

Outline

- 1 Introduction
- 2 Projection Methods
- 3 Arnoldi's Methods
- 4 Generalised Minimal Residual Method (GMRES)
- 5 Newton–Krylov Method
- 6 Preconditioning

$$K_m(A, \underline{r}^{(0)}) = \text{Span} \left\{ \underline{v}^{(0)}, A\underline{v}^{(0)}, \dots, A^{m-1}\underline{v}^{(0)} \right\}$$

ARNOLDI PROCESS

$$= \text{Span} \left\{ \underline{v}_1, \underline{v}_2, \dots, \underline{v}_m \right\}$$

ARNOLDI'S RELATION :

*Upper Hessenberg
mxm*

$$\begin{aligned}
 AV_m &= V_{m+1} \bar{H}_m \\
 &= (V_m : \underline{v}_{m+1}) \begin{pmatrix} H_m \\ \cdots \\ \cdots \\ h_{m+1, m} \underline{e}_m^T \\ \hline 0, 0, \dots, 0_{m \times m} \end{pmatrix} \\
 &= V_m H_m + h_{m+1, m} V_{m+1} \underline{e}_m^T
 \end{aligned}$$

Arnoldi's Method

- Arnoldi's method or the Arnoldi process makes use of the Gram-Schmidt process to generate an orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m\}$ for the Krylov subspace $\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$.
- The Arnoldi process produces the following decomposition:

$$\mathbf{A}\mathbf{V}_m = \mathbf{V}_m \mathbf{H}_m + h_{m+1,m} \mathbf{v}_{m+1} \mathbf{e}_m^T \quad (5)$$

or equivalently:

$$\mathbf{A}\mathbf{V}_m = \mathbf{V}_{m+1} \overline{\mathbf{H}}_m, \quad \overline{\mathbf{H}}_m = \begin{bmatrix} \mathbf{H}_m \\ \underbrace{h_{m+1,m} \mathbf{e}_m^T} \end{bmatrix} \quad (6)$$

where the columns of $\mathbf{V}_m = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m] \in \mathbb{R}^{n \times m}$ and $\mathbf{V}_{m+1} = [\mathbf{V}_m, \mathbf{v}_{m+1}] \in \mathbb{R}^{n \times (m+1)}$ form an orthonormal basis for $\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$ and $\mathcal{K}_{m+1}(\mathbf{A}, \mathbf{r}^{(0)})$, respectively.



Arnoldi's Method

- This means that $\mathbf{V}_m^T \mathbf{V}_m = \mathbf{I}$ and $\mathbf{V}_{m+1}^T \mathbf{V}_{m+1} = \mathbf{I}$, where \mathbf{I} is the identity matrix. Note also that $\mathbf{V}_m^T \mathbf{A} \mathbf{V}_m = \mathbf{H}_m$.
- The rectangular matrix $\overline{\mathbf{H}}_m \in \mathbb{R}^{(m+1) \times m}$ is an upper Hessenberg matrix:

$$\overline{\mathbf{H}}_m = \begin{bmatrix} h_{1,1} & h_{1,2} & \dots & h_{1,m-1} & h_{1,m} \\ h_{2,1} & h_{2,2} & \dots & h_{2,m-1} & h_{2,m} \\ h_{3,2} & \dots & h_{3,m-1} & h_{3,m} & \vdots \\ \vdots & & \vdots & \vdots & \vdots \\ h_{m,m-1} & h_{m,m} & & & \end{bmatrix}$$

Upper Hessenberg

m *m* *m+1*

Arnoldi's Method

- When the Classical Gram-Schmidt (CGS) Algorithm is implemented in a floating point environment the basis vectors (columns of \mathbf{V}_m) are sometimes not quite orthogonal due to rounding errors.

- This can be rectified by the small modification highlighted in blue in the algorithm below. This new version is referred to as Modified Gram-Schmidt (MGS).

CLASSICAL GRAM-SCHMIDT PROCESS (CGS)

$$\begin{aligned}\underline{\omega}_{m+1} &= \underline{A}\underline{v}_m - P_{K_m}(\underline{A}\underline{v}_m) \\ &= (\underline{A}\underline{v}_m) - \sum_{j=1}^{m+1} (\underline{v}_j^T \underline{A}\underline{v}_m) \underline{v}_j\end{aligned}$$

$$\underline{v}_{m+1} = \underline{\omega}_{m+1} / \|\underline{\omega}_{m+1}\|_2$$

MODIFIED GRAM-SCHMIDT PROCESS (MGS)

$$\underline{\omega}_{m+1} = (I - \underline{v}_m \underline{v}_m^T)(I - \underline{v}_{m-1} \underline{v}_{m-1}^T) \dots (I - \underline{v}_1 \underline{v}_1^T) \underline{A}\underline{v}_m$$

$$\underline{v}_{m+1} = \underline{\omega}_{m+1} / \|\underline{\omega}_{m+1}\|_2$$

MAIN OBSERVATION

$CGS :$

$$\begin{aligned}\underline{\omega}_{m+1} &= \left[I - \sum_{j=1}^m \underline{v}_j \underline{v}_j^T \right] \underline{A} \underline{v}_m \\ &= \left[I - \underline{v}_1 \underline{v}_1^T - \underline{v}_2 \underline{v}_2^T - \dots - \underline{v}_m \underline{v}_m^T \right] \underline{A} \underline{v}_m\end{aligned}$$

MGS : DUE TO ORTHOGONALITY

$$\begin{aligned}&(I - \underline{v}_m \underline{v}_m^T) (I - \underline{v}_{m-1} \underline{v}_{m-1}^T) \\ &= I - \underline{v}_{m-1} \underline{v}_{m-1}^T - \underline{v}_m \underline{v}_m^T + \underline{v}_m (\underline{v}_m^T \underline{v}_{m-1}) \underline{v}_{m-1}^T\end{aligned}$$

... CONTINUING THE PROCESS

$$\begin{aligned}\underline{\omega}_{m+1} &= (I - \underline{v}_m \underline{v}_m^T) (I - \underline{v}_{m-1} \underline{v}_{m-1}^T) \dots (I - \underline{v}_1 \underline{v}_1^T) \underline{A} \underline{v}_m \\ &= \boxed{\left[I - \underline{v}_m \underline{v}_m^T - \underline{v}_{m-1} \underline{v}_{m-1}^T - \dots - \underline{v}_1 \underline{v}_1^T \right] \underline{A} \underline{v}_m}\end{aligned}$$

a bases for K_m is $\{A_r^{(0)}, A_{\underline{r}}^{(0)}, \dots, A_{\underline{\underline{r}}}^{(0)}\}$
 $A K_m = \{A_r^{(0)}, A_{\underline{r}}^{(0)}, \dots, A_{\underline{\underline{r}}}^{(0)}\}$.

provided A is nonsingular then this
 is a basis for $A K_m$.

The only solution of

$$c_1 A_r^{(0)} + c_2 A_{\underline{r}}^{(0)} + \dots + c_n A_{\underline{\underline{r}}}^{(0)} = 0$$

is the trivial solution $c_1 = c_2 = \dots = c_n = 0$.

Consider

$$b_1 A_r^{(0)} + b_2 A_{\underline{r}}^{(0)} + \dots + b_n A_{\underline{\underline{r}}}^{(0)} = 0$$

$$A(b_1 A_r^{(0)} + b_2 A_{\underline{r}}^{(0)} + \dots + b_n A_{\underline{\underline{r}}}^{(0)}) = 0$$

2

If A is nonsingular, the only solution is
 $b_1 A_r^{(0)} + b_2 A_{\underline{r}}^{(0)} + \dots + b_n A_{\underline{\underline{r}}}^{(0)} = 0$
 $\therefore b_1 = b_2 = \dots = b_n = 0$ because $\{A_r^{(0)}, A_{\underline{r}}^{(0)}, \dots, A_{\underline{\underline{r}}}^{(0)}\}$
 is linearly indep. \square

Generalised Minimal Residual Method (GMRES)

- For the Generalised Minimal Residual Method (GMRES) the constraint space is chosen as $\mathcal{W}_m = \mathbf{A}\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$.
- An approximate solution $\mathbf{x}^{(m)}$ is sought from the affine space $\underline{\mathcal{X}}^{(m)} \in \underline{\mathbf{x}^{(0)} + \mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})}$ by imposing the Petrov-Galerkin condition:
$$\left\{ \begin{array}{l} \mathbf{A}\mathbf{y}_1, \mathbf{A}\mathbf{y}_2, \dots, \mathbf{A}\mathbf{y}_m \end{array} \right\} \perp \mathbf{A}\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)}).$$

$$\mathbf{r}^{(m)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(m)} \perp \mathbf{A}\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)}). \quad (7)$$

- Since we seek $\mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$ we assume the following form:

$$\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{V}_m \mathbf{y}_m$$
$$= \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_m \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}.$$

where $\mathbf{y}_m \in \mathbb{R}^m$ is a vector to be determined and the columns of \mathbf{V}_m are the orthonormal basis vectors of $\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$ generated using Arnoldi's method.

$$\begin{aligned}
 \underline{r}^{(n)} &= \underline{b} - A \left\{ \underline{x}^{(0)} + V_n \underline{y}_n \right\} \\
 &= \underline{r}^{(0)} - (AV_n) \underline{y}_n \\
 &= \underline{r}^{(0)} - V_{n+1} \overline{H}_n \underline{y}_n \\
 &= V_{n+1} \left\{ \beta_0 e_1 - \overline{H}_n \underline{y}_n \right\}.
 \end{aligned}$$

APPLY PETROV-GALERKIN CONDITION

$$(AV_n)^T \underline{r}^{(n)} = 0$$

SUBSTITUTION GIVES

$$\overline{H}_n^T (V_{n+1}^T V_{n+1}) \left\{ \beta_0 e_1 - \overline{H}_n \underline{y}_n \right\} = 0$$

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

"n × n"

Projection

(NORMAL EQUATIONS)

??

y_n is therefore a solution of a system of linear equations

ARNOLDI RELATION
 $A \bar{V}_k = \bar{V}_{k+1} \overline{H}_k$

$$y_1 = \frac{\underline{r}^{(0)}}{\beta_0}, \quad \beta_0 = \| \underline{r}^{(0)} \|_2$$

$$\beta_0 V_{n+1} e_1 = \underline{r}^{(0)}$$

HENCE

$$\overline{H}_n^T \overline{H}_n y_n = \beta_0 \overline{H}_n^T e_1$$

"Max"

Max

Generalised Minimal Residual Method (GMRES)

- The orthogonality condition (7) yields the following m -dimensional system to be solved for \mathbf{y}_m :

$$\bar{\mathbf{H}}_m^T \bar{\mathbf{H}}_m \mathbf{y}_m = \bar{\mathbf{H}}_m^T \beta \mathbf{e}_1. \quad (8)$$

where $\beta = \|\mathbf{r}^{(0)}\|$ and $\mathbf{e}_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^{m+1}$.

- Note that $\bar{\mathbf{H}}_m \in \mathbb{R}^{(m+1) \times m}$ so $\bar{\mathbf{H}}_m^T \bar{\mathbf{H}}_m \in \mathbb{R}^{m \times m}$.
- The system of linear equations (8) are the *normal equations* associated with the $(m+1) \times m$ linear system:

$$\boxed{\bar{\mathbf{H}}_m \mathbf{y}_m \approx \beta \mathbf{e}_1.}$$

(9)

$$\underline{x}^{(m)} = \underline{x}^{(0)} + V_m \mathbf{y}_m$$

Generalised Minimal Residual Method (GMRES)

- Hence the solution of (8) is equivalent to the *least squares solution* of (9), which be computed in MATLAB using the *backslash operator* $\mathbf{y}_m = \bar{\mathbf{H}}_m \backslash (\beta \mathbf{e}_1) = \bar{\mathbf{H}}_m^+ (\beta \mathbf{e}_1)$
- The GMRES approximate solution is therefore given by:

$$\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \beta \mathbf{V}_m \bar{\mathbf{H}}_m^\dagger \mathbf{e}_1 \quad (10)$$

where $\bar{\mathbf{H}}_m^\dagger$ is the pseudoinverse of $\bar{\mathbf{H}}_m$, which can be determined from the singular value decomposition of \mathbf{A} . The residual vector simplifies to:

$$\|\mathbf{r}^{(m)}\|_2^2 = \|\mathbf{b} - \mathbf{Ax}^{(m)} - \mathbf{V}_{m+1} (\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}_m)\|_2^2 = \varepsilon^T \varepsilon \quad (11)$$

and therefore:

$$\|\mathbf{r}^{(m)}\|_2 = \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}_m\|_2.$$

Generalised Minimal Residual Method (GMRES)

In summary, GMRES involves the following steps:

- 1 Choose $\mathbf{x}^{(0)}$ and compute $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(0)}$, $\beta = \|\mathbf{r}^{(0)}\|$ and $\mathbf{v}_1 = \mathbf{r}^{(0)} / \beta$.
- 2 Generate $\mathbf{AV}_m = \mathbf{V}_{m+1} \bar{\mathbf{H}}_m$ using the Arnoldi algorithm. (M65).
- 3 Solve the least squares problem $\min_{\mathbf{y} \in \mathbb{R}^m} \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}\|_2$ for \mathbf{y}_m .
- 4 Compute residual norm $\|\mathbf{r}^{(m)}\|_2 = \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}_m\|_2$.
Check if
$$\mathbf{y}_m = \arg \min_{\mathbf{y} \in \mathbb{R}^m} \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}\|_2$$
- and if so, go to step 5 else go back to step 2. A typical value of the tolerance tol is 10^{-8} .
- 5 Compute approximate solution $\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{V}_m \mathbf{y}_m$.



SOLUTION OF LEAST SQUARES PROBLEM

$$\min_{y \in \mathbb{R}^m} \| \beta_0 e_1 - \bar{H}_m y \|_2$$

USING SINGULAR VALUE DECOMPOSITION

(S.V.D.) $\underbrace{\quad}_{m \times m}$

$$\bar{H}_m = Q_{m+1} \sum_m (P_m^T) ; \quad Q_{m+1} = (Q_m : \tilde{q}_{m+1})$$

$$\sum_m = \begin{pmatrix} \sigma_1 q_1 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & \dots & \dots & 0 \end{pmatrix} = \begin{pmatrix} S_m \\ 0^T \end{pmatrix}$$

$$y_m = \bar{H}_m^+ (\beta_0 e_1) = P_m S_m^{-1} (Q_m^T (\beta_0 e_1))$$

$$= \sum_{j=1}^m \left[\frac{(\beta_0 e_1)^T e_j}{\sigma_j} \right] \beta_j$$

$$\| \underline{\epsilon}_m^{(cm)} \|_2 = \| \beta_0 e_1 - \bar{H}_m (P_m S_m^{-1} Q_m^T (\beta_0 e_1)) \|_2$$

$$= \|\beta_0 e_i - \frac{Q_{m+1} \sum_m P_m^T P_m}{Q_m S_m} S_m^{-1} Q_m^T \beta_0 e_i\|$$

$$= \left\| \left(I - Q_m Q_m^T \right) \beta_0 e_i \right\|$$

$$Q_{m+1}^T Q_{m+1} = \begin{pmatrix} Q_m^T \\ q_{m+1}^T \end{pmatrix} (Q_m : q_{m+1}) = I$$

$$Q_{m+1} Q_{m+1}^T = (Q_m : q_{m+1}) \begin{pmatrix} Q_m^T \\ q_{m+1}^T \end{pmatrix} = I$$

$$\therefore Q_m Q_m^T + q_{m+1} q_{m+1}^T = I$$

$$\text{i.e. } I - Q_m Q_m^T = \underline{\underline{q_{m+1} q_{m+1}^T}}$$

$$\therefore \|f^{(m)}\| = \|f_{m+1} (q_{m+1}^T \beta_0 e_i)\|_2$$

$$= \beta_0 |q_{m+1}^T e_i| \leftarrow$$

Note:

Generalised Minimal Residual Method (GMRES)

- Note that the above result is only true for the 2-norm. For a general norm, the result is:

$$\| \mathbf{r}^{(m)} \| = \| \mathbf{V}_{m+1} (\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}_m) \| . \quad (13)$$

- To compute the residual norm there is no need for the matrix-vector product $\mathbf{A}\mathbf{x}^{(m)}$.

Theorem (Minimum residual)

The GMRES approximate solution $\mathbf{x}^{(m)}$ minimises the 2-norm of the residual vector over the affine space $\mathbf{x}^{(0)} + \mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$.

Another way to view the behavior of GMRES.

$$\min_{\mathbf{x} \in \mathcal{K}_m} \| \underline{\mathbf{b}} - \underline{\mathbf{A}\mathbf{x}} \|_2$$

\Leftrightarrow

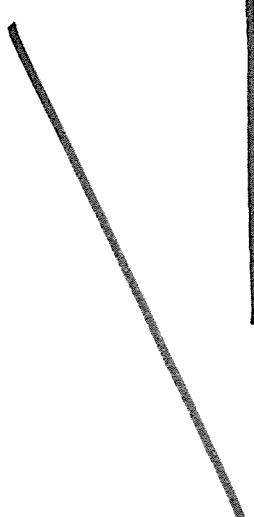
$$\min_{y \in \mathbb{R}^m} \| b - A \{ x^{(0)} + V_m y \} \|_2$$

$$= \min_{y \in \mathbb{R}^m} \| b - Ax^{(0)} - AV_m y \|_2$$

$$= \min_{y \in \mathbb{R}^m} \| (I_m - V_m H_m) y \|_2$$

$$= \boxed{\min_{y \in \mathbb{R}^m} \| V_m \{ (I_m - H_m) y \} \|_2}$$

$$\min_{y \in \mathbb{R}^m} \| (I_m - H_m) y \|_2$$



Preconditioning

- The basic idea is to choose a *preconditioning matrix* or preconditioner \mathbf{M} and solve a preconditioned version of the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$. $(\mathbf{A}\mathbf{M}^{-1}\mathbf{M}\tilde{\mathbf{x}}) = \mathbf{b}$, $\mathbf{A}\tilde{\mathbf{x}} = \mathbf{b}$
- Here we consider only right preconditioning:
Right preconditioning: The matrix \mathbf{M}^{-1} is actioned on the right of \mathbf{A} . The following right preconditioned system is then solved for $\tilde{\mathbf{x}}$:

$$(\mathbf{A}\mathbf{M}^{-1})\tilde{\mathbf{x}} = \mathbf{b}, \quad \tilde{\mathbf{x}} = \mathbf{M}\mathbf{x}. \quad (16)$$

- The required solution of the original linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ is then computed by solving $\mathbf{M}\mathbf{x} = \tilde{\mathbf{x}}$ for \mathbf{x} . *Very easy compute.*
- The preconditioner \mathbf{M} is chosen to be close to \mathbf{A} (in some sense) so that the matrix $\mathbf{A}\mathbf{M}^{-1}$ is close to the identity matrix, which produces faster convergence of the GMRES iterations.

Right-preconditioning

- In other words, \mathbf{M} should be some approximation to the matrix \mathbf{A} (or equivalently \mathbf{M}^{-1} should be some approximation to the inverse of the matrix \mathbf{A}). The preconditioner \mathbf{M} must also be cheap to generate and easy to invert. *With computations*
- Some common choices include:
 - ▶ Jacobi: $\mathbf{M} = \mathbf{D}$ $\mathbf{D} = \begin{pmatrix} d_{11} & & \\ & \ddots & \\ & & d_{nn} \end{pmatrix}$ $\mathbf{A} = \mathbf{L} + \mathbf{D} + \mathbf{U}$
 - ▶ Gauss-Seidel: $\mathbf{M} = \mathbf{D} + \mathbf{L}$ *forward solve*
 - ▶ SOR: $\mathbf{M} = \frac{1}{\omega} \mathbf{D} + \mathbf{L}$
 - ▶ Incomplete LU Factorisation: $\boxed{\mathbf{M} = \text{ilu}(\mathbf{A})}$
- where \mathbf{D} is the diagonal portion of \mathbf{A} , \mathbf{L} is the lower triangular portion of \mathbf{A} and ω is a chosen parameter.
- The incomplete LU factorisation produces sparse factors \mathbf{L} and \mathbf{U} such that $\mathbf{LU} \approx \mathbf{A}$.

Right-preconditioning

- Despite the knowledge of what a good preconditioner should do, the choice of an optimal \mathbf{M} for a particular system is still very much a trial and error process.
- In your group projects, \mathbf{M} is chosen as the full Jacobian matrix of \mathbf{F} but is held constant over several Newton iterations/time steps with heuristics used to determine when the preconditioner is updated.
- Note that for right preconditioning the residual vector does not change:

$$\tilde{\mathbf{r}}^{(m)} = \mathbf{b} - \mathbf{A}\mathbf{M}^{-1}\tilde{\mathbf{x}}^{(m)} = \mathbf{b} - \mathbf{A}\mathbf{M}^{-1}(\mathbf{M}\mathbf{x}^{(m)}) = \mathbf{b} - \mathbf{A}\mathbf{x}^{(m)} = \underline{\mathbf{r}^{(m)}} \quad (17)$$

Right-preconditioning GMRES

- For right-preconditioned GMRES an approximate solution $\mathbf{x}^{(m)}$ is sought from the affine space $\mathbf{x}^{(0)} + \mathbf{M}^{-1}\mathcal{K}_m(\underline{\mathbf{AM}^{-1}}, \mathbf{r}^{(0)})$ by imposing the Petrov-Galerkin condition:

$$\mathbf{r}^{(m)} = \mathbf{b} - \mathbf{Ax}^{(m)} \perp \mathbf{AM}^{-1}\mathcal{K}_m(\mathbf{AM}^{-1}, \mathbf{r}^{(0)}). \quad (18)$$

Right-preconditioned GMRES involves the following steps:

- Choose $\mathbf{x}^{(0)}$ and compute $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{Ax}^{(0)}$, $\beta = \|\mathbf{r}^{(0)}\|_2$ and $\mathbf{v}_1 = \mathbf{r}^{(0)}/\beta$.
- Generate $\boxed{\mathbf{AM}^{-1}\mathbf{V}_m} = \mathbf{V}_{m+1}\bar{\mathbf{H}}_m$ using the Arnoldi algorithm:

$$\mathbf{AM}^{-1}\mathbf{V}_m = \mathbf{V}_{m+1}\bar{\mathbf{H}}_m$$

$$\mathbf{AV}_m = \mathbf{V}_{m+1}\bar{\mathbf{H}}_m$$

$$\mathbf{AU} = \mathbf{V}_{m+1}\bar{\mathbf{H}}_m$$
- Solve the least squares problem $\min_{\mathbf{y} \in \mathbb{R}^m} \|\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}\|_2$ for \mathbf{y}_m .
- Compute residual norm $\|\mathbf{r}^{(m)}\|_2 = \|\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}_m\|_2$. If $\|\mathbf{r}^{(m)}\|_2 < tol/\|\mathbf{r}^{(0)}\|_2$ go to step 5 else go back to step 2. A typical value of the tolerance tol is 10^{-8} .
- Compute approximate solution $\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{M}^{-1}\boxed{\mathbf{V}_m \mathbf{y}_m}$

$$\mathbf{Solve} \mathbf{Mu} = \mathbf{V}_m \mathbf{y}_m \text{ for } \mathbf{u} \text{ then } \mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{u}$$

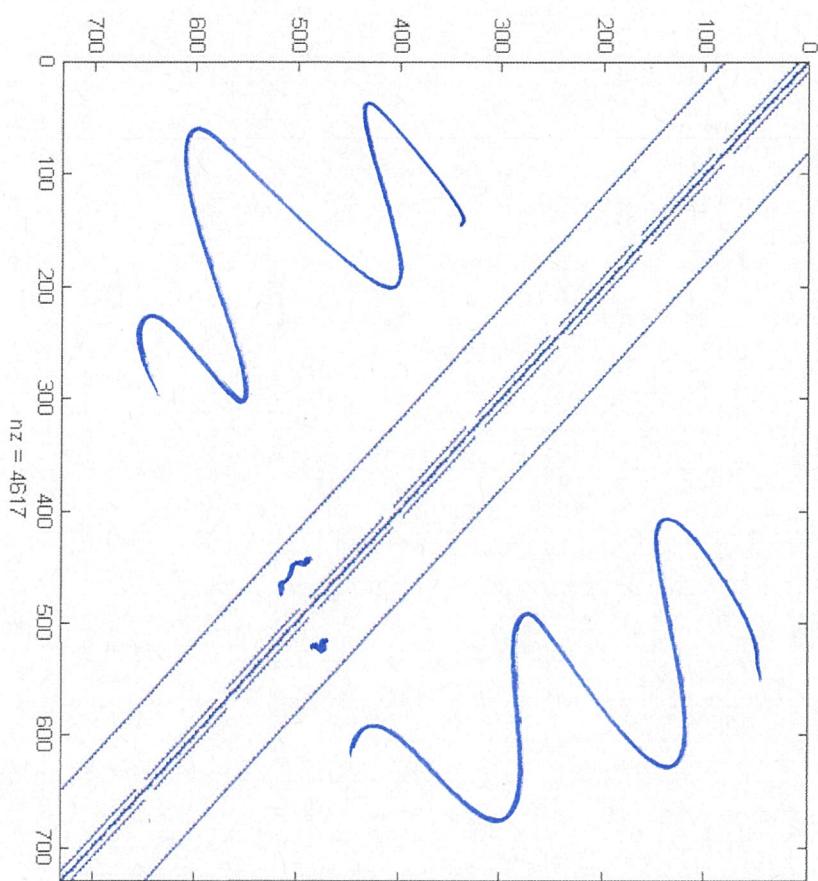
Case Studies:

Selected from the Matrix Market

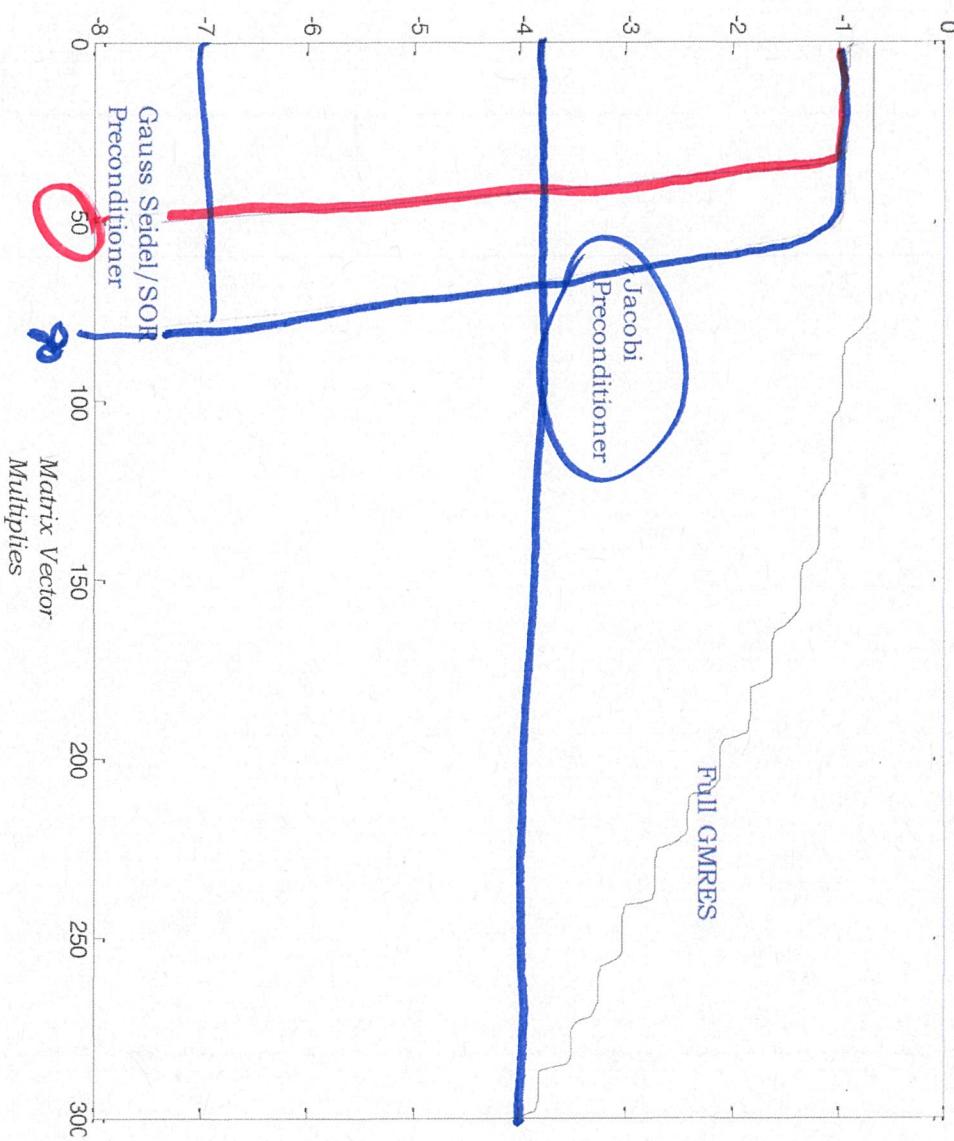
<http://math.nist.gov/MatrixMarket>

Nos7

$$\|\mathbf{b}\|_2 = 0.2313, n = 729, \|\mathbf{A}\|_2 = \underline{9.864 \times 10^6}, \text{cond}(\mathbf{A}) = \underline{2.3745 \times 10^9}$$



The Impact of (Right) Preconditioning



```

function [x,m] = pGMRESv01(A,b,x0,M,tol,MaxKrylov,diagnostics)
%Calculates the General Minimal Residual Method (GMRES) for a given matrix
%A and solution vector b.
%Input: Matrix A, vector b
%output: solution vector x and number of loops m

%Initialise
N = size(A,1);
H = zeros(MaxKrylov+1,MaxKrylov);
V = zeros(N,MaxKrylov+1);

r = b - A*x0;
beta = norm(r,2);
V(:,1) = r/beta;
m=0;
rnorm=inf;

while rnorm > beta*tol && m <= MaxKrylov
    m=m+1;
    %Arnoldi (Modified Gram-Schmidt)
    V(:,m+1) = A*(M\V(:,m));
    for j = 1:m
        H(j,m) = V(:,j)'*V(:,m+1);
        V(:,m+1) = V(:,m+1) - H(j,m)*V(:,j);
    end
    H(m+1,m) = norm(V(:,m+1),2);

    % Check for breakdown
    if abs(H(m+1,m)) < 1e-14
        fprintf('Invariant Krylov Subspace detected at m=%g\n',m);
        y = H(1:m,1:m) \ ([beta; zeros(m-1,1)]); % Invariant space detected
        break;
    else
        V(:,m+1) = V(:,m+1)/H(m+1,m);
    end
    % Solve small m dimensional least squares problem for y
    rhs= [beta; zeros(m,1)];
    y = H(1:m+1,1:m) \ rhs; ←
    % determine residual norm
    rnorm = norm(rhs-H(1:m+1,1:m)*y);

    if diagnostics, fprintf('m=%g ||r_m||=%g tol=%g\n',m,rnorm,beta*tol); end
end

%% Compute approximate solution
x = x0 + M\ (V(:,1:m)*y);
end

```

$$\frac{\|r^{(m)}\|}{\|L^{(0)}\|} < tol$$

m=m+1;

%Arnoldi (Modified Gram-Schmidt)

V(:,m+1) = A*(M\V(:,m));

for j = 1:m

H(j,m) = V(:,j)'*V(:,m+1);

V(:,m+1) = V(:,m+1) - H(j,m)*V(:,j);

end

H(m+1,m) = norm(V(:,m+1),2);

% Check for breakdown

if abs(H(m+1,m)) < 1e-14

"Happy"



fprintf('Invariant Krylov Subspace detected at m=%g\n',m);

y = H(1:m,1:m) \ ([beta; zeros(m-1,1)]); % Invariant space detected

break;

else

V(:,m+1) = V(:,m+1)/H(m+1,m);

end

% Solve small m dimensional least squares problem for y

rhs= [beta; zeros(m,1)];

y = H(1:m+1,1:m) \ rhs; ←

$$y_{\text{as}} = \bar{H}_m^+ (\beta e_1)$$

% determine residual norm

rnorm = norm(rhs-H(1:m+1,1:m)*y);

if diagnostics, fprintf('m=%g ||r_m||=%g tol=%g\n',m,rnorm,beta*tol); end

end

%% Compute approximate solution

x = x0 + M\ (V(:,1:m)*y);

end

SVD

==