MXB324 Computational Fluid Dynamics

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Introduction

- In this chapter we investigate methods for solving systems of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1}$$

where $\mathbf{A} \in \mathbb{R}^{n\times n}$ is nonsymmetric and $\mathbf{x}, \mathbf{b} \in \mathbb{R}^{n}$.

- Our motivation for considering such systems stems from Newton's method (as discussed in Chapter 2) which requires solving:

$$\mathbf{J}(\mathbf{x}^{(k)})\delta\mathbf{x}^{(k)} = -\mathbf{F}(\mathbf{x}^{(k)})$$

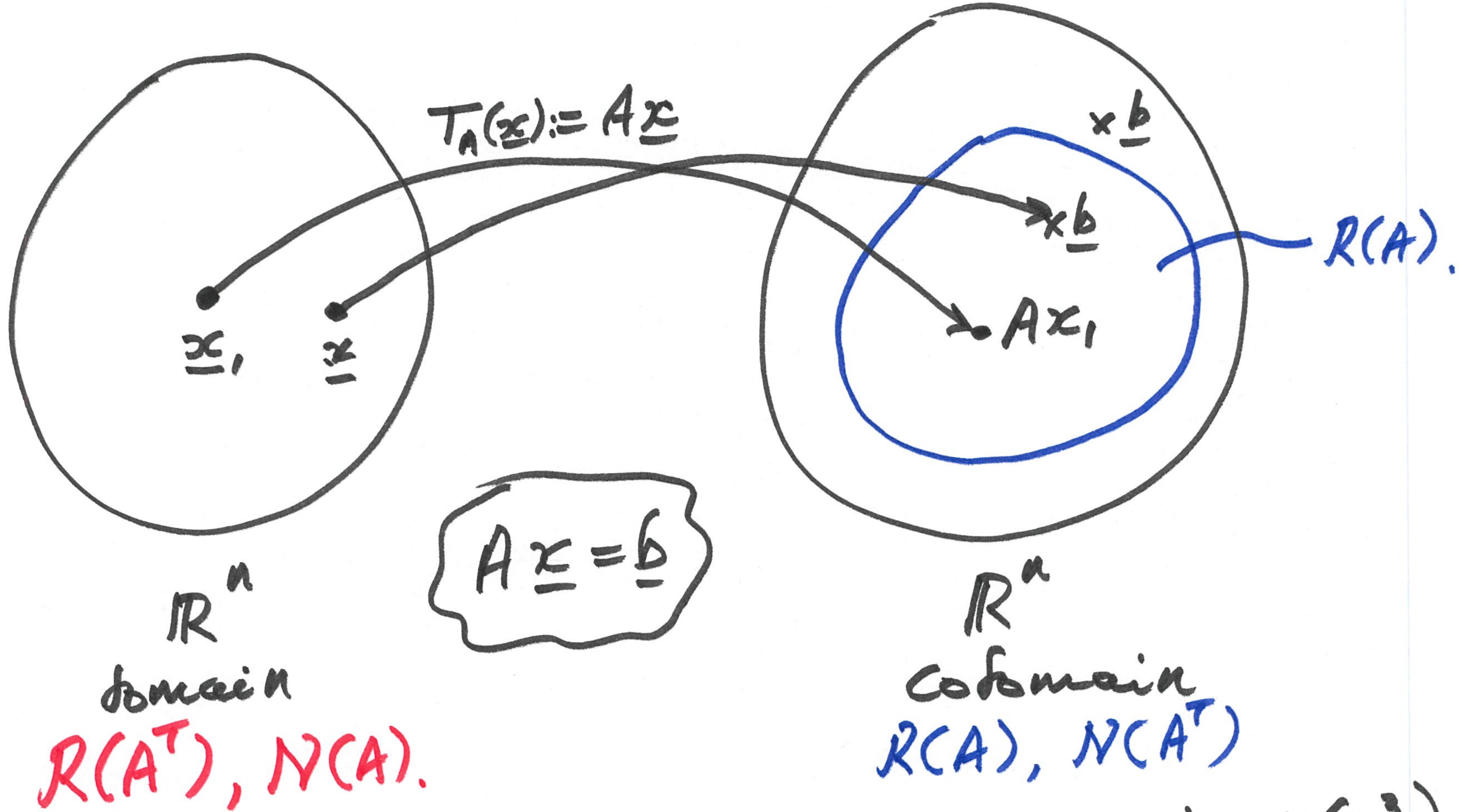
for $\delta\mathbf{x}^{(k)}$, at each Newton iteration.

$A \in \mathbb{R}^{n\times n}$, $\underline{b} \in \mathbb{R}^{n\times 1}$, $\underline{b} \neq \underline{0}$.

$\underline{x} \in \mathbb{R}^{n\times 1}$

$\text{rank}(A) = n$?

$\text{rank}(A) = r < n$



LU (Gaussian Elimination) $O(n^3)$.

NOT possible.

Introduction

- When the coefficient matrix $\mathbf{A}$ is large and sparse many iterative methods for solving (1) seek an approximate solution in a Krylov subspace.

Definition (Krylov subspace)

Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ *and* $\mathbf{b} \in \mathbb{R}^{n}$ *be any nonzero vector. The Krylov subspace generated by* $\mathbf{A}$ *and* $\mathbf{b}$ *is defined as*

$$\mathcal{K}_m(\mathbf{A},\mathbf{b}) = span\left\{\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^{m-1}\mathbf{b}\right\}.$$

Introduction

- The Krylov subspace naturally arises in the solution of linear systems of equations. To see why, recall the *Cayley-Hamilton* theorem, which states that any matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ satisfies it's characteristic equation, that is,

$$p(\mathbf{A}) = \mathbf{0}$$

where $p(\lambda) = \det(\lambda\mathbf{I} - \mathbf{A})$ is the characteristic polynomial of $\mathbf{A}$.

- The characteristic polynomial is a <u>monic polynomial</u> of <u>degree n</u> (i.e. the coefficient of λ^n is equal to 1) taking the form:

$$p(\lambda) = a_0 + a_1\lambda + a_2\lambda^2 \ldots + a_{n-1}\lambda^{n-1} + \overset{1}{\lambda^n}$$

where the coefficients a_i ($i = 0, \ldots, n-1$) are known.

The set of Annihilating polynomials for $A \in \mathbb{R}^{n\times n}$:

$$S_A = \left\{ p(t) \;\middle|\; \deg[p(t)] \leq n,\ p \text{ is monic polynomial},\ p(A) = 0_{n\times n} \right\}$$

- $S_A \neq \phi$ because by Cayley-Hamilton Th^{m} we have $c(t) \in S_A$.
- The monic polynomial of lowest degree in S_A, denoted $m(t)$, is called the minimal polynomial for A.
- $m(t)$, the minimal polynomial for A, is unique.

Proof: Suppose $\deg[m(t)] = k$, therefore if $m_1(t)$ was a minimal polynomial for A then

$$m_1(t) = t^k - \sum_{j=0}^{k-1} \alpha_j t^j$$

suppose that $m_2(t) = t^k - \sum_{j=0}^{k-1} \beta_j t^j$ is another minimal polynomial for A.

Define $d(t) = m_1(t) - m_2(t)$

Note $d(A) = m_1(A) - m_2(A) = O_{n\times n}$.

$\therefore$ $d(t)$ is an annihilating polynomial for A.

$$d(t) = \sum_{j=0}^{k-1} (\beta_j - \alpha_j) t^j = \sum_{j=0}^{k-2} (\beta_j - \alpha_j) t^j + (\beta_{k-1} - \alpha_{k-1}) t^{k-1}$$

Since $d(A) = O_{n\times n}$ we have that

$$\hat{d}(A) = \sum_{j=0}^{k-2} \left(\frac{\beta_j - \alpha_j}{\beta_{k-1} - \alpha_{k-1}}\right) A^j + A^{k-1} = O_{n\times n}.$$

$\Rightarrow$ $\hat{d}(t) = 1.\, t^{k-1} + \sum_{j=0}^{k-2} \gamma_j t^j$ is an annihilating polynomial for A monic, but $\deg[\tilde{d}(t)] = k-1 \implies$ contradiction !

$\therefore$ the minimal polynomial for A must be unique. $\square$

EXAMPLE :

$$A = \begin{pmatrix} 4 & -1 & 0 & -1 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ -1 & 0 & -1 & 4 \end{pmatrix} \in \mathbb{R}^{4\times 4}$$

CHARACTERISTIC POLYNOMIAL :

$-\mathrm{tr}(A)$ $\quad$ $(-1)^n \det(A)$

$$c(t) = \det(tI_4 - A) = t^4 - 16t^3 + 92t^2 - 224t \boxed{+ 192}$$

SPECTRUM : $\sigma(A) = \{2, 4, 6\}$ — set of distinct eigenvalues of A.

$$\left.\begin{aligned} \text{alg mult}_A(2) &= \text{geo mult}_A(2) = 1 \\ \text{alg mult}_A(4) &= \text{geo mult}_A(4) = 2 \\ \text{alg mult}_A(6) &= \text{geo mult}_A(6) = 1 \end{aligned}\right\} \; c(t) = (t-2)^1(t-4)^2(t-6)^1$$

A can be diagonalised as $A = XDX^{-1}$.

MINIMAL POLYNOMIAL :

$$m(t) = (t-2)(t-4)(t-6) = t^3 - 12t^2 + 44t - 48$$

$$c(A) = 0_{4\times 4} \quad \text{and} \quad m(A) = 0_{4\times 4} .$$

Next, we introduce minimal polynomial for $\underline{b} \in \mathbb{R}^{n\times 1}$ relative to $A \in \mathbb{R}^{n\times n}$.

$$\underbrace{A^{-1}A}\underline{x} = A^{-1}\underline{b}$$

$$I_n\underline{x} = \underline{x} = A^{-1}\underline{b}$$

$\underline{b} \neq \underline{0}$

$$q(A)\,\underline{b} = \underline{0}_{n\times 1}.$$

Suppose $A \in \mathbb{R}^{n\times n}$ is nonsingular then take $q(t) = t^k - \sum_{j=0}^{k-1} \alpha_j t^j$, $\deg[q(t)] = k$.

Note: $q(A)\,\underline{b} = A^k\underline{b} - \sum_{j=0}^{k-1} \alpha_j A^j \underline{b} = \underline{0}$

$\therefore$ $A^k\underline{b} - \sum_{j=1}^{k-1} \alpha_j A^j\underline{b} - \alpha_0 A^0 \underline{b} = \underline{0}$, $A^0 = I_n$.

i.e., $\alpha_0 A^{-1}\underline{b} = A^{k-1}\underline{b} - \sum_{j=1}^{k-1} \alpha_j A^{j-1}\underline{b}$.

$$A^{-1}A^k = A^k A^{-1} = A^{k-1}.$$

provided $\alpha_0 \neq 0$ we divide throughout to obtain

$$\underline{x} = A^{-1}\underline{b} = \frac{1}{\alpha_0} A^{k-1}\underline{b} - \sum_{j=1}^{k-1}\left(\frac{\alpha_j}{\alpha_0}\right) A^{j-1}\underline{b}$$

$$= \frac{1}{\alpha_0} A^{k-1}\underline{b} - \sum_{j=0}^{k-2}\left(\frac{\alpha_{j+1}}{\alpha_0}\right) A^{j}\underline{b}.$$

$$\therefore \quad \underline{x} = A^{-1}\underline{b} = \sum_{j=0}^{k-1} \beta_j A^j \underline{b}, \quad \beta_j = \frac{\alpha_{j+1}}{\alpha_0}, \; j = 0, \dots, k-2$$

$$\beta_{k-1} = \frac{1}{\alpha_0}.$$

<u>CONCLUSION</u>:

$$\underline{x} = \beta_0(\underline{b}) + \beta_1(A\underline{b}) + \dots + \beta_{k-1}(A^{k-1}\underline{b})$$

$$\therefore \quad \underline{x} \in \operatorname{span}\{\underline{b}, A\underline{b}, \dots, A^{k-1}\underline{b}\} \equiv K_k(A, \underline{b})$$

i.e., the solution of $A\underline{x} = \underline{b}$ lies in the Krylov subspace $K_k(A, \underline{b})$.

The great result is that

$$k = \deg[q(t)] := \operatorname{grade}(\underline{b}). \ll n.$$

GREAT PROMISE!!

Why is $\alpha_0 \neq 0$ when A is nonsingular?

Given $\quad q(t) = t^k - \sum_{j=0}^{k-1} \alpha_j t^j$

and $\quad q(A)\underline{b} = A^k \underline{b} - \sum_{j=1}^{k-1} \alpha_j A^j \underline{b} - \cancel{\alpha_0 \underline{b}} = \underline{0}$

Suppose $\alpha_0 = 0$ then

$$A^k \underline{b} - \sum_{j=1}^{k-1} \alpha_j A^j \underline{b} = \underline{0}$$

$$A \underbrace{\left[A^{k-1} \underline{b} - \sum_{j=1}^{k-1} \alpha_j A^{j-1} \underline{b} \right]}_{\underline{z}\,:\ \text{Vector in } \mathbb{R}^{n\times 1}} = \underline{0}$$

i.e, $\quad A\underline{z} = \underline{0} \implies \underline{z} \in N(A) = \{\underline{0}\}$.

It must therefore be that $\underline{z} = \underline{0}$.

i.e., $\quad A^{k-1} \underline{b} - \sum_{j=0}^{k-2} \alpha_{j+1} A^j \underline{b} = \underline{0}$

i.e, $\quad \left[A^{k-1} - \sum_{j=0}^{k-2} \alpha_{j+1} A^j \right] \underline{b} = \underline{0}$ which is a contradiction!

$\therefore \quad \alpha_0 \neq 0$.

Consider $\underline{b} = (3, 1, 3, 1)^T$, which can be expressed as a linear combination of the eigenvectors associated with the eigenvalues

$$\lambda = 2, 4.$$

In this case, the minimal polynomial for $\underline{b}$ relative to A is

$$q(t) = (t-2)(t-4) = t^2 - 6t + 8$$

we have that $q(A)\underline{b} = (A^2 - 6A + 8I_4)\underline{b} = \underline{0}$

$\text{grade}(\underline{b}) = 2 = \deg[q(t)]$.

Hence,

$$A^2\underline{b} - 6A\underline{b} + 8\underline{b} = \underline{0}$$

$$\therefore \cancel{8}\underline{b} = \frac{6}{8}A\underline{b} - \frac{1}{8}A^2\underline{b}$$

i.e, $\underline{x} = A^{-1}\underline{b} = \frac{3}{4}A^{-1}A\underline{b} - \frac{1}{8}A^{-1}A^2\underline{b}$

$$\underline{x} = \frac{3}{4}\underline{b} - \frac{1}{8}A\underline{b} \quad \therefore \underline{x} = \text{Span}\{\underline{b}, A\underline{b}\}$$

$$= \mathcal{K}_2(A, \underline{b}).$$

Projection Method

- To solve the large sparse linear system $\mathbf{Ax} = \mathbf{b}$, given some arbitrary initial estimate of the solution $\mathbf{x}^{(0)}$, projection methods seek an approximate solution $\mathbf{x}^{(m)}$ from the affine space $\mathbf{x}^{(0)} + \mathcal{S}_m$ where $\mathcal{S}_m$ is an m-dimensional search space.
- This is achieved by imposing the condition that the residual vector $\mathbf{r}^{(m)} = \mathbf{b} - \mathbf{Ax}^{(m)}$ be orthogonal to another m-dimensional subspace $\mathcal{W}_m$ called the *subspace of constraints*. In other words, we seek to:

$$\boxed{\textit{Find } \mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathcal{S}_m \textit{ such that } \mathbf{r}^{(m)} = \mathbf{b} - \mathbf{Ax}^{(m)} \perp \mathcal{W}_m.}$$

- The symbol $\perp$ denotes perpendicularity or orthogonality.

Projection Method

- Let $\mathbf{S}_m = [\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_m]$ and $\mathbf{W}_m = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_m]$ be matrices in $\mathbb{R}^{n \times m}$ having as their columns the basis vectors for the subspaces $\mathcal{S}_m$ and $\mathcal{W}_m$, respectively.
- If the approximate solution $\mathbf{x}^{(m)}$ is written as $\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{S}_m \mathbf{y}_m$ then the orthogonality condition is equivalent to enforcing that the residual vector $\mathbf{r}^{(m)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(m)}$ be orthogonal to each of the basis vectors of $\mathcal{W}_m$, that is,

$$\mathbf{W}_m^T \left(\mathbf{b} - \mathbf{A}\mathbf{x}^{(m)} \right) = \mathbf{0}\,.$$

Projection Method

- This leads to the following linear system for the vector $\mathbf{y}_m$:

$$\mathbf{W}_m^T \mathbf{A} \mathbf{S}_m \mathbf{y}_m = \mathbf{W}_m^T \mathbf{r}^{(0)} \qquad (2)$$

solve for y_m

and hence the approximate solution (provided $\mathbf{W}_m^T \mathbf{A} \mathbf{S}_m$ is nonsingular) is defined as

$y_m = (\beta_1, \beta_1, \ldots, \beta_m)^T$

$$\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{S}_m \boxed{\left(\mathbf{W}_m^T \mathbf{A} \mathbf{S}_m\right)^{-1} \mathbf{W}_m^T \mathbf{r}^{(0)}} \qquad (3)$$

- In this chapter, we consider some Krylov subspace methods for solving $\mathbf{A}\mathbf{x} = \mathbf{b}$, where the search space $\mathcal{S}_m$ is selected to be the Krylov subspace $\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$.

$\mathcal{S}_m = \text{span}\{\underline{s}_1, \underline{s}_2, \ldots, \underline{s}_m\} \subseteq \mathbb{R}^n$ Search space.

If $\underline{x}^{(m)} \in \underbrace{\underline{x}^{(0)} + \mathcal{S}_m}_{\text{Affine Space}} \iff \underline{x}^{(m)} = \underline{x}^{(0)} + \sum_{j=1}^{m} \beta_j \underline{s}_j$

QUESTION: how do we determine β_j's?

Let $S_m = \underbrace{[\underline{s}_1, \underline{s}_2, \ldots, \underline{s}_m]}_{\text{Matrix}} \in \mathbb{R}^{n \times m}$

$$\therefore \quad \underline{x}^{(m)} = \underline{x}^{(0)} + S_m \underline{y}^{(m)} \;;\quad \underline{y}^{(m)} = (\beta_1, \beta_2, \ldots, \beta_m)^T.$$

RESIDUAL:
$$\underline{r}^{(m)} = \underline{b} - A\underline{x}^{(m)}$$
$$= \underbrace{\underline{b} - A\underline{x}^{(0)}}_{\underline{r}^{(0)}} - A S_m \underline{y}^{(m)}.$$

$$\therefore \quad \underline{r}^{(m)} = \underline{r}^{(0)} - A S_m \underline{y}^{(m)}.$$

$$\mathcal{W}_m = \text{span}\{\underbrace{\underline{w}_1, \underline{w}_2, \ldots, \underline{w}_m}_{\text{basis vectors.}}\} \subseteq \mathbb{R}^n \quad \text{Constraint space.}$$

$$\boxed{\begin{array}{c}\text{Petrov-Galerkin Approach:} \\ \underline{r}^{(m)} \perp \mathcal{W}_m\end{array}}$$

$\therefore$ $\underline{r}^{(m)}$ must be orthogonal to basis vectors for $\mathcal{W}_m$

i.e.,

$$\left.\begin{array}{l} \underline{w}_1^T \underline{r}^{(m)} = 0 \\ \underline{w}_2^T \underline{r}^{(m)} = 0 \\ \vdots \\ \underline{w}_m^T \underline{r}^{(m)} = 0 \end{array}\right\}$$

$$W_m = [\underline{w}_1, \underline{w}_2, \ldots, \underline{w}_m] \in \mathbb{R}^{n \times m}$$

$$W_m^T \underline{r}^{(m)} = W_m^T(\underline{r}^{(0)} - AS_m \underline{y}^{(m)})$$
$$= \underline{0}$$

$$\therefore \boxed{\underbrace{W_m^T A S_m}_{m\times n\times n\times n\times n\times m} \underline{y}^{(m)} = W_m^T \underline{r}^{(0)}}$$

Note : This "projected system" is of size $\underline{m \times m}$. Much smaller than $\underline{n \times n}$

Ritz-Galerkin condition:

Orthogonal Projection

$$\mathcal{S}_k = \mathcal{K}_k(\mathbf{A}, \mathbf{b}); \mathcal{W}_k = \mathcal{K}_k(\mathbf{A}, \mathbf{b})$$

A unsymmetric - *FOM*

A symmetric - *Lanczos method*

A symmetric, positive-definite – *CG method*

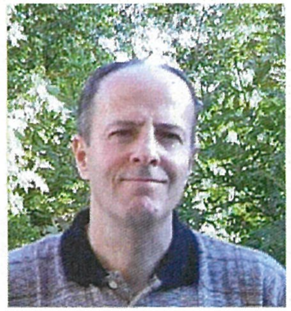
Petrov-Galerkin condition:

Oblique Projection

$$\mathcal{S}_k = \mathcal{K}_k(\mathbf{A}, \mathbf{b}); \mathcal{W}_k = \mathbf{A}\mathcal{K}_k(\mathbf{A}, \mathbf{b})$$

A unsymmetric – *GMRES (1986)*

A symmetric - *MINRES*



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