem 1.2 (Partial pivoting)** *Let $A$ be an invertible matrix. There exist a permutation matrix $P$, a matrix $L$ lower triangular with $l_{ii} = 1$ for all $i$, and a matrix $U$ upper triangular, such that*

$$PA = LU$$

### 1.1.4 Symmetric definite matrices : Cholewski decomposition

**Theorem 1.3** *If $A$ is symmetric definite positive, there exists a unique lower triangular matrix $R$ with positive entries on the diagonal, such that $A = RR^T$.*

### 1.1.5 Elimination with Givens rotations

This is meant to avoid pivoting. It is used often in connection with the resolution of least-square problems. In the $i$ step of the Gauss algorithm, we need to eliminate $x_i$ in equations $i+1$ to $n$ of the reduced system :

$$\begin{array}{rccccccc}
(i): & a_{ii}x_i & +\cdots & + & a_{in}x_n & = & b_i \\
 & \vdots & \vdots & & & & \\
(k): & a_{ki}x_i & +\cdots & + & a_{kn}x_n & = & b_k \\
 & \vdots & \vdots & & & & \\
(i): & a_{ni}x_i & +\cdots & + & a_{nn}x_n & = & b_n
\end{array}$$

If $a_{ki}=0$, nothing needs to be done. If $a_{ki}\neq 0$, we multiply equation$(i)$ with $\sin\alpha$ and equation $(k)$ with $\cos\alpha$ and add. This leads to replacing equation $(k)$ by the linear combination

$$(k)_{new} = -\sin\alpha\cdot(i)+\cos\alpha\cdot(k).$$

The idea is to choose $\alpha$ such that the first coefficient in the line vanishes, *i.e.*

$$-\sin\alpha\cdot a_{ii}+\cos\alpha\cdot a_{ki}=0.$$

Since $a_{ki}\neq 0$, this defines $\mathrm{cotg}\alpha_{ki}$, that is $\alpha_{ki}$ modulo $\pi$. For stability reasons, line $(i)$ is also modified, end we end up with

$$\begin{array}{rcll}
(i)_{new} & = & \cos\alpha\cdot(i) & +\sin\alpha\cdot(k) \\
(k)_{new} & = & -\sin\alpha\cdot(i) & +\cos\alpha\cdot(k)
\end{array}$$

From which the sine and cosine of $\alpha_{ki}$ are obtained through well-known trigonometric formulas

$$\sin\alpha_{ki}=1/\sqrt{1+\mathrm{cotg}^2\alpha_{ki}}, \quad \cos\alpha_{ki}=\sin\alpha_{ki}\,\mathrm{cotg}\alpha_{ki}.$$

$$\begin{array}{rcll}
A_{ij\,new} & = & \cos\alpha_{ki}\cdot A_{ij} & +\sin\alpha_{ki}\cdot A_{kj} \\
A_{kj\,new} & = & -\sin\alpha_{ki}\cdot A_{ij} & +\cos\alpha_{ki}\cdot A_{kj}
\end{array}$$

```
function x=BackSubstitutionSAXPY(U,b)
% BACKSUBSTITUTIONSAXPY solves linear system by backsubstitution
% x=BackSubstitutionSAXPY(U,b) solves Ux=b by backsubstitution by
% modifying the right hand side (SAXPY variant)n=length(b);
n=length(b);
for i=n:-1:1
x(i)=b(i)/U(i,i);
b(1:i-1)=b(1:i-1)-x(i)*U(1:i-1,i);
end
x=x(:);
```

```
function x=EliminationGivens(A,b);
% ELIMINATIONGIVENS solves a linear system using Givens-rotations
% x=EliminationGivens(A,b) solves Ax=b using Givens-rotations. Uses
% the function BackSubstitutionSAXPY.
n=length(A);
for i= 1:n
for k=i+1:n
if A(k,i)~=0
cot=A(i,i)/A(k,i); % rotation angle
si=1/sqrt(1+cot^2); co=si*cot;
A(i,i)=A(i,i)*co+A(k,i)*si; % rotate rows
h=A(i,i+1:n)*co+A(k,i+1:n)*si;
A(k,i+1:n)=-A(i,i+1:n)*si+A(k,i+1:n)*co;
A(i,i+1:n)=h;
h=b(i)*co+b(k)*si; % rotate right hand side
b(k)=-b(i)*si+b(k)*co; b(i)=h;
end
end;
if A(i,i)==0
error('Matrix is singular');
end;
end
x=BackSubstitutionSAXPY(A,b);
```

### 1.1.6 QR Decomposition

Note $G^{ik}$ which differs from identity only on the rows $i$ and $k$ where

$$g_{ii} = g_{kk} = \cos\alpha, \quad g_{ik} = -g_{ki} = \sin\alpha$$

Example for $n = 5$,

$$G^{24} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \cos\alpha & 0 & \sin\alpha & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -\sin\alpha & 0 & \cos\alpha & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Multipliying a vector $b$ by $G^{ik}$ changes only the components $i$ and $k$,

$$G^{ik}\begin{pmatrix}\vdots\\ b_i\\ \vdots\\ b_k\\ \vdots\end{pmatrix} = \begin{pmatrix}\vdots & \\ \cos\alpha\cdot b_i & +\sin\alpha\cdot b_k\\ \vdots & \\ -\sin\alpha\cdot b_i & +\cos\alpha\cdot b_k\\ \vdots & \end{pmatrix}$$

$$G^{ik}\boldsymbol{e}_i = \cos\alpha\,\boldsymbol{e}_i - \sin\alpha\,\boldsymbol{e}_k, \quad G^{ik}\boldsymbol{e}_k = \sin\alpha\,\boldsymbol{e}_i + \cos\alpha\,\boldsymbol{e}_k.$$

$G^{ik}$ represents the rotation of angle $\alpha$ in the plane generated by $\boldsymbol{e}_i$ and $\boldsymbol{e}_k$. $(G^{ik}(\alpha))^* = G^{ik}(-\alpha)$, $(G^{ik}(\alpha))^* G^{ik}(\alpha) = I$. Thus it is an orthogonal matrix. By applying successively $G_{21}, \dots, G_{n1}$ whereever $a_{k1}$ is not zero, we put zeros under the diagonal in the first column. We continue the process until the triangular matrix $R$ is obtained. Then there are orthogonal matrices $G_1, \cdots, G_N$ such that Then

$$Q^* = G_N \dots G_1, \quad QA = R.$$

Q is an orthogonal matrix,

$$Q^*Q = G_N \dots G_1 G_1^* \dots G_N^* = I.$$

then

$$A = QR,$$

we have reached the $QR$ decomposition of the matrix $A$.

## 1.2 Stationary iterative methods

For any splitting $A = M - N$, write $Mx = Nx + b$,

Define the sequence $Mx^{m+1} = Nx^m + b$.

$$\begin{aligned} Mx^{m+1} = Nx^m + b &\iff Mx^{m+1} = (M-A)x^m + b\\ &\iff x^{m+1} = (I - M^{-1}A)x^m + M^{-1}b\\ &\iff x^{m+1} = x^m - M^{-1}Ax^m + M^{-1}b\\ &\iff \text{fixed point algorithm to solve } x - M^{-1}Ax + M^{-1}b = x\\ &\iff \text{fixed point algorithm to solve } M^{-1}Ax = M^{-1}b. \end{aligned}$$

Again, $M$ is a preconditioner.

**Definition 1.1**

- *$e^m := x - x^m$ is the error at step $m$.*
- *$r^m := b - Ax^m = Ae^m$ is the residual at step $m$.*
- *$R = M^{-1}N = I - M^{-1}A$ is the iteration matrix.*

Then the sequence of the errors satisfies

$$Me^{m+1} = Ne^m, \quad e^{m+1} = M^{-1}Ne^m$$

**Stopping criterion** Usually, one stops if $\frac{\|r^m\|}{\|b\|} < \varepsilon$.

### 1.2.1 Classical methods

Use $A = D - E - F$.

| | | |
|---|---|---|
| Jacobi | $M = D$ | $R := J = I - D^{-1}A$ |
| Relaxed Jacobi | $M = \frac{1}{\omega}D$ | $R = I - \omega D^{-1}A$ |
| Gauss-Seidel | $M = D - E$ | $R := \mathcal{L}_1 = I - D^{-1}A$ |
| SOR | $M = \frac{1}{\omega}D - E,$ | $R := \mathcal{L}_\omega = (D-\omega E)^{-1}((1-\omega)D + \omega F)$ |
| Richardson | $M = \frac{1}{\rho}I$ | $R = I - \rho A$ |

The relaxed methods are obtained as follows : define $\hat{x}^m$ as an application of Jacobi or Gauss-Seidel, then take the centroid of $\hat{x}^m$ and $x^m$ as $x^{m+1} = \omega\hat{x}^m + (1-\omega)x^m$.
For symmetric positive definite matrices $A$, RIchardson is a gradient method with fixed parameter. There is an optimal value for this parameter, given by $\rho_{opt} = \frac{2}{\lambda_1+\lambda_n}$ where the $\lambda_j$ are the eigenvaues of $A$.

### 1.2.2 Fundamentals tools

Define the sequence

$$e^{m+1} = Re^m, \ R = M^{-1}N.$$

Then $e^m = R^m e_0$, and for any norm

$$\|e^{m+1}\| \leq \|R\|\|e^m\|, \quad \|e^m\| \leq \|R^m\|\|e^0\|.$$

**Definition 1.2**

- *$\rho(R) = \max\{|\lambda|, \lambda$ eigenvalue of $R\}$ is the spectral radius of $R$.*
- *$\rho_m(R) = \|R^m\|^{1/m}$ is the mean convergence factor of $R$.*
- *$\rho_\infty(R) = \lim_{m\to\infty}\|R^m\|^{1/m}$ is the asymptotic convergence factor of $R$.*

**Theorem 1.4**

- *For any matrix $R$, for any norm, for any $m$, $\rho_m(R) \geq \rho(R)$. The sequence $\rho_m(R)$ has a limit, called the asymptotic convergence factor of $R$ and denoted by $\rho_\infty(R)$.*
- *The sequence $x^m$ is convergent for any $x^0$ if and only if $\rho(R) < 1$.*

To reduce the initial error by a factor $\varepsilon$, we need $m$ iterations, defined by

$$\frac{\|e^m\|}{\|e^0\|} \leq (\rho_m(R))^m \sim \varepsilon.$$

So $m \sim \dfrac{\log\varepsilon}{\log\rho_m(R)}$. It is easier to use the asymptotic value relation, $m \sim \dfrac{\log\varepsilon}{\log\rho_\infty(R)}$. Then to obtain another decimal digit in the solution, one needs to choose $\varepsilon = 10^{-1}$, then $\bar{m} \sim -\dfrac{\ln(10)}{\ln(\rho(R))}$.

**Definition 1.3** *The asymptotic convergence rate is* $F = -\ln(\rho(R))$.

## Diagonally dominant matrices

**Theorem 1.5**

- *If $A$ is a matrix, either strictly diagonally dominant, or irreducible and strongly diagonally dominant, then the Jacobi algorithm converges.*
- *If $A$ is a matrix, either strictly diagonally dominant, or irreducible and strongly diagonally dominant, then for $0 < \omega \leq 1$, the SOR algorithm converges.*

## $M$- matrices

**Definition 1.4** $A \in \mathbb{R}^{n\times n}$ *is a $M$-matrix if*

1. $a_{ii} > 0$ *for* $i = 1, \ldots, n$,
2. $a_{ij} \leq 0$ *for* $i \neq j$, $i, j = 1, \ldots, n$,
3. *$A$ is invertible,*
4. $A^{-1} \geq 0$.

**Theorem 1.6** *If $A$ is a M-matrix and $A = M - N$ is a regular splitting ($M$ is invertible and both $M^{-1}$ and $N$ are nonnegative), then the stationary method converges.*

## Symmetric positive definite matrices

**Theorem 1.7 (Householder-John)** *Suppose $A$ is positive. If $M + M^T - A$ is positive definite, then $\rho(R) < 1$.*

**Corollary 1.1**

1. *If $D+E+F$ is positive definite, then Jacobi converges.*
2. *If $\omega \in (0, 2)$, then SOR converges.*

## Tridiagonale matrices

**Theorem 1.8**

1. $\rho(\mathcal{L}_1) = (\rho(J))^2$ *: Jacobi Gauss-Seidel converge or diverge simultaneously. If convergent, Gauss-Seidel is twice as fast.*
2. *Suppose the eigenvalues of $J$ are real. Then Jacobi and SOR converge or diverge simultaneously for $\omega \in ]0, 2[$.*
3. *Same assumptions, SOR has an optimal parameter* $\omega^* = \dfrac{2}{1 + \sqrt{1 - (\rho(J))^2}}$, *and then* $\rho(\mathcal{L}_{\omega^*}) = \omega^* - 1$.

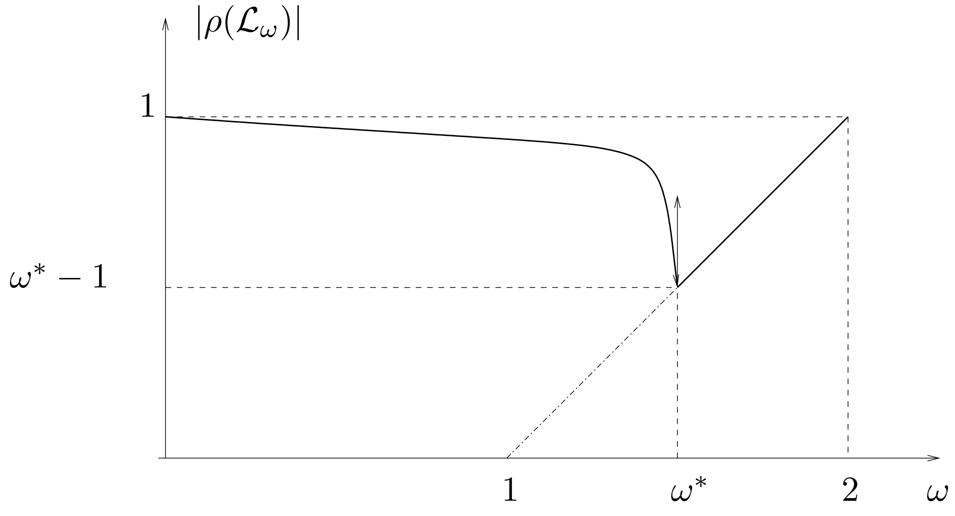


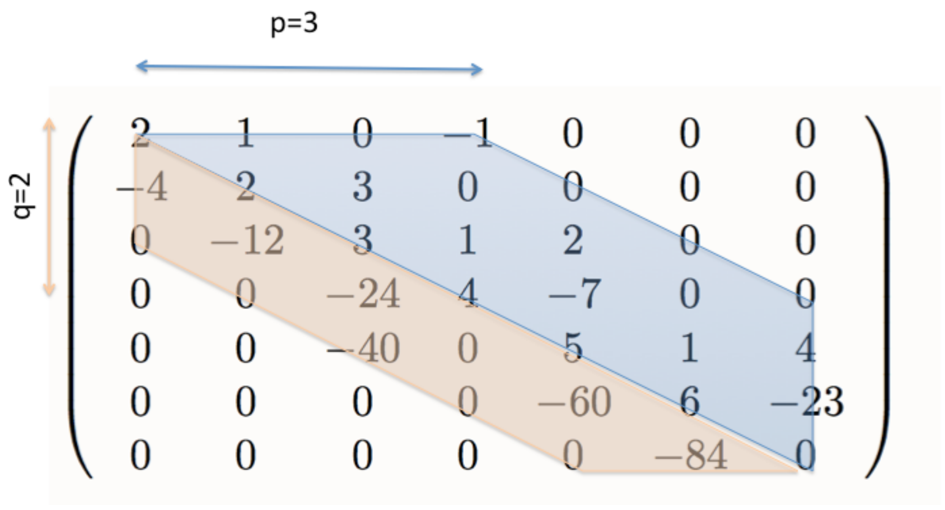
FIGURE 1.1 – Variations of $\rho(\mathcal{L}_\omega)$ as a fonction of $\omega$

## 1.3 Sparse and banded matrices

### 1.3.1 Direct methods

The first encounter of this name seems to be due to Wilkinson in 69 : *any matrix with enough zeros that it pays to take advantage of them.*

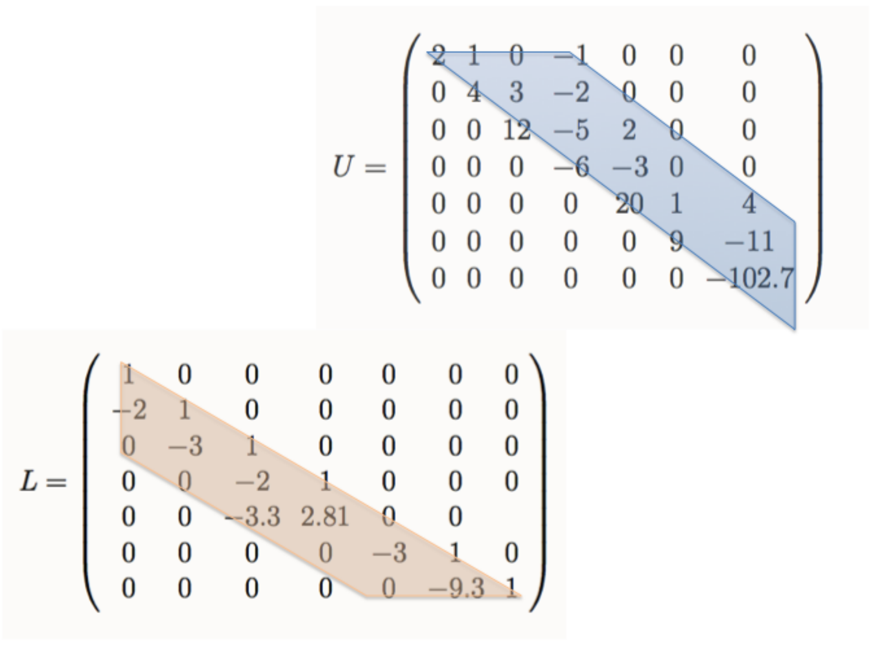
Example : a banded matrix, with upper bandwidth $p = 3$ and lower bandwidth $q = 2$, in total $p + q + 1$ nonzero diagonals.



$$\begin{pmatrix} 2 & 1 & 0 & -1 & 0 & 0 & 0 \\ -4 & 2 & 3 & 0 & 0 & 0 & 0 \\ 0 & -12 & 3 & 1 & 2 & 0 & 0 \\ 0 & 0 & -24 & 4 & -7 & 0 & 0 \\ 0 & 0 & -40 & 0 & 5 & 1 & 4 \\ 0 & 0 & 0 & 0 & -60 & 6 & -23 \\ 0 & 0 & 0 & 0 & 0 & -84 & 0 \end{pmatrix}$$

FIGURE 1.2 – A bandmatrix

Then $L$ is lowerbanded with $q = 2$, and $U$is upperbanded with $p = 3$.



$$U = \begin{pmatrix} 2 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 4 & 3 & -2 & 0 & 0 & 0 \\ 0 & 0 & 12 & -5 & 2 & 0 & 0 \\ 0 & 0 & 0 & -6 & -3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 20 & 1 & 4 \\ 0 & 0 & 0 & 0 & 0 & 9 & -11 \\ 0 & 0 & 0 & 0 & 0 & 0 & -102.7 \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & -3.3 & 2.81 & 0 & 0 & \\ 0 & 0 & 0 & 0 & -3 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -9.3 & 1 \end{pmatrix}$$

FIGURE 1.3 – LU decomposition

It is not the case anymore, when pivoting is used :

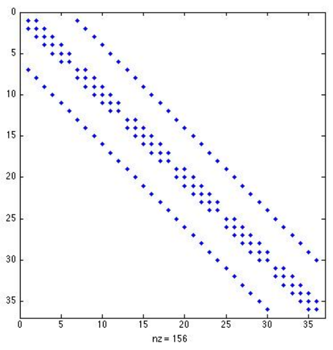
$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.6 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -0.5 & -0.17 & -0.05 & -0.21 & 0.025 & 0.0027 & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} -4 & 2 & 3 & 0 & 0 & 0 & 0 \\ 0 & -12 & 3 & 1 & 2 & 0 & 0 \\ 0 & 0 & -40 & 0 & 5 & 1 & 4 \\ 0 & 0 & 0 & 4 & -10 & -0.6 & -2.4 \\ 0 & 0 & 0 & 0 & -60 & 6 & -23 \\ 0 & 0 & 0 & 0 & 0 & -84 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.275 \end{pmatrix}$$

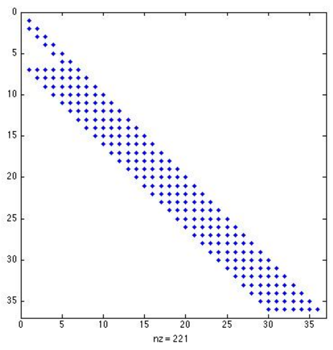
Here the permutation matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

In the Cholewsky decomposition, there is no need of permutation, unless some parameters are very small. Then if $A$ is banded, $R$ is banded with the same lower bandwidth, but it may be less sparse, in the sense that it can have more zeros. Consider as an example the $36 \times 36$ sparse matrix of $2 - D$ finite differences in a square. With the command `spy` de matlab, the nonzero terms appear in blue :



A bandmatrix sparse matrix



Corresponding Cholewski

Even though $R$ has the same bandwidth as $A$, nonzero diagonals appear.

EXERCISE Write the Gauss and Givens algorithms for a tridiagonal matrix $A = diag(c, -1) + diag(d, 0) + diag(e, 1)$.

**LU factorization** : verify that

$$c_k = l_k\, u_k,\ \ d_{k+1} = l_k\, f_k + u_{k+1},\ \ e_k = f_k.$$

then it is not necessary to compute $f_k$, and only recursively

$$c_k = l_k\, u_k, \quad u_{k+1} = d_{k+1} - l_k\, e_k.$$

```
n=length(d);
for k=1:n-1 % LU-decomposition with no pivoting
        c(k)=c(k)/d(k);
        d(k+1)=d(k+1)-c(k)*e(k);
end
for k=2:n % forward substitution
        b(k)=b(k)-c(k-1)*b(k-1);
end
b(n)=b(n)/d(n); % backward substitution
for k=n-1:-1:1
        b(k)=(b(k)-e(k)*b(k+1))/d(k);
end
```

**Givens** : verify that the process inserts an extra updiagonal.

```
n=length(d);
e(n)=0;
for i=1: n-1 % elimination
        if c(i)~=0
                t=d(i)/c(i); si=1/sqrt(1+t*t); co=t*si;
                d(i)=d(i)*co+c(i)*si; h=e(i);
                e(i)=h*co+d(i+1)*si; d(i+1)=-h*si+d(i+1)*co;
                c(i)=e(i+1)*si; e(i+1)=e(i+1)*co;
                h=b(i); b(i)=h*co+b(i+1)*si;
                b(i+1)=-h*si+b(i+1)*co;
        end;
end;
b(n)=b(n)/d(n); % backsubstitution
b(n-1)=(b(n-1)-e(n-1)*b(n))/d(n-1);
for i=n-2:-1:1,
        b(i)=(b(i)-e(i)*b(i+1)-c(i)*b(i+2))/d(i);
end;
```

**Creation and manipulation of sparse matrices in matlab**

```
>>S=sparse([2 3 1 2],[1 1 2 3],[2 4 1 3])

 S =
   (2,1)        2
   (3,1)        4
   (1,2)        1
   (2,3)        3

>>S=speye(2,3)

S =

   (1,1)        1
   (2,2)        1

>>n=4;
>>e=ones(n,1)
e =

     1
     1
     1
     1

>>A=spdiags([e -2*e e],-1:1,n,n)
A =

   (1,1)       -2
   (2,1)        1
   (1,2)        1
   (2,2)       -2
   (3,2)        1
   (2,3)        1
   (3,3)       -2
   (4,3)        1
   (3,4)        1
   (4,4)       -2

>>full(A)
ans =

    -2     1     0     0
     1    -2     1     0
     0     1    -2     1
     0     0     1    -2


>>S=sparse([2 3 1 2],[1 1 2 3],[2 4 1 3])
```

```
 S =

   (2,1)        2
   (3,1)        4
   (1,2)        1
   (2,3)        3

>>S=speye(2,3)

S =

   (1,1)        1
   (2,2)        1

>>n=4;
>>e=ones(n,1)
e =

     1
     1
     1
     1

>>A=spdiags([e -2*e e],-1:1,n,n)
A =

   (1,1)       -2
   (2,1)        1
   (1,2)        1
   (2,2)       -2
   (3,2)        1
   (2,3)        1
   (3,3)       -2
   (4,3)        1
   (3,4)        1
   (4,4)       -2

>>full(A)
ans =

    -2     1     0     0
     1    -2     1     0
     0     1    -2     1
     0     0     1    -2
```

The direct methods first transform the original system into a triangular matrix, and then solve the simpler triangular system. Therefore a direct method leads, modulo truncation errors, to the exact solution, after a number of operations which is a function of the size of the matrix. Thereby, when the matrix is sparse, the machine performs a large number of redundant operations due to the large number of multiplication by zero it performs.

### 1.3.2 Iterative methods

The iterative methods rely on a product matrix vector, therefore are easier to perform in a *sparse* way. They have gain a lot of popularity for sparse matrix, in conjunction with preconditioning and and domain decomposition. However their success relies on the convergence speed of the algorithm.

### 1.3.3 Implementation issues

To minimize computing costs and storage of a sparse matrix, it can be useful to renumber the matrix coefficients. There are (for the moment) no absolute ideal renumbering algorithms but one of the most efficient is the Reverse Cuthill Mackee algorithm.

It is also called the bandwidth reduction problem, also known in the field of sparse matrix applications as the bandwidth minimization problem (or BMP in short) :

For a given symmetric sparse matrix, A(nxn), the problem is to reduce its bandwidth B by permuting rows and columns so as to move all the non-zero elements of A in a band as close as possible to the diagonal.

In other words, the problem consists in transforming through successive row and column permutations as for example matrix A1 (8x8 input matrix) into A2 :

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

A1 A2

**Notions of Graph**

The graph G(A) corresponding to the matrix A we will have n nodes labelled i = 1,2, ... ,n. For each non-zero element aij, $i < j$ of A there will be an edge connecting nodes i and j. From the graph of A we can determine the position of all off-diagonal non-zero elements of A.

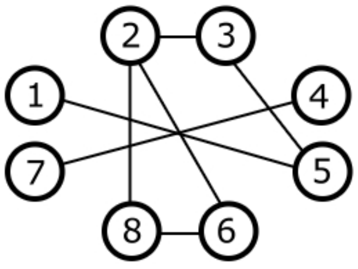
Two nodes of G(A) are said to be adjacent if they are connected by an edge.

Two nodes of G(A) are said to be connected if there is a sequence of edges joining them such that consecutive edges have a common end point. A graph is said to be connected if every pair of nodes of the graph are connected. If G(A) is connected, the corresponding matrix is irreducible.

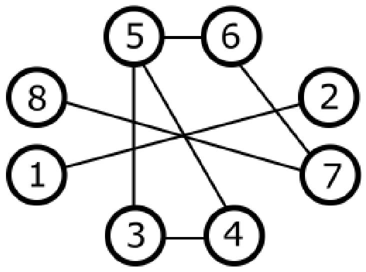
A component of a graph is a connected subgraph which is not contained in a larger connected subgraph.

The degree of a node i of G(A) is the number of edges meeting at i. For the corresponding matrix, this is the number of non-zero off diagonal elements in row i.

For example, the corresponding graphs of A1 and A2 are



Graph(A1)



Graph(A2)

The two graph structures are identical, the only thing that is different is the node (vertex) labelling. In other words the bandwidth reduction problem can also be viewed as a graph labelling problem :

Find the node labelling that minimizes the bandwidth B of the adjacency matrix of the graph G(A) , where we can formally define : B=max|Li-Lj|, i,j=1..n and Li is the label of node i, Lj is the label of node j and nodes i and j are adjacent.

**The Reverse Cuthill Mackee algorithm (RCM)**

This algorithm was presented by E. Cuthill and J. McKee in 1969 in REDUCING THE BANDWIDTH OF SPARSE SYMMETRIC MATRICES and improved by A. George

**Algorithm** RCM

```
Step 0 : Prepare an empty queue Q and an empty result array R. ;
Step 1 : Select the node in G(A) with the lowest degree (ties are
  broken arbitrarily) that hasn't previously been inserted in the result
  array. Let us name it P (for Parent). ;
Step 2 : Add P in the first free position of R. ;
Step 3 : Add to the queue all the nodes adjacent with P in the
  increasing order of their degree. ;
Step 4.1 : Extract the first node from the queue and examine it. Let
  us name it C (for Child). ;
Step 4.2 : If C hasn't previously been inserted in R, add it in the first
  free position and add to Q all the neighbours of C that are not in R
  in the increasing order of their degree. ;
Step 5 : If Q is not empty repeat from Step 4.1 . ;
Step 6 : If there are unexplored nodes (the graph is not connected)
  repeat from Step 1 . ;
Step 7 : Reverse the order of the elements in R. Element R[i] is
  swaped with element R[n+1-i]. ;
```

The result array will be interpreted like this : R[L] = i means that the new label of node i (the one that had the initial label of i) will be L.
Nodes are explored in the increasing order of their degree. Step 7 is not mandatory, it is the modification introduced by George to the initial algorithm (it has the purpose of further reducing the profile of a matrix).

Such a renumbering is also a good technique to reduce computing costs and storage space.

**Storage schemes**

The main goal is to represent only the non zero elements, and to be able to perform the common matrix operations. In the following, $N_Z$ denotes the total number of non zero elements. Only the most popular schemes are covered here.

— Compressed Sparse Row (CSR)
A real array AA that contains the real non zero values $a_{ij}$ stored row by row, from row 1 to n. The length of AA is $N_Z$
An integer array JA that contains the column indices of elements $a_{ij}$ as stored in AA. The length of JA is $N_Z$.
An integer array IA that contains the pointers to the beginning of each row in the arrays AA and JA. IA(1) = 0, IA(2) = number of

non zero elements in row 1, IA(ii+1)= IA(ii) + number of non zero elements in row ii. The length of IA is n+1, and IA(n+1) = $N_Z$

— Compressed Sparse Column (CSC)
A variation of CSR but based on storing columns instead of rows.

For example , matrix

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

FIGURE 1.4 – Matrix A

will be stored as follows/

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA | 1. | 2. | 3. | 4. | 5. | 6. | 7. | 8. | 9. | 10. | 11. | 12. |
| JA | 1 | 4 | 1 | 2 | 4 | 1 | 3 | 4 | 5 | 3 | 4 | 5 |
| IA | 1 | 3 | 6 | 10 | 12 | 13 | | | | | | |

FIGURE 1.5 – Sparse Matrix A storage

The case of a CSR storage leads to an efficient matrix vector product. The following Fortran 90 segment shows the main loop of the matrix-by-vector operation for matrices stored in the Compressed Sparse Row stored format.

```
DO I=1, N
   K1 = IA(I)
   K2 = IA(I+1)-1
   Y(I) = DOTPRODUCT(A(K1:K2),X(JA(K1:K2)))
ENDDO
```

FIGURE 1.6 – Sparse Matrix vector product

Notice that each iteration of the loop computes a different component of the resulting vector. This is advantageous because each of these components can be computed independently.

Solving a lower or upper triangular system is another important kernel in sparse matrix computations. The following segment of code shows a simple and parallel routine for solving LX = Y for the CSR storage format.

```
X(1) = Y(1)
DO I = 2, N
   K1 = IAL(I)
   K2 = IAL(I+1)-1
   X(I)=Y(I)-DOTPRODUCT(AL(K1:K2),X(JAL(K1:K2)))
ENDDO
```

FIGURE 1.7 – Computing LX = Y

# Chapitre 2

# Nonstationary methods

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## 2.1 Non-Stationary iterative methods. Symmetric definite positive matrices

**Descent methods**

### 2.1.1 Definition of the iterative methods

Suppose the descent directions $p_m$ are given beforehand. Define

$$\boxed{x^{m+1} = x^m + \alpha_m p^m, \quad e^{m+1} = e^m - \alpha_m p^m, \quad r^{m+1} = r^m - \alpha_m A p^m.}$$

Define the $A$ norm : $\boxed{\|y\|_A^2 = (Ay, y).}$

**Theorem 2.1** *$x$ is the solution of $Ax = b \iff$ it minimizes over $\mathbb{R}^N$ the functional $J(y) = \frac{1}{2}(Ay, y) - (b, y)$.*

This is equivalent to minimizing $G(y) = \frac{1}{2}(A(y-x), y-x) = \frac{1}{2}\|y-x\|_A^2$. At step $m$, $\alpha_m$ is defined such as to minimize $J$ in the direction of $p_m$. Define the quadratic function of $\alpha$

$$\varphi_m(\alpha) = J(x^m + \alpha p^m) = J(x^m) - \alpha(r^m, p^m) + \frac{1}{2}\alpha^2(Ap^m, p^m).$$

Minimizing $\varphi_m$ leads to

$$\boxed{\alpha_m = \frac{(p^m, r^m)}{(Ap^m, p^m)}, \quad (p^m, r^{m+1}) = 0}$$

$$G(x^{m+1}) = G(x^m)(1-\mu_m), \quad \mu_m = \frac{(r^m, p^m)^2}{(Ap^m, p^m)(A^{-1}r^m, r^m)}$$

- **Steepest descent (gradient à pas optimal)** $p^m = r^m$.

$$x^{m+1} = x^m + \alpha_m r^m, \quad e^{m+1} = e^m - \alpha_m r^m, \quad r^{m+1} = (I - \alpha_m A)p^m.$$

$$\boxed{\alpha_m = \frac{\|r^m\|^2}{(Ar^m, r^m)}, \quad (r^m, r^{m+1}) = 0}$$

$$G(x^{m+1}) = G(x^m)\left(1 - \frac{\|r^m\|^4}{(Ar^m, r^m)(A^{-1}r^m, r^m)}\right) \leq \left(\frac{\kappa(A)-1}{\kappa(A)+1}\right)^2 G(x^m)$$

- **Conjugate gradient**

$$x^{m+1} = x^m + \alpha_m p^m, \quad \alpha_m = \frac{(p^m, r^m)}{(Ap^m, p^m)}, \quad (r^m, p^{m-1}) = 0.$$

Search $p^m$ as $p^m = r^m + \beta_m p^{m-1}$

$$G(x^{m+1}) = G(x^m)(1-\mu_m)$$

$$\mu_m = \frac{(r^m, p^m)^2}{(Ap^m, p^m)(A^{-1}r^m, r^m)} = \frac{\|r^m\|^4}{(Ap^m, p^m)(A^{-1}r^m, r^m)}$$

Maximize $\mu_m$, or minimize

$$(Ap^m, p^m) = \beta_m^2(Ap^{m-1}, p^{m-1}) + 2\beta_m(Ap^{m-1}, r^m) + (Ar^m, r^m)$$

$$\beta_m = -\frac{(Ap^{m-1}, r^m)}{(Ap^{m-1}, p^{m-1})} \quad \Rightarrow (Ap^{m-1}, p^m) = 0$$

$$(r^m, r^{m+1}) = 0, \quad \beta_m = \frac{\|r^m\|^2}{\|r^{m-1}\|^2}.$$

**Properties of the conjugate gradient** Choose $p^0 = r^0$. Then $\forall m \geq 1$, if $r^i \neq 0$ for $i < m$.

1. $(r^m, p^i) = 0$ for $i \leq m-1$.
2. $\mathrm{vec}(r^0, \dots, r^m) = \mathrm{vec}(r^0, Ar^0, \dots, A^m r^0)$.
3. $\mathrm{vec}(p^0, \dots, p^m) = \mathrm{vec}(r^0, Ar^0, \dots, A^m r^0)$.
4. $(p^m, Ap^i) = 0$ for $i \leq m-1$.
5. $(r^m, r^i) = 0$ for $i \leq m-1$.

**Definition 2.1** *Krylov space $\mathcal{K}_m = vec(r^0, Ar^0, \dots, A^{m-1}r^0)$.*

**Theorem 2.2 (optimality of CG)** *A symétrique définie positive,*

$$\|x^m - x\|_A = \inf_{y \in x^0 + \mathcal{K}_m} \|y - x\|_A, \quad \|x\|_A = \sqrt{x^T A x}.$$

**Theorem 2.3** *Convergence in at most $N$ steps (size of the matrix). Furthermore*

$$G(x^m) \leq 4 \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^2 G(x^{m-1})$$

**The conjugate gradient algorithm**

$$x^0 \text{chosen}, \quad p^0 = r^0 = b - Ax^0.$$

while $m < Niter$ or $\|r^m\| \geq tol$, do

$$\begin{aligned}
\alpha_m &= \frac{\|r^m\|^2}{(Ap^m, p^m)}, \\
x^{m+1} &= x^m + \alpha_m p^m, \\
r^{m+1} &= r^m - \alpha_m A p^m, \\
\beta_{m+1} &= \frac{\|r^{m+1}\|^2}{\|r^m\|^2}, \\
p^{m+1} &= r^{m+1} - \beta_{m+1} p^m.
\end{aligned}$$

end.

### 2.1.2 Comparison of the iterative methods

**Basic example :**. 1-D Poisson equation $-u'' = f$ on $(0,1)$, with Dirichlet boundary conditions $u(0) = g_g, \; u(1) = g_d$. Introduce the second order finite difference stencil.

$$(0,1) = \cup (x_j, x_{j+1}), \quad x_{j+1} - x_j = h = \frac{1}{n+1}, \quad j = 0, \dots, n.$$

$$-\frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} \sim f(x_i), \quad i = 1, \dots n$$

$$u_0 = g_g, \quad u_{n+1} = g_d.$$

$$|u_i - u(x_i)| \leq h^2 \frac{\sup_{x\in[a,b]} |u^{(4)}(x)|}{12}$$

.

The vector of discrete unknowns is $u =^t (u_1, \dots, u_n)$.

$$A = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \quad b = \begin{pmatrix} f_1 - \frac{g_g}{h^2} \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n - \frac{g_d}{h^2} \end{pmatrix}$$

The matrix $A$ is symmetric definite positive.

The discrete problem to be solved is

$$Au = b$$

### 2.1.3 Condition number and error

$$Ax = b, \quad A\hat{x} = \hat{b}$$

Define $\kappa(A) = \|A\|_2 \|A^{-1}\|_2$. If $A$ is symmetric $> 0$, $\kappa(A) = \frac{\max \lambda_i}{\min \lambda_i}$.

**Theorem 2.4**

$$\frac{\|\hat{x} - x\|_2}{\|x\|_2} \leq \kappa(A) \frac{\|\hat{b} - b\|_2}{\|b\|_2}$$

*and there is a $b$ such that it is equal.*

Eigenvalues and eigenvectors of $A$ ($h \times (n+1) = 1$).

$$\mu_k = \frac{4}{h^2} \sin^2 \frac{k\pi h}{2}, \quad \Phi^{(k)} = \left(\sin \frac{jk\pi}{n+1}\right)_{1 \leq j \leq n},$$

$$\kappa(A) = \frac{\sin^2 \frac{n\pi h}{2}}{\sin^2 \frac{\pi h}{2}} = \frac{\cos^2 \frac{\pi h}{2}}{\sin^2 \frac{\pi h}{2}} \sim \frac{4}{\pi^2 h^2}$$

For any iterative method, the eigenfunctions of the iteration matrix are equal to those of $A$.

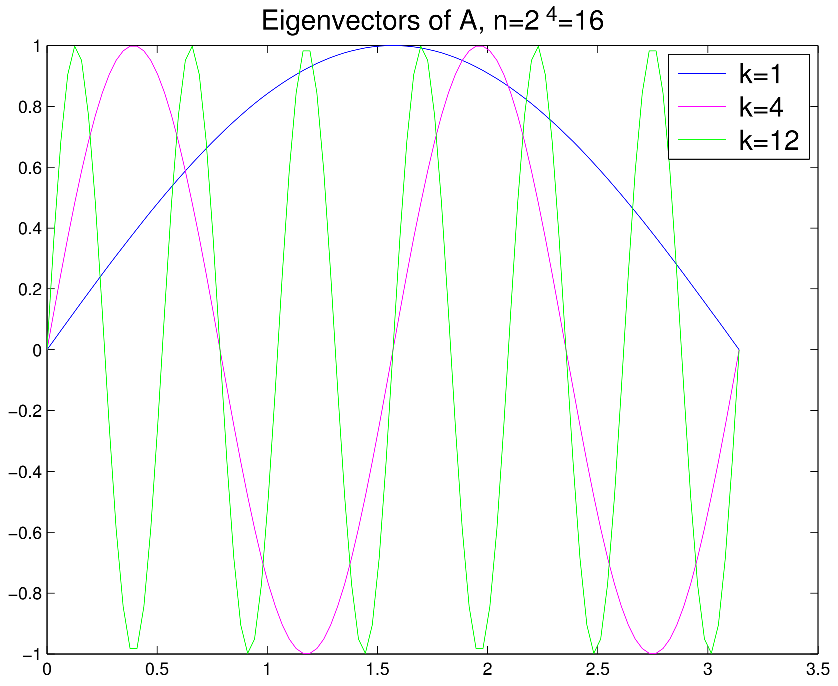

FIGURE 2.1 – Eigenvectors of $A$

| **Algorithm** | **Eigenvalues of the iteration matrix** $R$ |
|---|---|
| Jacobi | $\lambda_k(J) = 1 - \frac{h^2}{2}\mu_k = cos(k\pi h)$ |
| Gauss-Seidel | $\lambda_k(\mathcal{L}_1) = (\lambda_k(J))^2 = cos^2(k\pi h)$ |
| SOR | $\eta = \lambda_k(\mathcal{L}_\omega)$ solution of $(\eta + \omega - 1)^2 = \eta\omega(\lambda_k(J))^2$. |

TABLE 2.1 – Eigenvalues of the iteration matrix

| **Algorithm** | **Convergence factor** | $n = 5$ | $n = 30$ | $n = 60$ |
|---|---|---|---|---|
| Jacobi | $\cos \pi h$ | 0.81 | 0.99 | 0.9987 |
| Gauss-Seidel | $\cos^2 \pi h$ | 0.65 | 0.981 | 0.9973 |
| SOR | $\dfrac{1 - \sin \pi h}{1 + \sin \pi h}$ | 0.26 | 0.74 | 0.9021 |
| steepest descent | $\dfrac{K(A) - 1}{K(A) + 1} = \cos \pi h$ | 0.81 | 0.99 | 0.9987 |
| conjugate gradient | $\dfrac{\sqrt{K(A)} - 1}{\sqrt{K(A)} + 1} = \dfrac{\cos \pi h - \sin \pi h}{\cos \pi h + \sin \pi h}$ | 0.51 | 0.86 | 0.9020 |

TABLE 2.2 – Convergence factor

| Algorithm | convergence factor $\rho_\infty$ | convergence rate $F$ |
|---|---|---|
| Jacobi | $1-\frac{\varepsilon^2}{2}$ | $\frac{\varepsilon^2}{2}$ |
| Gauss-Seidel | $1-\varepsilon^2$ | $\varepsilon^2$ |
| SOR | $1-2\varepsilon$ | $2\varepsilon$ |
| Steepest descent | $1-\varepsilon^2$ | $1\varepsilon^2$ |
| conjugate gradient | $1-2\varepsilon$ | $2\varepsilon$ |

TABLE 2.3 – Asymptotic behavior in function of $\varepsilon = \pi h$

| $n$ | Jacobi and steepest descent | Gauss-Seidel | SOR | conjugate gradient |
|---|---|---|---|---|
| 10 | 56 | 28 | 4 | 4 |
| 100 | 4760 | 2380 | 38 | 37 |

TABLE 2.4 – Reduction factor for one digit $M \sim -\dfrac{\ln(10)}{F}$

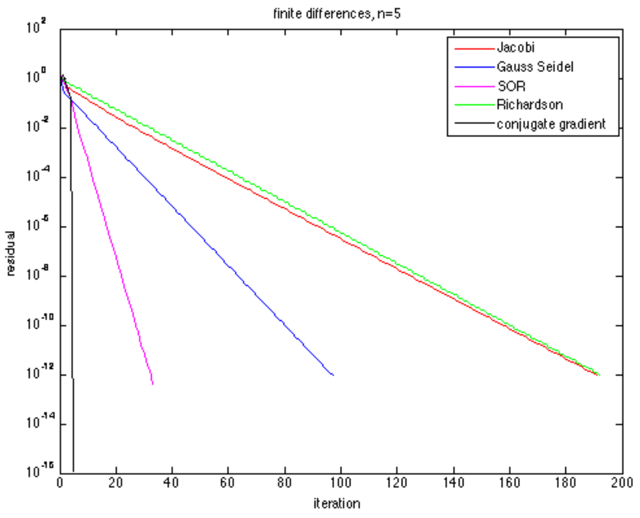

FIGURE 2.2 – Convergence history, $n = 5$

| | |
|---|---|
| Gauss elimination | $n^2$ |
| optimal overrelaxation | $n^{3/2}$ |
| FFT | $n\ln_2(n)$ |
| conjugate gradient | $n^{5/4}$ |
| multigrid | $n$ |

TABLE 2.5 – Asymptotic order of the number of elementary operations needed to solve the $1-D$ problem as a function of the number of grid points

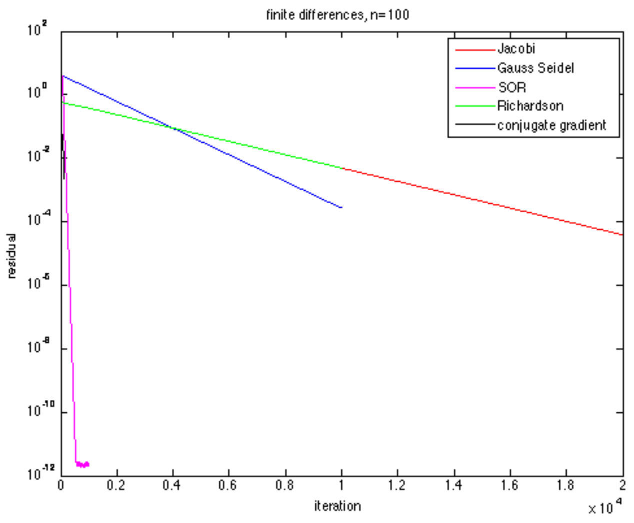

FIGURE 2.3 – Convergence history, $n = 100$

Not only the conjugate gradient is better, but the convergence rate being $\mathcal{O}(h^{1/2})$, the number of iterations necessary to increases the precision of one digit is multiplied by $\sqrt{10}$ when the mesh size is divided by 10, whereas for the Jacobi or Gauss-Seidel it is divided by 100. The miracle of multigrids, is that the convergence rate is independent of the mesh size.

## 2.2 Krylov methods for non symmetric matrices, Arnoldi algorithm

### 2.2.1 Gram-Schmidt orthogonalization and $QR$ decomposition

Starting with a free family $(v_1, \cdots, v_m, \cdots)$ in a vector space $E$ with a scalar product $(\cdot,\cdot)$, the process builds an orthonormal family $(w_1, \cdots, w_m, \cdots)$ recursively.

•. Define $w_1 = \dfrac{v_1}{\|v_1\|}$.

•. Note $r_{1,2} = (v_2, w_1)$, and define $u_2 = v_2 - r_{1,2}w_1$. By construction $u_2$ is orthogonal to $w_1$. It only remains to make it of norm 1 by defining $r_{2,2} = \|u_2\|$, $w_2 = \dfrac{u_2}{r_{2,2}}$.

•. Suppose we have built $(w_1, \cdots, w_{j-1})$ an orthonormal basis of $\mathcal{L}(v_1, \cdots, v_{j-1})$. Take $v_j$

and define $r_{i,j} = (v_j, w_i)$ for $1 \leq i \leq j-1$, and

$$u_j = v_j - \sum_{i=1}^{j-1} r_{i,j} w_i, \quad r_{j,j} = \|u_j\|, \quad w_j = \frac{u_j}{r_{j,j}}.$$

Then $(w_1, \cdots, w_j)$ is orthonormal. Furthermore, we can rewrite the previous equality as

$$v_j = r_{j,j} w_j + \sum_{i=1}^{j-1} r_{i,j} w_i,$$

which gives for each $j$ ;

$$v_j = \sum_{i=1}^{j} r_{i,j} w_i \, . \tag{2.1}$$

Define the matrix $K$ whose columns are the $v_j$, the matrix $Q$ whose columns are the $w_j$, and the upper triangular matrix $R$ whose coefficients are $r_{i,j}$ for $i \leq j$, and 0 otherwise. Then (2.1) takes the matrix form

$$K_{k,j} = \sum_{i=1}^{j} r_{i,j} Q_{k,i} \qquad K = QR \tag{2.2}$$

The matrix $Q$ is orthogonal, so this is exactly the so-called $QR$ decomposition of the matrix $K$. Note that the matrix K DOES NOT NEED TO BE SQUARE, nor the matrix $Q$, but the matrix $R$ has size $m \times m$.

### 2.2.2 Arnoldi algorithm

Let $A$ a $N \times N$ matrix. The purpose is to build recursively a orthonormal basis of the Krylov space $\mathcal{K}_m = vect(r, Ar, \cdots, A^{m-1}r)$ for $r \in \mathbb{R}^N$. We will take advantage of the special form of the generating family to proceed a slight modification of Gram Schmidt.
•. Define $q_1 = \dfrac{r}{\|r\|}$.
•. Now we must orthogonalize $q_1$ and $Ar$, or equivalently $q_1$ and $Aq_1$ :

$$h_{1,1} = (Aq_1, q_1), \quad u_2 = Aq_1 - h_{1,1} q_1, \quad h_{2,1} = \|u_2\|, \quad q_2 = \frac{u_2}{h_{2,1}}.$$

Then $q_2 \in Vec(q_1, Aq_1) = Vec(r, Ar) = \mathcal{K}_2$ and $(q_1, q_2)$ is an orthonormal basis of $\mathcal{K}_2$. All this can be rewritten as

$$Aq_1 = h_{1,1} q_1 + h_{2,1} q_2.$$

Then $\mathcal{K}_3 = Vec(q_1, q_2, A^2 r) = Vec(q_1, q_2, Aq_2)$. Therefore, instead of orthonormalizing with the new vector $A^2 r$, we can do it with the new vector $Aq_2$. Define

$$u_3 = Aq_2 - h_{1,2} q_1 - h_{2,2} q_2, \quad h_{2,2} = (Aq_2, q_2), \quad h_{1,2} = (Aq_2, q_1), \quad h_{3,2} = \|u_3\|, \; q_3 = \frac{u_3}{h_{3,2}}.$$

This generalizes in building an orthonormal basis of $\mathcal{K}_{j+1}$ by

$$u_{j+1} = Aq_j - \sum_{i=1}^{j} h_{i,j} q_i \; , \quad h_{i,j} = (Aq_j, q_i), \quad h_{j+1,j} = \|u_{j+1}\|, \; q_{j+1} = \frac{u_{j+1}}{h_{j+1,j}}.$$

**Theorem 2.5** *If the algorithm goes through $m$, then $(q_1, \ldots, q_m)$ is a basis of $\mathcal{K}_m$.*

Below is the matlab script

```
for j=1:m do
            h(i,j)=(A*v(j,:),v(i,:)) , i=1:i
      w(j,:)=A*v(j,:)—sum(h(i,j)v(i,:)
      h(j+1,j)=norm(w(j,:),2)
      If h(j+1,j) == 0 stop
      v(j+1,:)= w(j,:)/h(j+1,j)
```

The definition of the $q_j$ above can be rewritten as

$$Aq_j = \sum_{i=1}^{j+1} h_{i,j} q_i \ , \tag{2.3}$$

$$[Aq_1, \cdots, Aq_m] = [q_1, \cdots, q_m, q_{m+1}] \underbrace{\begin{bmatrix} h_{1,1} & & \cdots & & h_{1,m} \\ h_{2,1} & h_{2,2} & & \cdots & h_{2,m} \\ 0 & h_{3,2} & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & h_{m,m-1} & h_{m,m} \\ 0 & 0 & 0 & 0 & h_{m+1,m} \end{bmatrix}}_{\text{Hessenberg matrix } \widetilde{H}_m}$$

Define $V_m = [q_1, \cdots, q_m] \in \mathcal{M}_{N,m}(\mathbb{R})$ . $H_m$ is the $m \times m$ matrix obtained from the $(m+1) \times m$ matrix $\widetilde{H}_m$ by deleting the last row.

**Proposition 2.1**

$$AV_m = V_{m+1}\widetilde{H}_m = V_m H_m + h_{m+1,m} q_{m+1} e_m^T, \quad V_m^T A V_m = H_m. \tag{2.4}$$

Proof The first identity is just rewriting (2.3). As for the second one, rewrite the first one in blocks as

$$V_{m+1}\widetilde{H}_m = [V_m, q_{m+1}] \begin{bmatrix} H_m \\ h_{m+1,m} e_m^T \end{bmatrix} = V_m H_m + h_{m+1,m} q_{m+1} e_m^T.$$

Use this now in the first equality to obtain

$$AV_m = V_m H_m + h_{m+1,m} q_{m+1} e_m^T.$$

Multiply on the left by $V_m^T$. Since $V_m$ is orthogonal, and $V_m^T q_{m+1} = [(q_1, q_{m+1}), \cdots, (q_m, q_{m+1})]^T = 0$, we obtain

$$V_m^T A V_m = H_m.$$

■

### 2.2.3 Full orthogonalization method or FOM

Search for an approximate solution in $x_0 + \mathcal{K}_m(A, r_0)$ in the form $x_m = x_0 + V_m y$, and impose $r_m \perp \mathcal{K}_m(A, r_0)$. This is equivalent to $V_m^T r_m = 0$, which by

$$r_m = b - A(x_0 + V_m y) = r_0 - AV_m y$$

can be written by (2.4) as

$$V_m^T A V_m y = V_m^T r_0 \text{ or } H_m y = \|r_0\| e_1.$$

The small Hessenberg system

$$H_m y = \|r_0\| e_1 \tag{2.5}$$

can be solved at each step using a direct method : suppose all the principal minors of $H_m$ are nonzero. Due to the special structure of $H_m$, the $LU$ factorization of $H_m$ has the form

$$L = \begin{pmatrix} 1 & & \cdots & & 0 \\ l_1 & 1 & & \cdots & 0 \\ 0 & l_2 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & l_{m-1} & 1 \end{pmatrix}, \quad U = \begin{pmatrix} u_{11} & & \cdots & & u_{1m} \\ 0 & u_{22} & & \cdots & u_{2m} \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & u_{mm} \end{pmatrix}$$

The following matlab code gives the $LU$ factorization

```
 u(1,:)=h(1,:);
 for i=1:m-1
 l(i)=h(i+1,i)/u(i,i);
  for j=i+1:n
u(i+1,j)=h(i+1,j)-l(i)*u(i,j)
end
end
```

```
u(1,:)=h(1,:);
for i=1:m-1
l(i)=h(i+1,i)/u(i,i);
       for j=i+1:n
       u(i+1,j)=h(i+1,j)-l(i)*u(i,j)
       end
end
```

The computational cost is $m^2 + 2m - 1$ operations.

**Theorem 2.6** *At each step $m$, $r_m$ is parallel to $q_{m+1}$.*

**Proof**

$$r_m = r_0 - AV_my = r_0 - (V_mH_m + h_{m+1,m}q_{m+1}e_m^T)y = r_0 - V_mH_my - h_{m+1,m}y_mq_{m+1}.$$

But $H_my = \|r_0\|e_1$, therefore $r_0 - V_mH_my = r_0 - \|r_0\|V_me_1 = r_0 - \|r_0\|q_1 = 0$. Therefore $r_m = -h_{m+1,m}y_mq_{m+1}$ is parallel to $q_{m+1}$.

■

```
function [X,R,H,Q]=FOM(A,b,x0);
% FOM full orthogonalization method
% [X,R,H,Q]=FOM(A,b,x0) computes the decomposition A=QHQ?, Q
    orthogonal
% and H upper Hessenberg, Q(:,1)=r/norm(r), using Arnoldi in order to
% solve the system Ax=b with the full orthogonalization method. X
    contains
% the iterates and R the residuals
n=length(A); X=x0;
r=b-A*x0; R=r; r0norm=norm(r);
Q(:,1)=r/r0norm;
for k=1:n
    v =A*Q(:,k);
    for j=1:k
        H(j,k)=Q(:,j)'*v; v=v-H(j,k)*Q(:,j);
    end
    e0=zeros(k,1); e0(1)=r0norm; % solve system
    y=H\e0; x= x0+Q*y;
    X=[X x];
    R=[R b—A*x];
    if k<n
        H(k+1,k)=norm(v); Q(:,k+1)=v/H(k+1,k);
    end
end
```

### 2.2.4 GMRES algorithm

Here we minimize at each step the residual $r_m$ in $\mathcal{K}_m(A, r_0)$, which is equivalent to the minimization of $J(y) = \|r_0 - AV_m y\|_2$ for $y$ in $\mathbb{R}^m$, Use the Proposition to write

$$r_0 - AV_m y = \|r_0\|q_1 - V_{m+1}\widetilde{H}_m y = V_{m+1}(\|r_0\|e_1 - \widetilde{H}_m y).$$

Since $V_{m+1}$ is orthogonal, then

$$\|r_0 - AV_m y\| = \|\|r_0\|e_1 - \widetilde{H}_m y\|.$$

So in FOM we solve EXACTLY the square system $H_m y = \|r_0\|e_1$, while in GMRES we solve the LEAST SQUARE problem $\inf \|\|r_0\|e_1 - \widetilde{H}_m y\|$. This small minimization problem has a special form with a upper Hessenberg form, and is best solved by the Givens reflection method. Let us consider the case of $m = 3$ ($\sigma_0 = \|r_0\|$).

$$z = \widetilde{H}_3 y - \sigma_0 e_1 = \begin{pmatrix} h_{1,1} & h_{1,2} & h_{1,3} \\ h_{2,1} & h_{2,2} & h_{2,3} \\ 0 & h_{3,2} & h_{3,3} \\ 0 & 0 & h_{4,3} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} - \begin{pmatrix} \sigma_0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Multiply successively by the three $(m+1) \times (m+1)$ Givens matrices

$$Q_1 = \begin{pmatrix} c_1 & s_1 & 0 & 0 \\ -s_1 & c_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad Q_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & c_2 & s_2 & 0 \\ 0 & -s_2 & c_2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad Q_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_3 & s_3 \\ 0 & 0 & -s_3 & c_3 \end{pmatrix},$$

to make the system triangular, and even better

$$Q_3 Q_2 Q_1 z = \left(\begin{array}{ccc} \tilde{h}_{1,1} & \tilde{h}_{1,2} & \tilde{h}_{1,3} \\ 0 & \tilde{h}_{2,2} & \tilde{h}_{2,3} \\ 0 & 0 & \tilde{h}_{3,3} \\ \hline 0 & 0 & 0 \end{array}\right) \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} - \left(\begin{array}{c} c_1 \\ c_2 \\ c_3 \\ \hline c_4 \end{array}\right)$$

Therefore

$$\|z\|^2 = \|Q_3 Q_2 Q_1 z\|^2 = \|Ry - c^I\|^2 + (c_4)^2$$

where $R$ is the upperblock of the matrix, and $c^I$ the upperblock of the vector. Now we have a regular system, and $y$ is THE solution of

$$Ry = c^I,$$

which is now an upper triangular system.

```
function [x,iter,resvec] = GMRES(A,b,restart,tol,maxit)
%GMRES  Generalized Minimum Residual Method for Schwarz methods
%   [x,iter]=GMRES(A,b,RESTART,TOL,MAXIT) uses gmres to solve a
    system
```

```
%   Ax=b where A is defined as the procedure 'A'.
%   This is an adapted copy of Matlabs GMRES.

n = length(b);

n2b = norm(b);                    % Norm of rhs vector, b

% x0=rand(n,1);
% x0 = ones(n,1);
f=1;                              % all frequencies to initialize
x0 = sin((1:n/2)'/(n/2+1)*pi*f); x0=[x0; x0];
for f=2:n/2,
  x0 = x0+[sin((1:n/2)'/(n/2+1)*pi*f); sin((1:n/2)'/(n/2+1)*pi*f)];
end;

x = x0;

% Set up for the method
flag = 1;
xmin = x;                         % Iterate which has minimal residual
    so far
imin = 0;                         % Outer iteration at which xmin was
    computed
jmin = 0;                         % Inner iteration at which xmin was
    computed
tolb = tol * n2b;                 % Relative tolerance
if tolb==0,
  tolb=tol;                       % use absolute error to find zero
      solution
end;
r = b - feval(A,x);               % Zero-th residual
normr = norm(r);                  % Norm of residual

if normr <= tolb                  % Initial guess is a good enough
    solution
  flag = 0;
  relres = normr / n2b;
  iter = 0;
  resvec = normr;
  os = sprintf(['The initial guess has relative residual %0.2g' ...
                ' which is within\nthe desired tolerance %0.2g' ...
                ' so GMRES returned it without iterating.'], ...
                relres,tol);
  disp(os);
  return;
end


resvec = zeros(restart*maxit+1,1); % Preallocate vector for norm of
    residuals
```

```
resvec(1) = normr;                 % resvec(1) = norm(b-A*x0)
normrmin = normr;                  % Norm of residual from xmin
rho = 1;
stag = 0;                          % stagnation of the method

% loop over maxit outer iterations (unless convergence or failure)

for i = 1 : maxit
  V = zeros(n,restart+1);          % Arnoldi vectors
  h = zeros(restart+1,1);          % upper Hessenberg st A*V = V*H ...
  QT = zeros(restart+1,restart+1); % orthogonal factor st QT*H = R
  R = zeros(restart,restart);      % upper triangular factor st H = Q*R
  f = zeros(restart,1);            % y = R\f => x = x0 + V*y
  W = zeros(n,restart);            % W = V*inv(R)
  j = 0;                           % inner iteration counter

  vh = r;
  h(1) = norm(vh);
  V(:,1) = vh / h(1);
  QT(1,1) = 1;
  phibar = h(1);

  for j = 1 : restart
    j
%   MapU(x,sqrt(n),sqrt(n));

    u = feval(A,V(:,j));         % matrix multiply
    for k = 1 : j
      h(k) = V(:,k)' * u;
      u = u - h(k) * V(:,k);
    end
    h(j+1) = norm(u);
    V(:,j+1) = u / h(j+1);
    R(1:j,j) = QT(1:j,1:j) * h(1:j);
    rt = R(j,j);

% find cos(theta) and sin(theta) of Givens rotation
    if h(j+1) == 0
      c = 1.0;                      % theta = 0
      s = 0.0;
    elseif abs(h(j+1)) > abs(rt)
      temp = rt / h(j+1);
      s = 1.0 / sqrt(1.0 + temp^2); % pi/4 < theta < 3pi/4
      c = - temp * s;
    else
      temp = h(j+1) / rt;
      c = 1.0 / sqrt(1.0 + temp^2); % -pi/4 <= theta < 0 < theta <= pi/4
      s = - temp * c;
    end

    R(j,j) = c * rt - s * h(j+1);
%   zero = s * rt + c * h(j+1);

    q = QT(j,1:j);
    QT(j,1:j) = c * q;
    QT(j+1,1:j) = s * q;
    QT(j,j+1) = -s;
    QT(j+1,j+1) = c;
    f(j) = c * phibar;
    phibar = s * phibar;

    if j < restart
      if f(j) == 0                 % stagnation of the method
        stag = 1;
      end
      W(:,j) = (V(:,j) - W(:,1:j-1) * R(1:j-1,j))/ R(j,j);
% Check for stagnation of the method
      if stag == 0
        stagtest = zeros(n,1);
        ind = (x ~= 0);
        if ~(i==1 & j==1)
          stagtest(ind) = W(ind,j) ./ x(ind);
          stagtest(~ind & W(:,j) ~= 0) = Inf;
          if abs(f(j))*norm(stagtest,inf) < eps
            stag = 1;
          end
        end
      end
      x = x + f(j) * W(:,j);       % form the new inner iterate
    else % j == restart
      vrf = V(:,1:j)*(R(1:j,1:j)\f(1:j));
% Check for stagnation of the method
      if stag == 0
        stagtest = zeros(n,1);
        ind = (x0 ~= 0);
        stagtest(ind) = vrf(ind) ./ x0(ind);
        stagtest(~ind & vrf ~= 0) = Inf;
        if norm(stagtest,inf) < eps
          stag = 1;
        end
      end
      x = x0 + vrf;                % form the new outer iterate
    end
    normr = norm(b-feval(A,x));
    resvec((i-1)*restart+j+1) = normr;

    if normr <= tolb               % check for convergence
```

```
      if j < restart
        y = R(1:j,1:j) \ f(1:j);
        x = x0 + V(:,1:j) * y;     % more accurate computation of xj
        r = b - feval(A,x);
        normr = norm(r);
        resvec((i-1)*restart+j+1) = normr;
      end
      if normr <= tolb             % check using more accurate xj
        flag = 0;
        iter = [i j];
        break;
      end
    end

    if stag == 1
      flag = 3;
      break;
    end

    if normr < normrmin            % update minimal norm quantities
      normrmin = normr;
      xmin = x;
      imin = i;
      jmin = j;
    end
  end                              % for j = 1 : restart

  if flag == 1
    x0 = x;                        % save for the next outer
       iteration
    r = b - feval(A,x0);
  else
    break;
  end

end                                % for i = 1 : maxit

% returned solution is that with minimum residual

if n2b==0,
  n2b=1;          % here we solved for the zero solution and thus show
end;              % the absolute residual !

if flag == 0
  relres = normr / n2b;
else
  x = xmin;
  iter = [imin jmin];
  relres = normrmin / n2b;
end
```

```

% truncate the zeros from resvec
if flag <= 1 | flag == 3
  resvec = resvec(1:(i−1)∗restart+j+1);
else
  if j == 0
    resvec = resvec(1:(i−1)∗restart+1);
  else
    resvec = resvec(1:(i−1)∗restart+j);
  end
end


% only display a message if the output flag is not used
switch(flag)
    case 0,
      os = sprintf(['GMRES(%d) converged at iteration %d(%d) to a' ...
                    ' solution with relative residual %0.2g'], ...
                    restart,iter(1),iter(2),relres);

    case 1,
      os = sprintf(['GMRES(%d) stopped after the maximum %d iterations' ...
                    ' without converging to the desired tolerance %0.2g' ...
                    '\n         The iterate returned (number %d(%d))' ...
                    ' has relative residual %0.2g'], ...
                    restart,maxit,tol,iter(1),iter(2),relres);

    case 2,
      os = sprintf(['GMRES(%d) stopped at iteration %d(%d)' ...
                    ' without converging to the desired tolerance %0.2g' ...
                    '\n         because the system involving the' ...
                    ' preconditioner was ill conditioned.' ...
                    '\n         The iterate returned (number %d(%d))' ...
                    ' has relative residual %0.2g'], ...
                    restart,i,j,tol,iter(1),iter(2),relres);

    case 3,
      os = sprintf(['GMRES(%d) stopped at iteration %d(%d)' ...
                    ' without converging to the\n         desired' ...
                    ' tolerance %0.2g because the method stagnated.' ...
                    '\n         The iterate returned (number %d(%d))' ...
                    ' has relative residual %0.2g'], ...
                    restart,i,j,tol,iter(1),iter(2),relres);

end                             % switch(flag)
if flag == 0
  disp(os);
else
  warning(os);
end

semilogy(0:length(resvec)-1,resvec);
```

**Remark** If $A$ is symmetric, $H_m$ is tridiagonale.

**Restarted GMRES** For reasons of storage cost, the GMRES algorithm is mostly used by restarting every $M$ steps :

Compute $x_1, \cdots, x_M$.

If $r_M$ is small enough, stop,

else restart with $x_0 = x_M$.

# Chapitre 3

# Preconditioning

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## 3.1 Introduction

**Preconditioning : purpose**

Take the system $AX = b$, with $A$ symmetric definite positive, and the conjugate gradient algorithm. The speed of convergence of the algorithm deteriorates when $\kappa(A)$ increases. The purpose is to replace the problem by another system, better conditioned. Let $M$ be a symmetric regular matrix. Multiply the system on the left by $M^{-1}$.

$$AX = b \iff M^{-1}AX = M^{-1}b \iff (M^{-1}AM^{-1})MX = M^{-1}b$$

Define

$$\tilde{A} = M^{-1}AM^{-1}, \quad \tilde{X} = MX, \quad \tilde{b} = M^{-1}b,$$

and the new problem to solve $\tilde{A}\tilde{X} = \tilde{b}$. Since $M$ is symmetric, $\tilde{A}$ is symmetric definite positive. Write the conjugate gradient algorithm for this “tilde“ problem.

**The algorithm for $\tilde{A}$**

$$\tilde{X}^0 \text{ given}, \quad \tilde{p}^0 = \tilde{r}^0 = \tilde{b} - \tilde{A}\tilde{X}^0.$$

While $m < Niter$ or $\|\tilde{r}^m\| \geq tol$, do

$$\begin{aligned}
\alpha_m &= \frac{\|\tilde{r}^m\|^2}{(\tilde{A}\tilde{p}^m, \tilde{p}^m)}, \\
\tilde{X}^{m+1} &= \tilde{X}^m + \alpha_m \tilde{p}^m, \\
\tilde{r}^{m+1} &= \tilde{r}^m - \alpha_m \tilde{A}\tilde{p}^m, \\
\beta_{m+1} &= \frac{\|\tilde{r}^{m+1}\|^2}{\|\tilde{r}^m\|^2}, \\
\tilde{p}^{m+1} &= \tilde{r}^{m+1} - \beta_{m+1}\tilde{p}^m.
\end{aligned}$$

Now define

$$p^m = M^{-1}\tilde{p}^m, \quad X^m = M^{-1}\tilde{X}^m, \quad r^m = M\tilde{r}^m,$$

and replace in the algorithme above.

**The algorithm for $A$**

$$Mp^0 = M^{-1}r^0 = M^{-1}b - M^{-1}AM^{-1}MX^0 \iff \begin{cases} p^0 = M^{-2}r^0, \\ r^0 = b - AX^0. \end{cases}$$

$$\|\tilde{r}^m\|^2 = (M^{-1}r^m, M^{-1}r^m) = (M^{-2}r^m, r^m)$$

Define $\boxed{z^m = M^{-2}r^m}$. Then $\boxed{\beta_{m+1} = \dfrac{(z^{m+1}, r^{m+1})}{(z^m, r^m)}}$.

$$(\tilde{A}\tilde{p}^m, \tilde{p}^m) = (M^{-1}AM^{-1}Mp^m, Mp^m) = (Ap^m, p^m)$$

$$\Rightarrow \boxed{\alpha_m = \frac{(z^m, r^m)}{(Ap^m, p^m)}}.$$

$$MX^{m+1} = MX^m + \alpha_m Mp^m \iff \boxed{X^{m+1} = X^m + \alpha_m p^m}.$$

$$M^{-1}r^{m+1} = M^{-1}r^m - \alpha_m M^{-1}AM^{-1}Mp^m \iff \boxed{r^{m+1} = r^m - \alpha_m Ap^m}.$$

$$Mp^{m+1} = M^{-1}r^{m+1} - \beta_{m+1}Mp^m \iff \boxed{p^{m+1} = z^{m+1} - \beta_{m+1}p^m}.$$

**The algorithm for $A$**
Define $C = M^2$.

$$X^0 \text{ given}, \quad r^0 = b - AX^0, \quad \text{solve } Cz^0 = r^0, \quad p^0 = z^0.$$

While $m < Niter$ or $\|r^m\| \geq tol$, do

$$\begin{aligned} \alpha_m &= \frac{(z^m, r^m)}{(Ap^m, p^m)}, \\ X^{m+1} &= X^m + \alpha_m p^m, \\ r^{m+1} &= r^m - \alpha_m Ap^m, \\ \text{solve } Cz^{m+1} &= r^{m+1}, \\ \beta_{m+1} &= \frac{(z^{m+1}, r^{m+1})}{(z^m, r^m)}, \\ p^{m+1} &= z^{m+1} - \beta_{m+1}p^m. \end{aligned}$$

**How to choose $C$**
$C$ must be chosen such that

1. $\tilde{A}$ is better conditioned than $A$,
2. $C$ is easy to invert.

Use an iterative method such that $A = C - N$ with symmetric $C$. For instance it can be a symmetrized version of SOR, named SSOR, defined for $\omega \in (0, 2)$ by

$$C = \frac{1}{\omega(2-\omega)}(D - \omega E)D^{-1}(D - \omega F).$$

Notice that if $A$ is symmetric definite positive, so is $D$ and its coefficients are positive, then its square root $\sqrt{D}$ is defined naturally as the diagonal matrix of the square roots of the coefficients. Then $C$ can be rewritten as

$$C = SS^T, \quad \text{with } S = \frac{1}{\sqrt{\omega(2-\omega)}}(D - \omega E)D^{-1/2},$$

yielding a natural Cholewski decomposition of $C$.

Another possibility is to use an incomplete Cholewski decomposition of $A$. Even if $A$ is sparse, that is has many zeros, the process of LU or Cholewski decomposition is very expensive, since it creates non zero values.

**Example : Matrix of finite differences in a square**

Poisson equation

$$-(\Delta_h u)_{i,j} = -\frac{1}{h^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) - \frac{1}{h^2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) = f_{i,j}, \quad 1 \le i \le M, 1 \le j \le M$$

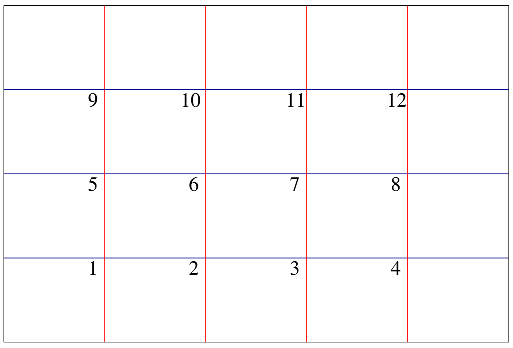


FIGURE 3.1 – Numbering by line

The point $(x_i, y_j)$ has for number $i+(j-1)M$. A vector of all unknowns $X$ is created :

$$Z = (u_{1,1}, u_{2,1}, u_{M,1}), (u_{1,2}, u_{2,2}, u_{M,2}), \cdots (u_{1,M}, u_{2,M}, u_{M,M})$$

with $Z_{i+(j-1)*M} = u_{i,j}$.
If the equations are numbered the same way (equation #$k$ is the equation at point $k$), the matrix is block-tridiagonal :

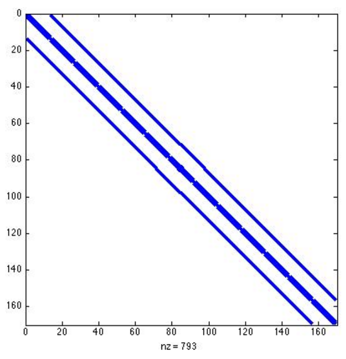
$$A = \frac{1}{h^2}\begin{pmatrix} B & -C & & 0_M & \\ -C & B & -C & & \\ & \ddots & \ddots & \ddots & \\ & & -C & B & -C \\ & 0_M & & -C & B \end{pmatrix} \tag{3.1}$$

$$C = I_M, \quad B = \begin{pmatrix} 4 & -1 & & 0 & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & 0 & & -1 & 4 \end{pmatrix}$$

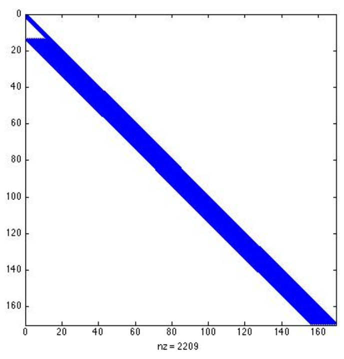
The righthand side is $b_{i+(j-1)*M} = f_{i,j}$, and the system takes the form $AZ = b$.

**Cholewski decomposition of $A$**

The block-Cholewski decomposition of $A$, $A = RR^T$, is block-bidiagonale, but the blocks are not tridiagonale as in $A$, as the `spy` command of matlab can show, in the case where $M = 15$.



spy(A)



spy(R)

However, if we look closely to the values of $R$ between the main diagonales where $A$ was non zero, we see that where the coefficients of $A$ are zero, the coefficients of $R$ are small. Therefore the incomplete Cholewski preconditioning computes only the values of $R$ where the coefficient of $A$ is not zero, and gains a lot of computational time.

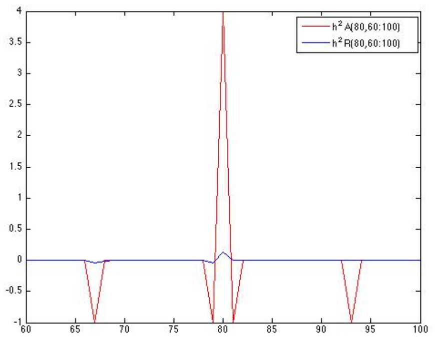


FIGURE 3.2 – Variation of the coefficients of Cholewski in the line 80 for $M = 15$

The matlab codes are as follows ([3])

**Cholewski**

```
Ch=tril(A);
for k=1:nn
    Ch(k,k)=sqrt(Ch(k,k));
    Ch(k+1:nn,k)=Ch(k+1:nn,k)/Ch(k,
        k);
    for j=k+1:nn
        Ch(j:nn,j)=Ch(j:nn,j)-Ch(j:
            nn,k)*Ch(j,k);
    end
end
```

**Incomplete Cholewski**

```
ChI=tril(A);
for k=1:nn
    ChI(k,k)=sqrt(ChI(k,k));
    for j=k+1:nn
        if ChI(j,k) ~= 0
            ChI(j,k)=ChI(j,k)/ChI(k,k);
        end
    end
    for j=k+1:nn
        for i=j:n
            if ChI(i,j) ~= 0
                ChI(i,j)=ChI(i,j)-ChI(i,k)*ChI(j,k);
            end
        end
    end
end
```

Then use $C = R * R^T$.

**Comparison** For the 2-D finite differences matrix and $n = 25$ internal points in each direction, we compare the convergence of the conjugate gradient and various preconditioning : Gauss-Seidel, SSOR with optimal parameter, and incomplete Cholewski. The gain even with $\omega = 1$ is striking. Furthermore Gauss-Seidel is comparable with Incomplete Cholewski.

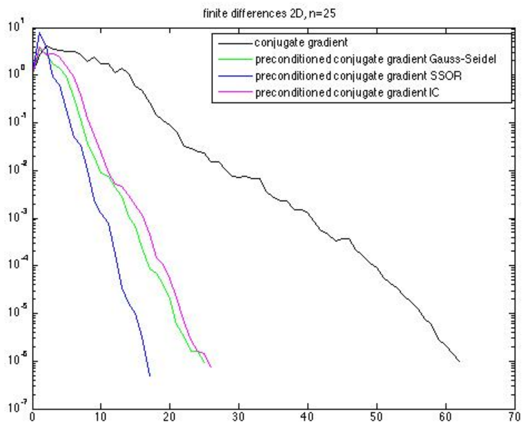


FIGURE 3.3 – Convergence history, influence of preconditioning

## 3.2 Deflation method for GMRES

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Recall the restarted GMRES algorithm to solve $Ax = b$ :

```
Algorithm GMRES(m)
Choose $x_0$ ;
1. $r_0 = b - Ax_0$ , $\beta = \|r_0\|$, $v_1 := r_0/\beta$ ;
2. Generate the Arnoldi basis applied to $A$ and the associated Hessenberg matrix
   $\tilde{H_m}$ starting with $v_1$;
3. Compute $y_m$ which minimises $\|\beta e_1 - \tilde{H_m} y\|$ and $x_m = x_0 + V_m y_m$ ;
4. If convergence Stop, else set $x_0 = x_m$ and Go To 1 ;
```

Here we choose a right preconditioning $M$ in order to garantee a non increasing residual. This would not be true with a left preconditioner since the residual is multiplied by $M-1$
This preconditioner can change at each restart. The algorithm becomes

```
Algorithm PRECGMRES(m)
Choose $x_0$ ;
Choose $M$ ;
1. $r_0 = b - Ax_0$ , $\beta = \|r_0\|$, $v_1 := r_0/\beta$ ;
2. Generate the Arnoldi basis applied to $AM^{-1}$ and the associated Hessenberg
   matrix $\tilde{H_m}$ starting with $v_1$;
3. Compute $y_m$ which minimises $\|\beta e_1 - \tilde{H_m} y\|$ and $x_m = x_0 + M^{-1} V_m y_m$ ;
4. If convergence Stop, else set $x_0 = x_m$ update $M$ and Go To 1 ;
```

The objective of deflation is to remove the smallest eigenvalues of $A$ which slow down the GMRES convergence. With a restarted GMRES, information on these eigenvalues is lost which explains why restarted GMRES can be quite slow and even fail to converge. Deflation aims to replace them by real positive eigenvalues equal to the largest modulus of the eigenvalues.

## 3.2.1 Building the preconditioner

In the following we assume that A is diagonalizable in $\mathbb{C}$ with eigenvalues $|\lambda_1| \leq |\lambda_2| \leq |\lambda_n|$.
Let P be an invariant subspace of dimension r corresponding to the r smallest eigenvalues of A and U an orthonormal basis of P. The deflating preconditioner is based on the idea that the linear system is solved exactly in space P.

**Theorem 3.1** *if $T = U^T AU$ and $M = I_n + U(1/|\lambda_n| T - I_r)U^T$ then $M$ is non singular and $M^{-1} = I_n + U(|\lambda_n| T^{-1} - I_r)U^T$ and the eigenvalues of $AM^{-1}$ are $\lambda_{r+1}, \lambda_{r+2}, ..., \lambda_r, |\lambda_n|$, and $|\lambda_n|$ is an eigenvalue of multiplicity at least r.*

**Note** : If only a close approximation $\tilde{P}$ is known , an improved convergence rate is still to be obtained.

## 3.2.2 Computing the invariant subspace

The GMRES algorithm provides the Hesssenberg matrix $H_k = {V_k}^T AV_k$, which is the restriction of A onto the Krylov subspace $K(k, A, r_0)$. The eigenvalues of $H_k$ are called Ritz values. Let $H_k = SRS^T$ be the Schur canonical form of $H_k$ with the eigenvalues ordered by increasing values. Then vectors $U = V_k S$ approximate the Schur vectors of

A. The largest Ritz value approximates the largest eigenvalue of A thus providing a first approximation of $M$.

After each restart new Ritz values can be estimated approximating eigenvalues of $AM^{-1]}$ also approximating remaining eigenvalues of A. By increasing the invariant subspace at each restart , a more powerful preconditioner is thus built.
To avoid loss of orthogonality , these vectors are orthogonalized against the previous basis $U$ .

**Note** : In some sense this algorithm recovers the superlinear convergence of the full GMRES version which behaves as if the smallest eigenvalues were removed. The preconditioner keeps the information on the smallest Ritz values which would be lost by restarting.

```
**Algorithm** DEFLGMRES(m)
Choose $x_0$ ;
$M = I_n$ ;
U= ;
1. $r_0 = b - Ax_0$ , $\beta = \|r_0\|$, $v_1 := r_0/\beta$ ;
2. Generate the Arnoldi basis applied to $AM^{-1}$ and the associated Hessenberg
  matrix $\tilde{H_m}$ starting with $v_1$;
3. Compute $y_m$ which minimises $\|\beta e_1 - \tilde{H_m} y\|$ and $x_m = x_0 + M^{-1}V_m y_m$ ;
4. If convergence Stop, else set ;
      $x_0 = x_m$ ;
      Compute l Schur vectors of $H_m$ noted $S_l$ ;
      Compute the approximation of $|\lambda_n|$ ;
      Orthogonalize $V_m S_l$ against $U$ ;
      Increase $U$ with $V_m S_l$ ;
      $T = U^T AU$ ;
      $M^{-1} = I_n + U(|\lambda_n| T^{-1} - I_r)U^T$ ;
      Go To 1 ;
```

### 3.2.3 Numerical results

Results on two matrices of dimension 100 are given . A has the form $A = SDS^{-1}$ with $S = (1, \beta)$ an upper bidiagonal matrix.
Case 1 : $\beta = 0.9$ and $D = diag(1, 2, ..., 100)$
Case 2 : $\beta = 0.9$ and $D = diag(1, 100, 200, ..., 10000)$

DEFLGMRES(10,1) is compared with GMRES(10) and full GMRES . Tolerance is set to $10^{-8}$

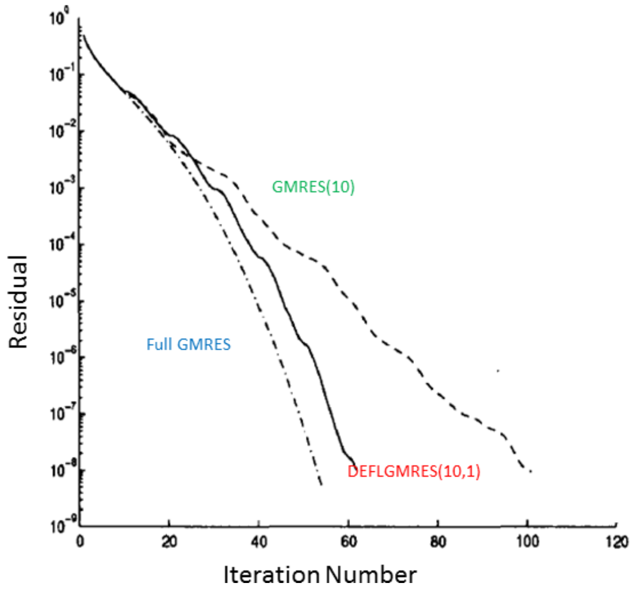

FIGURE 3.4 – Convergence history, Case 1

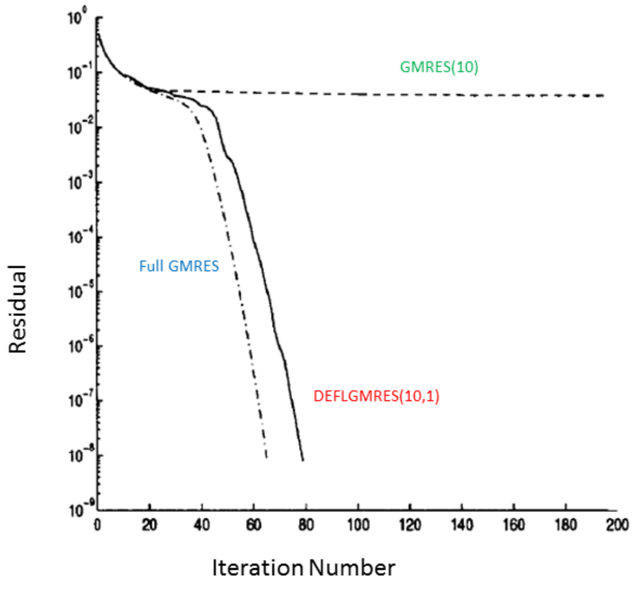

FIGURE 3.5 – Case 2

## 3.3 Fast methods using Fast Fourier Transform

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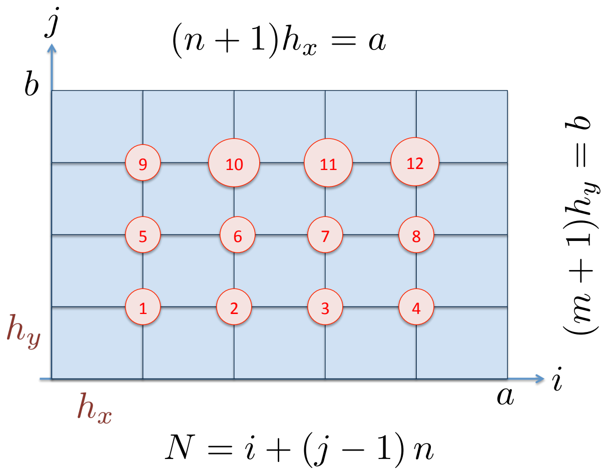
## 3.3.1 Presentation of the method

We'll work with the finite difference approximation of the Laplace equation in dimension 2.



$$A = \begin{pmatrix} B & C & 0 \\ C & B & C \\ 0 & C & B \end{pmatrix}$$

FIGURE 3.6 – Pavage de $[0,a] \times [0,b]$, $n = 4$ and $m = 3$

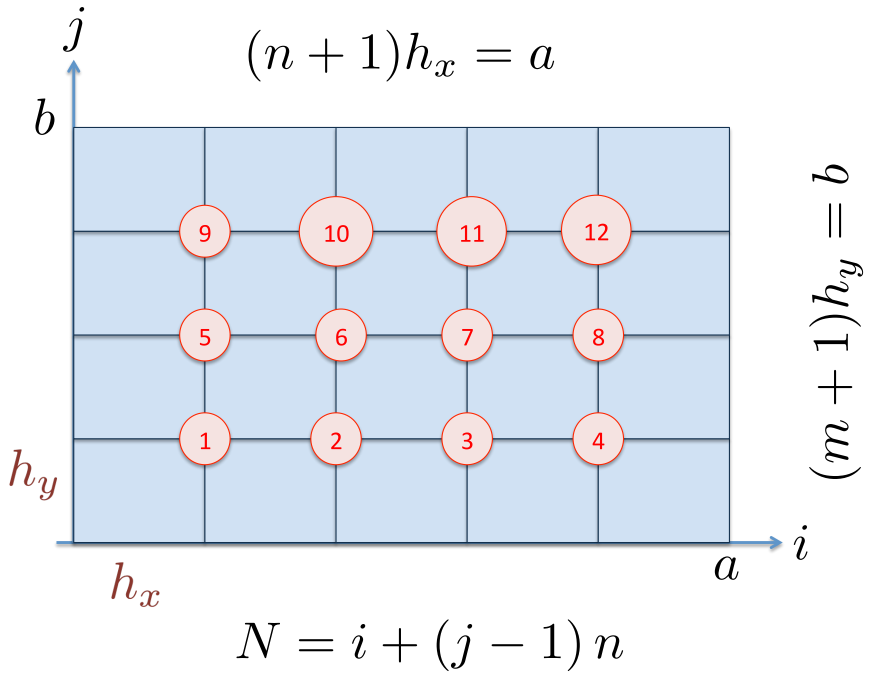


FIGURE 3.7 – Pavage de $[0, a] \times [0, b]$, $n = 4$ and $m = 3$

$$\left(\begin{array}{cccc|cccc|cccc}
\frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 \\
\hline
-\frac{1}{h_y^2} & 0 & 0 & 0 & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 \\
0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 \\
0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 \\
0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & 0 & 0 & 0 & -\frac{1}{h_y^2} \\
\hline
0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2}
\end{array}\right)$$

$$A = \begin{pmatrix} B & C & 0 \\ C & B & C \\ 0 & C & B \end{pmatrix}$$

$$B = \begin{pmatrix} \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 \\ -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 \\ 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} \\ 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} \end{pmatrix} = A_1(h_x)+\frac{2}{h_y^2}\, I_n$$

$$C = -\begin{pmatrix} \frac{1}{h_y^2} & 0 & 0 & 0 \\ 0 & \frac{1}{h_y^2} & 0 & 0 \\ 0 & 0 & \frac{1}{h_y^2} & 0 \\ 0 & 0 & 0 & \frac{1}{h_y^2} \end{pmatrix} = -\frac{1}{h_y^2}\, I_n.$$

Consider now the general problem $Ax = b$, where $A$ is a $nm \times nm$ symmetric matrix $A$, block tridiagonal in the form

$$A = A(B,C) = \begin{pmatrix} B & C & & 0 & \\ C & B & C & & \\ & \ddots & \ddots & \ddots & \\ & & C & B & C \\ & 0 & & C & B \end{pmatrix}. \tag{3.2}$$

Each block is a $n \times n$ matrix. The vectors $\boldsymbol{b}$ and $\boldsymbol{x}$ can be split by block of size $n$ as well, $x^j$ is the sought solution on the ligne $j$.

$$\boldsymbol{b} = \begin{pmatrix} \boldsymbol{b}^1 \\ \vdots \\ \boldsymbol{b}^m \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} \boldsymbol{x}^1 \\ \vdots \\ \boldsymbol{x}^m \end{pmatrix}$$

The system can be rewritten as

$$\begin{pmatrix} B & C & & 0 & \\ C & B & C & & \\ & \ddots & \ddots & \ddots & \\ & & C & B & C \\ & 0 & & C & B \end{pmatrix} \begin{pmatrix} \boldsymbol{x}^1 \\ \boldsymbol{x}^2 \\ \vdots \\ \boldsymbol{x}^{m-1} \\ \boldsymbol{x}^m \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^{m-1} \\ \boldsymbol{b}^m \end{pmatrix}$$

which is a system of $m$ systems of dimension $n$ :

$$\begin{array}{rcl} B\boldsymbol{x}^1 + C\boldsymbol{x}^2 & = & \boldsymbol{b}^1 \\ \ddots & & \\ C\boldsymbol{x}^{i-1} + B\boldsymbol{x}^i + C\boldsymbol{x}^{i+1} & = & \boldsymbol{b}^i \\ \ddots & & \\ C\boldsymbol{x}^{m-1} + B\boldsymbol{x}^m & = & \boldsymbol{b}^m \end{array}$$

Suppose $B$ and $C$ are symmetric, and diagonalise in the same orthonormal basis $(\boldsymbol{q}^1, \dots, \boldsymbol{q}^n)$. This is the case for our previous example. Denote by $Q$ the corresponding orthogonal matrix $Q = [\boldsymbol{q}^1, \dots, \boldsymbol{q}^n]$. There exist two diagonal matrices $D^1$ and $D^2$ such that

$$B = QD^1Q^T, \quad C = QD^2Q^T.$$

Take for example the first equation

$$B\boldsymbol{x}^1 + C\boldsymbol{x}^2 = \boldsymbol{b}^1$$

and replace $B$ and $C$ :

$$QD^1Q^T\boldsymbol{x}^1 + QD^2Q^T\boldsymbol{x}^2 = \boldsymbol{b}^1$$

Multiply by $Q^T$ :

$$D^1Q^T\boldsymbol{x}^1 + D^2Q^T\boldsymbol{x}^2 = Q^T\boldsymbol{b}^1$$

Denote by $(\boldsymbol{c}^i, \boldsymbol{y}^i)$ the coordinates of $(\boldsymbol{b}^i, \boldsymbol{x}^i)$ in the new basis :

$$Q^T\boldsymbol{b}^i = \boldsymbol{c}^i, \quad Q^T\boldsymbol{x}^i = \boldsymbol{y}^i, \quad 1 \le i \le m.$$

Then the problem takes the form

$$\begin{array}{rcl} D^1\boldsymbol{y}^1 + D^2\boldsymbol{y}^2 & = & \boldsymbol{c}^1 \\ \ddots & & \\ D^2\boldsymbol{y}^{i-1} + D^1\boldsymbol{y}^i + D^2\boldsymbol{y}^{i+1} & = & \boldsymbol{c}^i \\ \ddots & & \\ D^2\boldsymbol{y}^{m-1} + D^1\boldsymbol{y}^m & = & \boldsymbol{c}^m \end{array}$$

These are all diagonal systems. Take the component number $j$ in each block of the previous system, for $1 \le j \le n$ :

$$\begin{array}{rcl} D^1_jy^1_j + D^2_jy^2_j & = & c^1_j \\ \ddots & = & \\ D^2_jy^{i-1}_j + D^1_jy^i_j + D^2_jy^{i+1}_j & = & c^i_j \\ \ddots & & \\ D^2_jy^{m-1}_j + D^1_jy^m_j & = & c^m_j \end{array}$$

which is written in matrix form as

$$\begin{pmatrix} D^1_j & D^2_j & & 0 & \\ D^2_j & D^1_j & D^2_j & & \\ & \ddots & \ddots & \ddots & \\ & & D^2_j & D^1_j & D^2_j \\ & 0 & & D^2_j & D^1_j \end{pmatrix} \begin{pmatrix} y^1_j \\ y^2_j \\ \vdots \\ y^{m-1}_j \\ y^m_j \end{pmatrix} = \begin{pmatrix} c^1_j \\ c^2_j \\ \vdots \\ c^{m-1}_j \\ c^m_j \end{pmatrix}$$

For each $j$, $1 \le j \le n$, define the tridiagonal $m \times m$ matrix

$$T_j = \begin{pmatrix} D_j^1 & D_j^2 & & 0 & \\ D_j^2 & D_j^1 & D_j^2 & & \\ & \ddots & \ddots & \ddots & \\ & & D_j^2 & D_j^1 & D_j^2 \\ & 0 & & D_j^2 & D_j^1 \end{pmatrix}$$

and 2 vectors in $\mathbb{R}^m$

$$\boldsymbol{d}^j = \begin{pmatrix} c_j^1 \\ \vdots \\ c_j^m \end{pmatrix}, \quad \boldsymbol{z}^j = \begin{pmatrix} y_j^1 \\ \vdots \\ y_j^m \end{pmatrix}$$

We have now $n$ tridiagonal systems of size $m$,

$$T_j \boldsymbol{z}^j = \boldsymbol{d}^j, \quad 1 \le j \le n.$$

which can be solved in parallel with a $LU$ decomposition for instance. For the 2D Laplace equation with equidistant grid, the computation of the $c^j$ and the reconstruction of $x$ can be done by Fast Fourier transform.

We have to compute for each $j$, $\boldsymbol{x}^j = Q\boldsymbol{y}^j$. The matrice $C$ is $-\dfrac{1}{h_y^2}I_n$, the matrix $B$ is $A_1(h_x) + \frac{2}{h_y^2}I_n$. The eigenvalues of $B$ are those of $A_1 + \frac{2}{h_y^2}$, which are $\frac{2}{h_y^2} + \frac{4}{h_x^2}\sin^2\frac{k\pi h_x}{2}$, the eigenvectors of $B$ and $C$ are those of $A_1$, given by (after orthonormalisation)

$$\Phi_j^{(k)} = \sqrt{\frac{2}{n+1}} \sin\frac{jk\pi}{n+1}, \quad 1 \le j \le n,$$

Define the matrix $Q$ as the matrix of eigenvectors

$$Q = [\boldsymbol{\Phi}^{(1)}, \cdots, \boldsymbol{\Phi}^{(n)}].$$

By

$$Q\boldsymbol{v} = \sum_{k=1}^{n} v_k \boldsymbol{\Phi}^{(k)},$$

we obtain

$$(Q\boldsymbol{v})_j = (Q^T\boldsymbol{v})_j = \sqrt{\frac{2}{n+1}} \sum_{k=1}^{n} v_k \sin\frac{kj\pi}{n+1}.$$

Note that the sum can be extended to $k = 0$ and $k = n+1$ since the sinus vanishes.

$$(Q\boldsymbol{v})_j = (Q^T\boldsymbol{v})_j = \sqrt{\frac{2}{n+1}} \sum_{k=1}^{n+1} v_k \sin\frac{kj\pi}{n+1}. \tag{3.3}$$

The next section is occupied with the FFT, we'll come back to the algorithm later.

### 3.3.2 Discrete and Fast Fourier Transform

Let $n' = n+1$. The Discrete Fourier Transform of length $n'$ is defined by

$$w_j = \sum_{k=1}^{n'} v_k \, e^{-2i\frac{kj\pi}{n'}}, \quad j = 1, \cdots, n'.$$

Define $r = e^{2i\frac{\pi}{n'}}$ the basic root of unity, then we rewrite the formula above as

$$w_j = \sum_{k=1}^{n'} v_k \, r^{-kj}, \quad j = 1, \cdots, n'. \tag{3.4}$$

**Lemma 3.1 (Inverse DFT)** *If $w = (w_j)_{1\le j\le n'}$ is the discrete Fourier transform of $v = (v_j)_{1\le j\le n'}$ from (3.4), then the inverse discrete Fourier transform is given by*

$$v_j = \frac{1}{n'}\sum_{k=1}^{n'} w_k \, r^{kj}, \quad j = 1, \cdots, n'. \tag{3.5}$$

**Proof** Just replace

$$\sum_{k=1}^{n'}\left(\frac{1}{n'}\sum_{p=1}^{n'} w_p \, r^{kp}\right) r^{-kj} \quad = \quad \frac{1}{n'}\sum_{p=1}^{n'} w_p \sum_{k=1}^{n'} r^{k(p-j)}$$

Since $z = r^{p-j}$ is a $n'-$ root of unity,

$$\begin{cases} \text{for } z \neq 1, & \sum_{k=1}^{n'} z^k = 0, \\ \text{for } z = 1, & \sum_{k=1}^{n'} z^k = n'. \end{cases}$$

Therefore

$$\frac{1}{n'}\sum_{p=1}^{n'} w_p \sum_{k=1}^{n'} r^{k(p-j)} = w_j$$

and the lemma is proven. ■

We now suppose that $n' = 2p$. We need to specify more $r$, that we call $r_{n'}$. Note for further use that $r_{n'}^{n'} = 1$ and $r_{n'}^{p} = -1$. Split the sum above into even ($k = 2\ell, \ell = 1 : p$) and odd terms ($k = 2\ell - 1, \ell = 1 : p$). For $j = 1, \cdots, 2p$,

$$\begin{aligned} w_j &= \sum_{k=1}^{n'} v_k \, r_{n'}^{-kj} \\ w_j &= \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell j} + \sum_{\ell=1}^{p} v_{2\ell-1} \, r_{n'}^{-(2\ell-1)j} \\ &= \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell j} + r^j \sum_{\ell=1}^{p} v_{2\ell-1} \, r_{n'}^{-2\ell j}. \end{aligned}$$

Defining for $j = 1, \cdots, 2p$,

$$u_j = \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell j}, \quad t_j = \sum_{\ell=1}^{p} v_{2\ell-1} \, r_{n'}^{-2\ell j}.$$

Then

$$w_j = u_j + r_{n'}^j t_j.$$

We verify that for each $j$, $u_{j+p} = u_j$ and $t_{j+p} = t_j$ :

$$u_{j+p} = \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell(j+p)} = r_{n'}^{-2\ell p} u_j = u_j.$$

This implies that we only need to compute $(u_j, t_j)$ for $1 \le j \le p$. Furthermore

$$w_{j+p} = u_{j+p} + r_{n'}^{j+p} t_{j+p} = u_j + r_{n'}^j r_{n'}^p t_j = u_j - r_{n'}^j t_j.$$

To compute $u_j$ and $t_j$ note that

$$\sum_{\ell=1}^{p} v_{2\ell}\, r_{n'}^{-2\ell j} = \sum_{\ell=1}^{p} v_{2\ell}\, (r_{n'}^2)^{-\ell j}$$

But $r_{n'}^2 = (e^{-\frac{2i\pi}{2p}})^2 = e^{-\frac{2i\pi}{p}} : r_{n'}^2 = r_p$. Therefore

$$u_j = \sum_{\ell=1}^{p} v_{2\ell}\, r_p^{-\ell j}, \quad t_j = \sum_{\ell=1}^{p} v_{2\ell-1}\, r_p^{-\ell j}.$$

The sums above are similar sums as that defining $w_j$, but with $p = n'/2$. This is the starting point for a dyadic computation of the $w_j$ : the Fast Fourier Transform.

To obtain $\{w_j\}_{1\leq j\leq 2p}$ from $\{v_j\}_{1\leq j\leq 2p}$, do

Compute $r_{n'}^j \qquad j = 1, \cdots, p$

Compute $u_j = \sum_{\ell=1}^{p} v_{2\ell}\, r_p^{-\ell j}, \quad t_j = \sum_{\ell=1}^{p} v_{2\ell-1}\, r_p^{-\ell j} \qquad j = 1, \cdots, p$

Compute $w_j = u_j + r_{n'}^j t_j, \quad w_{j+p} = u_j - r_{n'}^j t_j \qquad j = 1, \cdots, p.$

$$r = e^{2i\frac{\pi}{n'}}, w_j = \sum_{k=1}^{n'} v_k\, r^{-kj}, \quad j = 1, \cdots, n'.$$

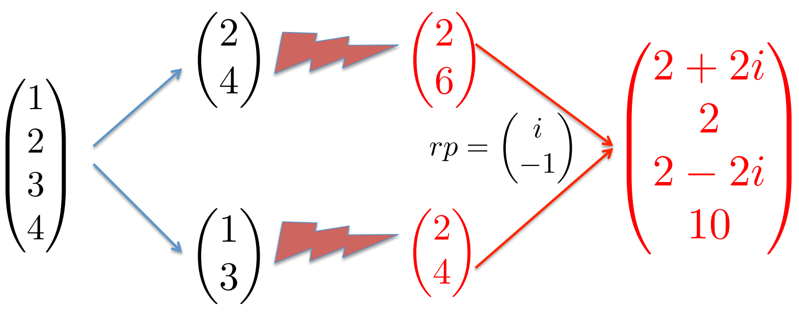
$n' = 2$, $r = -1$, initialization $w_1 = -v_1 + v_2, \quad w_2 = v_1 + v_2$.

```
function w=myFFT(v)
% MYFFT fast Fourier transform
% w=myFFT(v); computes recursively the Fourier tranform of
% the vector v whose length must be a power of 2.
n=length(v);
if n==2,
        w=[-v(1)+v(2);v(1)+v(2)];
else
        rp=exp(2i*pi/n*(1:n/2)');
        t=myFFT(v(1:2:n-1));
        u=myFFT(v(2:2:n));
        w=[u+rp.*t; u-rp.*t];
end;
```

$$r = e^{2i\frac{\pi}{n'}}, w_j = \sum_{k=1}^{n'} v_k \, r^{-kj}, \quad j = 1, \cdots, n'.$$

$n' = 2$, $r = -1$, initialization $w_1 = -v_1 + v_2, \quad w_2 = v_1 + v_2$.

```matlab
function w=myFFT(v)
% MYFFT fast Fourier transform
% w=myFFT(v); computes recursively the Fourier tranform of
% the vector v whose length must be a power of 2.
n=length(v);
if n==2,
        w=[-v(1)+v(2);v(1)+v(2)];
else
        rp=exp(2i*pi/n*(1:n/2)');
        t=myFFT(v(1:2:n-1));
        u=myFFT(v(2:2:n));
        w=[u+rp.*t; u-rp.*t];
end;
```



$\begin{pmatrix}1\\2\\3\\4\end{pmatrix}$
$\begin{pmatrix}2\\4\end{pmatrix}$
$\begin{pmatrix}1\\3\end{pmatrix}$
$\begin{pmatrix}2\\6\end{pmatrix}$
$\begin{pmatrix}2\\4\end{pmatrix}$
$rp = \begin{pmatrix}i\\-1\end{pmatrix}$
$\begin{pmatrix}2+2i\\2\\2-2i\\10\end{pmatrix}$

FIGURE 3.8 – FFT for $n' = 4$

It is easy to count the number of operations in the algorithm to be $\mathcal{O}(n\log_2(n))$, which is much better than *blockLU*.

### 3.3.3 The algorithm

We now show how to obtain the computation of $Qv$ in (3.3) with FFT.

$$
\begin{array}{lll}
\boldsymbol{v} \in \mathbb{R}^n,\ n' = n+1 \text{ EVEN} & & \\
Q\boldsymbol{v} = \sqrt{\tfrac{2}{n+1}}\ \boldsymbol{z} \in \mathbb{R}^n, & z_j = \sum\limits_{k=1}^{n} v_k \sin \tfrac{kj\pi}{n'} & 1 \le j \le n, \\
\tilde{\boldsymbol{v}} = [v; 0] \in \mathbb{R}^{n'}, & & \\
DFT(\tilde{\boldsymbol{v}}) = \boldsymbol{w} \in \mathbb{R}^{n'}, & w_j = \sum\limits_{k=1}^{n'} \tilde{v}_k\, e^{-2i\frac{kj\pi}{n'}} & 1 \le j \le n'
\end{array}
$$

Note first that $z_j = \sum\limits_{k=1}^{n'} \tilde{v}_k \sin \frac{kj\pi}{n'}$ as well. Consider first the even indices $z_2, \cdots, z_{n-1}$ :

$$
z_{2\ell} = \sum_{k=1}^{n'} \tilde{v}_k \sin \frac{2\ell k\pi}{n'} = -\mathcal{I}\mathrm{m} w_\ell, \quad \ell = 1, \cdots, \frac{n-1}{2}.
$$

Consider now the odd indices, $z_1, \cdots, z_n$

$$
\begin{aligned}
z_{2\ell-1} &= -\mathcal{I}\mathrm{m} \sum_{k=1}^{n'} \tilde{v}_k e^{-i\frac{k(2\ell-1)\pi}{n'}} = -\mathcal{I}\mathrm{m} \sum_{k=1}^{n'} (\tilde{v}_k e^{i\frac{k\pi}{n'}}) e^{-2i\frac{k\ell\pi}{n'}} \\
&= -\mathcal{I}\mathrm{m}(DFT(\{\tilde{v}_k e^{i\frac{k\pi}{n'}}\}_k))_\ell, \quad \ell = 1, \cdots, \tfrac{n+1}{2}.
\end{aligned}
$$

Resuming with matlab notations

QFFT

$$
\begin{aligned}
\boldsymbol{r_0} &= e^{i\frac{\pi}{n'}} \\
(Q\boldsymbol{v})_{2\ell} &= -\sqrt{\tfrac{2}{n+1}}\ \mathcal{I}\mathrm{m}(FFT(\tilde{\boldsymbol{v}}))_\ell, & \ell = 1, \cdots, \tfrac{n-1}{2} \\
(Q\boldsymbol{v})_{2\ell-1} &= -\sqrt{\tfrac{2}{n+1}}\ \mathcal{I}\mathrm{m}(FFT(\tilde{\boldsymbol{v}} \mathbin{.*} \boldsymbol{r_0}^{(1:n')'}))_\ell, & \ell = 1, \cdots, \tfrac{n+1}{2}
\end{aligned}
\tag{3.6}
$$

Summarizing the solution of

$$
\begin{pmatrix}
B & C & & 0 & \\
C & B & C & & \\
 & \ddots & \ddots & \ddots & \\
 & & C & B & C \\
 & 0 & & C & B
\end{pmatrix}
\begin{pmatrix}
\boldsymbol{x}^1 \\ \boldsymbol{x}^2 \\ \vdots \\ \boldsymbol{x}^{m-1} \\ \boldsymbol{x}^m
\end{pmatrix}
=
\begin{pmatrix}
\boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^{m-1} \\ \boldsymbol{b}^m
\end{pmatrix}
$$

**Step 1 : FFT** Compute $\boldsymbol{c}^j = Q^T \boldsymbol{b}^j$ by (3.6) for $1 \le j \le m$.

**Step 2 : Sort** $\{\boldsymbol{c}^1, \cdots, \boldsymbol{c}^m\}$ The righthand side has been build by rows in the mesh : $\boldsymbol{b}^j$ is the vector of the values of the forcing term on the line $y = j * h_y$.

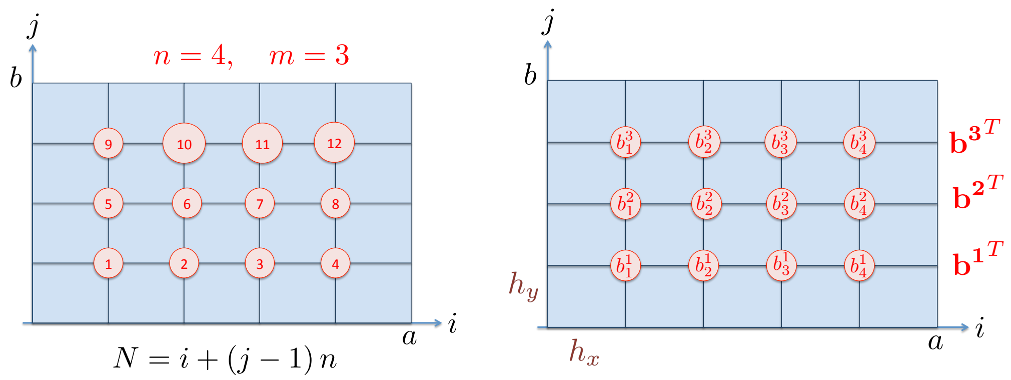


FIGURE 3.9 – Numbering

$$\begin{pmatrix} \begin{pmatrix} c_1^1 \\ c_2^1 \\ c_3^1 \\ c_4^1 \end{pmatrix} \\ \begin{pmatrix} c_1^2 \\ c_2^2 \\ c_3^2 \\ c_4^2 \end{pmatrix} \\ \begin{pmatrix} c_1^3 \\ c_2^3 \\ c_3^3 \\ c_4^3 \end{pmatrix} \end{pmatrix} \longrightarrow \boxed{\begin{pmatrix} c_1^1 & c_1^2 & c_1^3 \\ c_2^1 & c_2^2 & c_2^3 \\ c_3^1 & c_3^2 & c_3^3 \\ c_4^1 & c_4^2 & c_4^3 \end{pmatrix}} \longrightarrow \begin{pmatrix} \begin{pmatrix} c_1^1 \\ c_1^2 \\ c_1^3 \end{pmatrix} \\ \begin{pmatrix} c_2^1 \\ c_2^2 \\ c_2^3 \end{pmatrix} \\ \begin{pmatrix} c_3^1 \\ c_3^2 \\ c_3^3 \end{pmatrix} \\ \begin{pmatrix} c_4^1 \\ c_4^2 \\ c_4^3 \end{pmatrix} \end{pmatrix}$$

FIGURE 3.10 – Renumbering

The total vector $\boldsymbol{\sigma}$ is numbered from 1 to $nm$, with $N = i + (j-1) * n$. The matrix $C$ is built as follows

$$\begin{aligned} \boldsymbol{\sigma}(1:n) \quad &\rightarrow C(:,1) \\ \boldsymbol{\sigma}(n+1:2n) \quad &\rightarrow C(:,2) \\ &\vdots \\ \boldsymbol{\sigma}((m-1)n+1:mn) \quad &\rightarrow C(:,m) \end{aligned}$$

```
for j=1:m
        C(:,j)=sig((j−1)*n+1:j*n )
end
```

and then instead of reading the columns, we read the rows.

**Step 3 : Solving the $n$ tridiagonal systems** of size $m$,

$$T_j \boldsymbol{z}^j = \boldsymbol{d}^j, \quad 1 \le j \le n.$$

with $\boldsymbol{d}^j = C(j,:)$, and

$$T_j = \begin{pmatrix} D_j^1 & D_j^2 & & 0 & \\ D_j^2 & D_j^1 & D_j^2 & & \\ & \ddots & \ddots & \ddots & \\ & & D_j^2 & D_j^1 & D_j^2 \\ & 0 & & D_j^2 & D_j^1 \end{pmatrix},$$

$$D_j^2 = -\frac{1}{h_y^2}, \quad D_j^1 = \frac{2}{h_y^2} + \frac{4}{h_x^2}\sin^2\frac{j\pi h}{2(n+1)}.$$

**Step 4 : Reordering the $\boldsymbol{z}^j$** into $\boldsymbol{y}^j$

**Step 5 : Recovering $\boldsymbol{x}^j$** $= Q\boldsymbol{y}^j$ by (3.6).

For this method, we talk about FFT preconditioning, since the system $A\boldsymbol{u} = \boldsymbol{b}$ is premultiplied by the block-diagonal matrix

$$\mathcal{Q} = \begin{pmatrix} Q^T & & & \\ & Q^T & 0 & \\ & & \ddots & \\ & 0 & & Q^T \end{pmatrix}$$

That is we write

$$\mathcal{Q}A\mathcal{Q}^T\mathcal{Q}\boldsymbol{u} = \mathcal{Q}\boldsymbol{b}.$$