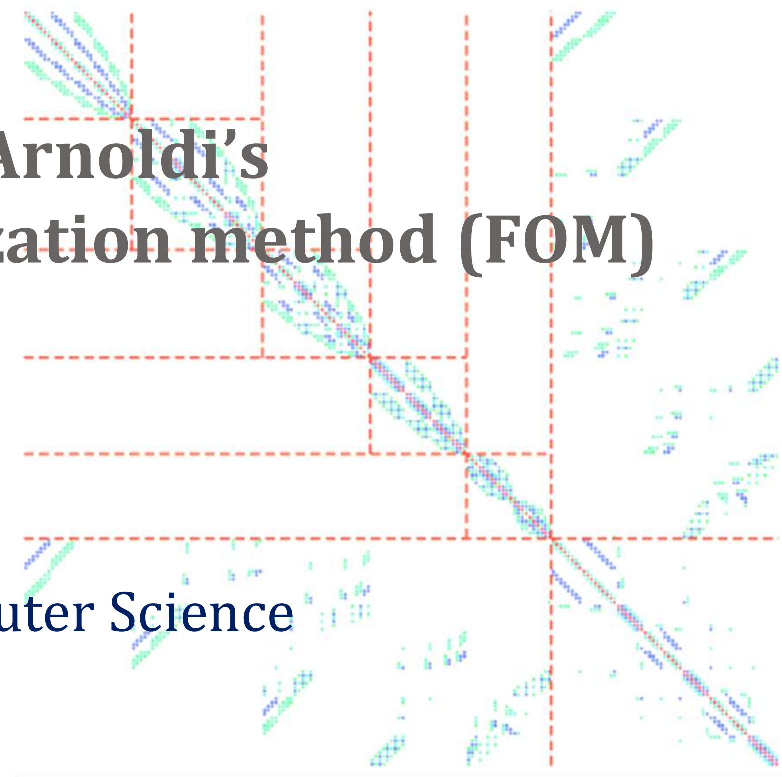
Numerical Methods of Linear Algebra for Sparse Matrices

Lecture 13

Krylov subspace methods based on Arnoldi's orthogonalization. Full Orthogonalization method (FOM)



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Krylov Subspace methods based on Arnoldi's orthogonalization

- Definition of Krylov subspace and Krylov subspace projection method
- Arnoldi's method of orthogonalization
- Full Orthogonalization method (FOM)

Multi-dimensional projection method

For the linear system $Ax = b$, $A \in \mathbb{C}^{n \times n}$, $b \in \mathbb{C}^n$
consider the case when $m > 1$ and $m \ll n$.
Search the approximate solution $x_m \in x_0 + K_m$, where

- x_0 is the initial guess, $r_0 = b - Ax$ is the initial residual
- K_m is the search subspace, $\dim(K_m) = m$
- L_m is the subspace of constraints, $\dim(L_m) = m$
- $r_m = b - Ax_m \perp L_m$ is the residual

Approximate solution $x_m = x_0 + \delta_m$, $\delta_m \in K_m$ is correction vector.
$r_m = r_0 - A\delta_m \perp L_m$
How to choose δ_m? Ideally it should give zero residual:
$r_m = r_0 - A\delta_m = 0$. Hence $\delta_m^{best} = A^{-1} r_0$
Computing δ_m^{best} from solving the system $A\delta_m = r_0$ is not efficient.
In projection method $\delta_m = V_m y$, where $y \in \mathbb{C}^m$, $V_m \in \mathbb{C}^{n \times m}$
$\delta_m \approx A^{-1} r_0$

Krylov subspace projection method

Take $K_m = K_m(A, r_0)$, where K_m is Krylov subspace

Krylov subspace of dimension m, induced by the matrix A and the vector v, is defined as $K_m(A, v) = span\{v, Av, A^2v, \dots, A^{m-1}v\}$

In Krylov subspace methods, the search subspace is the Krylov subspace, induced by the matrix A and the initial residual vector r_0: $K_m = K_m(A, r_0)$

Any Krylov subspace method implicitly generates a polynomial $q_{m-1}(A)$ of a degree $m - 1$:
$q_{m-1}(A)r_0 = \alpha_0 r_0 + \alpha_1 A r_0 + \alpha_2 A^2 r_0 + \cdots + \alpha_{m-1} A^{m-1} r_0$

Approximate solution
$x_m = x_0 + q_{m-1}(A)r_0 \approx A^{-1}b$

Arnoldi method of orthogonalization

How to build Krylov subspace $K_m = K_m(A, v_1)$? The subspace is defined by its basis.

The basis for Krylov subspace can be constructed by Arnoldi process.

Arnoldi process is the Gram-Schmidt process which builds *orthonormal* set of vectors $\{v_1, v_2, ..., v_m\} = V_m$ for a given vector v_1 and given matrix A that is the basis of $K_m(A, v_1)$

Recall the definition of orthonormal set $\{v_1, v_2, ..., v_m\}$: $(v_i, v_j) = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}$; $\|v_i\|_2 = 1,\ i = \overline{1, m}$

Basic algorithm of Arnoldi orthogonalization

1) Choose v_1: $\|v_1\|_2 = 1$. Matrix A and dimension of subspace m are given.

2) Loop for j from 1 to m.

2.1) $h_{ij} := (Av_j, v_i),\ i = \overline{1, j}$

2.2) $w_j := Av_j - \sum_{i=1}^{j} h_{ij} v_i$

2.3) $h_{j+1,j} := \|w_j\|_2$. If $h_{j+1,j} = 0 \Rightarrow$ stop, else

2.4) $v_{j+1} := \dfrac{w_j}{h_{j+1,j}}$

Arnoldi process for numerical implementation

- Arnoldi process is the modified Gram-Schmidt process applied to Krylov subspace $K_m(A, v_1)$ induced by matrix A and vector v_1

1) Choose $v_1 : \ \|v_1\|_2 = 1$. Matrix A and dimension of subspace m are given.

2) Loop for j from 1 to m.

 2.1) $w_j = Av_j$

 2.2) Loop for i from 1 to j $h_{ij} := (w_j, v_i),\ w_j := w_j - h_{ij} v_i$

 2.3) $h_{j+1,j} := \|w_j\|_2$. If $h_{j+1,j} = 0 \Rightarrow$ stop, else

 2.4) $v_{j+1} := \dfrac{w_j}{h_{j+1,j}}$

Properties of Arnoldi process

Property 1. If all m steps of Arnoldi process are complited, then the set of vectors $\{v_1, v_2, \ldots, v_m\}$ is the orthonormalized basis of Krylov subspace $K_m(A, v_1)$.

Property 2. From Arnoldi algorithm form the matrices:

$$V_m = \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \ldots & v_m \\ | & | & & | \end{pmatrix} \in \mathbb{C}^{n\times m};\; V_{m+1} = \begin{pmatrix} | & | & & | & | \\ v_1 & v_2 & \ldots & v_m & v_{m+1} \\ | & | & & | & | \end{pmatrix} \in \mathbb{C}^{n\times(m+1)}$$

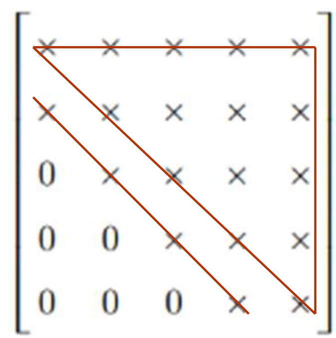
$$\overline{H}_m = \{\tilde{h}_{ij}\},\; \tilde{h}_{ij} = \begin{cases} 0, & i > j+1 \\ h_{ij}, & i \le j+1 \end{cases};\; H_m = \begin{pmatrix} \tilde{h}_{11} & \ldots & \tilde{h}_{1m} \\ \ldots & & \ldots \\ \tilde{h}_{m1} & \ldots & \tilde{h}_{mm} \end{pmatrix};\; H_m \in \mathbb{C}^{m\times m}$$

$\overline{H}_m \in \mathbb{C}^{(m+1)\times m}$ is Hessenberg matrix of the size $m+1$ by m

Then the following Arnoldi relation holds:

1) $AV_m = V_m H_m + w_m e_m^T = V_{m+1} \overline{H}_m$

2) $V_m^H A V_m = H_m$



Upper Hessenberg

Arnoldi relation 1

1) $AV_m = V_m H_m + w_m e_m^T = V_{m+1} \overline{H}_m$

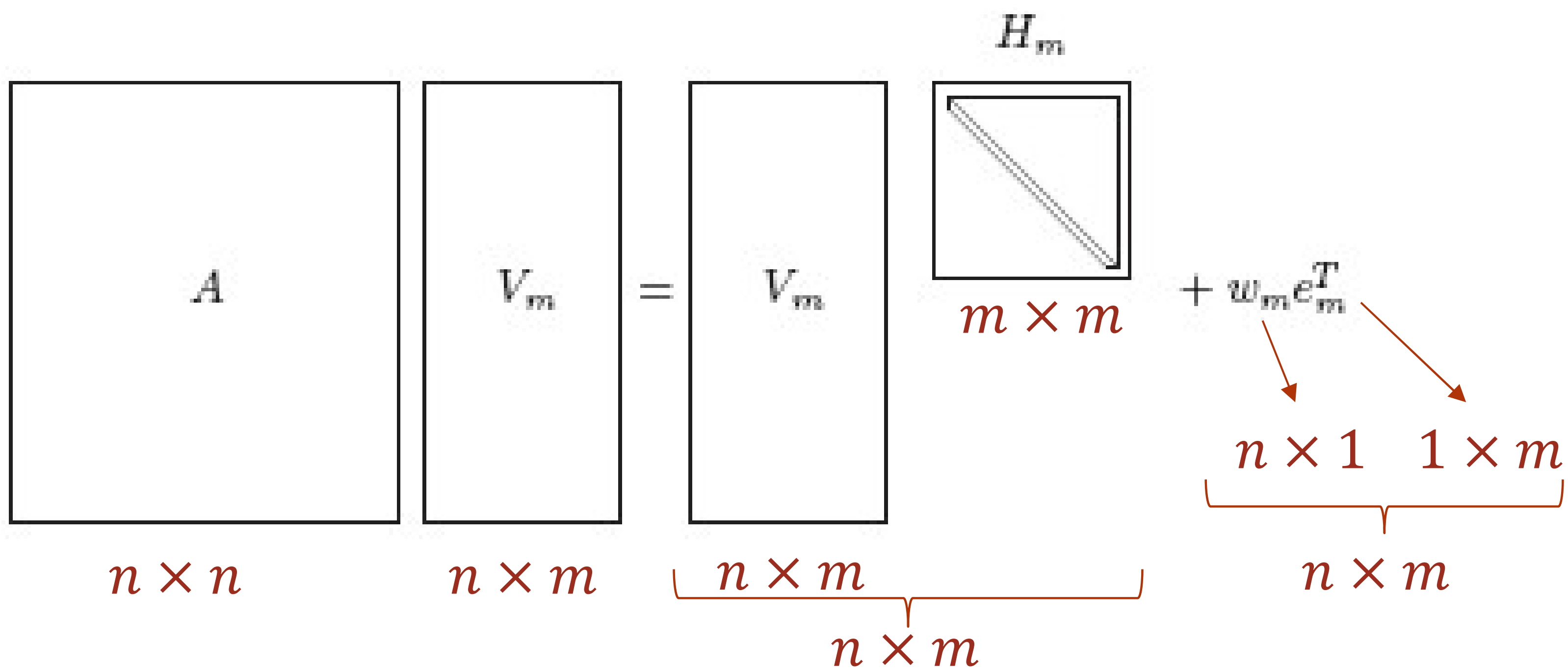
FOM GMRES

Recall that at the last step of Arnoldi algorithm when $j = m$: $v_{m+1} = \dfrac{w_m}{h_{m+1,m}}$

From (1) we can derive two methods:

a) FOM: $AV_m = V_m H_m + w_m e_m^T = V_m H_m + v_{m+1}\, h_{m+1,m}\, e_m^T$

b) GMRES: $AV_m = V_{m+1} \overline{H}_m$



Arnoldi relation 2

2) $V_m^H A\, V_m = H_m$; $V_{m+1}^H A\, V_m = \overline{H}_m$

V_m is unitary non-square matrix (orthonormal columns):
$V_m^H V_m = I_m$

(2) shows that A can be transformed to H_m: $A \sim H_m$

$$\underset{m\times m}{H_m} = \underset{m\times n}{V_m^H} * \underset{n\times n}{A} * \underset{n\times m}{V_m}$$

$$\underset{(m+1)\times m}{\overline{H}_m} = \underset{(m+1)\times n}{V_{m+1}^H} * \underset{n\times n}{A} * \underset{n\times m}{V_m}$$

Arnoldi process for solving the linear system Ax=b

- When applied to solving the system $Ax = b$, Arnoldi process constructs an orthonormal basis for the search subspace $K_m = K_m(A, r)$, where K_m is the Krylov subspace and $r = b - Ax$ is the residual vector

Arnoldi algorithm

1. define zero matrix $\underline{H}_m \in \mathbb{R}^{(m+1)\times m}$ and zero matrix $V_{m+1} \in \mathbb{R}^{n\times(m+1)}$
2. $\beta := \|r\|_2$
 $v_1 := r/\beta$
3. for $j = 1, 2, \ldots, m$ do

   every loop cycle gives $v_{j+1} =$ `V(:,j+1)` and $(h_{1,j}, \ldots, h_{j+1,j})^T =$ `H(1:j+1,j)`

4. $\quad w_j := Av_j$
5. $\quad$ for $i = 1, 2, \ldots, j$ do
6. $\qquad h_{ij} := (w_j, v_i)$
7. $\qquad w_j := w_j - h_{ij} v_i$
8. $\quad$ endfor
9. $\quad h_{j+1,j} := \|w_j\|_2$.
 $\quad$ If $h_{j+1,j} = 0$ stop.
10. $\quad v_{j+1} := w_j / h_{j+1,j}$
11. endfor

Arnoldi in Matlab

```
H=zeros(m+1,m);
V=zeros(n,m+1);
beta=norm(r);
V(:,1)=(1/beta)*r;
for j=1:m,
   wj=A*V(:,j);
   for i=1:j,
      H(i,j)=(V(:,i))'*wj;
      wj=wj-H(i,j)*V(:,i);
   end
   H(j+1,j)=norm(wj);
   if(H(j+1,j)==0), break, end
V(:,j+1)=(1/H(j+1,j))*wj;
end
```

Arnoldi process for solving the linear system Ax=b

- Classical examples of methods based on Arnold orthogonalization process are FOM (Full Orthogonalization Method) and GMRES (Generalized Minimal Residual)

- In these methods, the solution is searched in the form $x_m = x_0 + \delta_m$, $\delta_m \in K_m(A, r_0)$ is correction vector,

  $K_m(A, r_0) = span\{r_0, Ar_0, A^2 r_0, \dots, A^{m-1} r_0\}$ is Krylov subspace

- Orthogonal basis of $K_m(A, r_0)$ is produced by Arnoldi process, where the basis vectors are the columns of V_m:

  $\delta_m \in K_m(A, r_0) \Leftrightarrow \exists y \in C^m\!: \delta_m = V_m y$

- FOM uses the first part of Arnoldi relation: $AV_m = V_m H_m + w_m e_m^T$ and solves the linear system of the size m with matrix H_m

- GMRES uses the second part of Arnoldi relation: $AV_m = V_{m+1} \overline{H}_m$ and solves the linear system of size the $m + 1$ by m with matrix $\overline{H}_m$

Derivation of Full Orthogonalization method (FOM)

Consider projection method with Krylov subspace as the search subspace.

Search subspace is Krylov subspace $K_m(A, r_0) = span\{r_0, Ar_0, A^2 r_0, ..., A^{m-1} r_0\}$

Subspace of constraints is $L_m = K_m = K_m(A, r_0)$

$$V_m = \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_m \\ | & | & & | \end{pmatrix}$$ is the basis in K_m, $W_m = V_m$ is the basis in $L_m = K_m$

Approximate solution is given by $x_m = x_0 + \delta_m = x_0 + V_m y_m;\ \delta_m \in K_m(A, r_0)$

y_m can be found from solving the system $(W_m{}^H A V_m) y = W_m{}^H r_0 \Rightarrow$

formally $y_m = (W_m{}^H A V_m)^{-1} W_m{}^H r_0$. When $W_m = V_m$ we have:

$y_m = (V_m{}^H A V_m)^{-1} V_m{}^H r_0 = H_m^{-1} V_m^H r_0$ from Arnoldi relation

Derivation of Full Orthogonalization method (FOM)

We build orthonormal basis in Arnoldi process: $\|v_1\|_2 = 1$

As we take Krylov subspace induced by initial residual, we can take

the first vector as normalized initial residual: $v_1 = \dfrac{r_0}{\|r_0\|_2}$

Denote $\beta = \|r_0\|_2$, then $r_0 = \beta v_1$

Hence $y_m = H_m^{-1} V_m^H r_0 = H_m^{-1} V_m^H \beta v_1 = H_m^{-1} \beta e_1$, because

$$V_m^H \beta v_1 = \beta V_m^H v_1 = \beta \begin{pmatrix} -v_1- \\ -v_2- \\ \dots \\ -v_m- \end{pmatrix} \begin{pmatrix} | \\ v_1 \\ | \end{pmatrix} = \beta \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \end{pmatrix} = \beta e_1 \text{ (e_1 is the unit ort)}$$

So $y_m = H_m^{-1} \beta e_1$, and we find y_m from solving the system

$$H_m y = \beta e_1$$

Here $H_m \in \mathbb{C}^{m \times m}$, $y \in \mathbb{C}^m$, $e_1 \in \mathbb{R}^m$ is the unit ort

We have small linear system with m equations and m unknowns, which is easier to solve than initial system $Ax = b$ with large matrix A.

Small system in FOM

We find y from the system $H_m y = \beta e_1$ with m equations and m unknowns

$$y^T = y_m{}^T = \left(y_m^1, \quad y_m^2, \quad \dots \quad y_m^m \right),$$

where $y_m^1, \quad y_m^2, \quad \dots \quad y_m^m$ are the unknowns to be found from the system

$$\begin{cases} h_{11} y_m^1 + h_{12} y_m^2 + \quad \dots \quad + h_{1m} y_m^m = \beta \\ h_{21} y_m^1 + h_{22} y_m^2 + \quad \dots \quad + h_{2m} y_m^m = 0 \\ \dots \\ h_{m,m-1} y_m^{m-1} + h_{mm} y_m^m = 0 \end{cases}$$

For example for $m = 4$ the matrix form of the system is:

$$\begin{pmatrix} h_{11} & h_{12} & h_{13} & h_{14} \\ h_{21} & h_{22} & h_{23} & h_{24} \\ 0 & h_{32} & h_{33} & h_{34} \\ 0 & 0 & h_{43} & h_{44} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} \beta \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Full Orthogonalization method (FOM)

1. Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$,

calculate residual norm $\beta = \|r_0\|_2$, and the first vector $v_1 = \dfrac{r_0}{\beta}$

2. Define $H_m = \{h_{ij}\} \in \mathbb{C}^{m\times m}$, $V_m \in \mathbb{C}^{n\times m}$. Set $H_m = 0$

3. Build the basis for Krylov subspace using Arnoldi process:

Loop for j from 1 to m.

3.1) $w_j = Av_j$

3.2) Loop for i from 1 to j $h_{ij} := (w_j, v_i)$, $w_j := w_j - h_{ij}v_i$

3.3) $h_{j+1,j} := \|w_j\|_2$. If $h_{j+1,j}=0 \Rightarrow m := j$, go to step 4, else

3.4) $v_{j+1} := \dfrac{w_j}{h_{j+1,j}}$

4. Find y_m from solving the system $H_m y = \beta e_1$

5. Calculate residual r_m, estimate residual norm: $\|r_m\|_2 < \varepsilon$.

6. Calculate new approximate solution $x_m = x_0 + V_m y_m$

The residual in FOM can be calculated **without** general formula $r_m = b - Ax_m$

Calculating residual in FOM

FOM depends on the dimension of Krylov subspace m.

It is possible to select m so, that $\|r_m\|_2 < \varepsilon$

In fact, the residual can be computed inexpensively, without having to compute approximate solution x_m

Proposition. The residual vector r_m of the approximate solution x_m computed by FOM algorithm is defined as

$r_m = -h_{m+1,m} e_m^T y_m v_{m+1}$ and residual norm as $\|r_m\|_2 = h_{m+1,m} \left| e_m^T y_m \right|$

△ Proove the formula for residual norm: 2) $\|r_m\|_2 = h_{m+1,m} \left| e_m^T y_m \right|$

As from 1) $r_m = -h_{m+1,m} e_m^T y_m v_{m+1} \Rightarrow$

$$\|r_m\|_2 = \left\| -h_{m+1,m} e_m^T y_m v_{m+1} \right\|_2 = h_{m+1,m} \left| e_m^T y_m \right| \|v_{m+1}\|_2 = h_{m+1,m} \left| e_m^T y_m \right|$$

because $h_{m+1,m}$ is computed as a norm, so $h_{m+1,m} > 0$,

v_{m+1} is the basis vector from orthonormal basis, so $\|v_{m+1}\|_2 = 1$, $e_m^T y_m$ is a scalar. □

Calculating residual in FOM

▵ Proove the formula for residual: 1) $r_m = -h_{m+1,m} e_m^T y_m v_{m+1}$

Recall that $r_m = b - Ax_m = b - A(x_0 + V_m y_m) = b - Ax_0 - AV_m y_m =$

$= r_0 - AV_m y_m$

From Arnoldi relation $AV_m = V_m H_m + w_m e_m^T = V_m H_m + v_{m+1} h_{m+1,m} e_m^T$,

from FOM algorithm $r_0 = \beta v_1 \Rightarrow$

$r_m = r_0 - AV_m y_m = \beta v_1 - (V_m H_m + v_{m+1} h_{m+1,m} e_m^T) y_m = \beta v_1 - \underline{V_m H_m y_m} - v_{m+1} h_{m+1,m} e_m^T y_m.$

From Arnoldi algorithm $y_m = H_m^{-1} \beta e_1 \Rightarrow$

$r_m = \beta v_1 - \underline{V_m H_m H_m^{-1} \beta e_1} - v_{m+1} h_{m+1,m} e_m^T y_m = \beta v_1 - \underline{\underline{V_m \beta e_1}} - v_{m+1} h_{m+1,m} e_m^T y_m$

$$V_m \beta e_1 = \beta V_m e_1 = \beta \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_m \\ | & | & & | \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \end{pmatrix} = \beta v_1 \Rightarrow$$

$r_m = \beta v_1 - V_m \beta e_1 - v_{m+1} h_{m+1,m} e_m^T y_m = \beta v_1 - \beta v_1 - v_{m+1} h_{m+1,m} e_m^T y_m =$

$= -v_{m+1} h_{m+1,m} e_m^T y_m \Rightarrow r_m = -h_{m+1,m} e_m^T y_m v_{m+1}$ □

Modifications of FOM

A step of FOM costs approximately $2Nz(A)+2mn$, where $Nz(A)$ is the number of nonzero entries in A.

Together with storing the basis V_m, Hessenberg matrix H_m, additional vectors for the current solution and right-hand side, the total is roughly $(m+3)n+\frac{m^2}{2}$

As m increases, the computational cost increases as $O(m^2 n)$. The memory cost increases as $O(mn)$.

The idea of Krylov subspace methods is to use $m << n$.

So in order not to increase m to the value of n, there are two variations of FOM:

1) restart FOM for the fixed value of m

2) truncate the orthogonalization in Arnoldi process (see details in Yosef Saad book, p. 168)

Restarted FOM(m)

1. Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$,

calculate residual norm $\beta = \|r_0\|_2$, and the first vector $v_1 = \frac{r_0}{\beta}$

2. Define $H_m = \{h_{ij}\} \in \mathbb{C}^{m \times m}$, $V_m \in \mathbb{C}^{n \times m}$. Set $H_m = 0$

3. Build the basis for Krylov subspace using Arnoldi process.

4. Find y_m from solving the system $H_m y = \beta e_1$

5. Calculate residual r_m, estimate residual norm: $\|r_m\|_2 < \varepsilon$.

6. Calculate new approximate solution $x_m = x_0 + V_m y_m$

If satisfied, then stop. Else

7. Set $x_0 := x_m$ and go to step 1.

- Convergence of restarted FOM: sometimes small m is sufficient, sometimes the largest possible m is necessary
- Variation of restarted FOM: start with $m = 1$ and for every run of the algorithm increment m by 1 until certain m_{max} is reached