Krylov Subspace Methods

$Ax = b \quad , \; A \in \mathbb{C}^{n \times n}$

$\Rightarrow \quad x = A^{-1} b$

Gaussian elimination $\quad O(n^3)$

This is a DIRECT METHOD
to solve $Ax = b$

ITERATIVE ALGORITHMS solve for $x = A^{-1}b$
by repeated applications of fixed point
iterations

$$x_{k+1} = \Phi(x_k) \qquad k \geq 0$$

Norms

- vector norms: A vector norm $\|\cdot\|: \mathbb{K}^n \longrightarrow \mathbb{R}$ has ~~the~~ the following properties

$\forall\ x, y \in \mathbb{K}^n$, and $\alpha \in \mathbb{C}$

(1) $\|x\| \geq 0$, with $\|x\| = 0 \iff x = 0$

(2) $\|\alpha \cdot x\| = |\alpha| \cdot \|x\|$

(3) $\|x + y\| = \|x\| + \|y\|$

Vector norms

Euclidean norm $\|x\|_2$

where $(x, y) = y^{+} \cdot x = \sum_{i=1}^{n} y_i^{*} x_i$

Hölder norm (P norms)

$$\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{\frac{1}{p}}$$

$$\lim_{p \to \infty} \|x\|_p = \max_{i=1,\dots,n} |x_i|$$

Matrix Norms

A matrix norm

$$\|\cdot\| : \mathbb{C}^{n \times m} \longrightarrow \mathbb{R}$$

has properties

(1) $\|A\| \geq 0$, with $\|A\| = 0 \iff A = 0$

(2) $\|\alpha A\| = |\alpha| \cdot \|A\|$

(3) $\|A + B\| \leq \|A\| + \|B\|$

$\forall \; A, B \in \mathbb{C}^{n \times m}$, $\alpha \in \mathbb{C}$

Given 2-vector norms one defines an induced matrix norm

$$\|A\|_{pq} = \max_{x \in \mathbb{C}^n, x \neq 0} \frac{\|Ax\|_p}{\|x\|_q}$$

if $p = q$ $\|A\|_{pp} = \|A\|_p$

- Key property of matrix p-norm

(1) $\|A \cdot B\|_p \leq \|A\|_p \cdot \|B\|_p$

(2) $\|A^k\|_p \leq \|A\|_p^k$

Examples

$$\|A\|_1 = \max_{j=1,\dots,n} \{ |a_{1j}| + |a_{2j}| + \dots + |a_{nj}| \} = \max_j \{ \sum_i |a_{ij}| \}$$

$$\|A\|_\infty = \max_i \{ \sum_j |a_{ij}| \}$$

$$\|A\|_2 = \sqrt{\rho(A^+A)} = \sqrt{\rho(AA^+)}$$

Definition

The spectral radius $\rho(B)$ of $B \in \mathbb{C}^{n \times n}$ is given by

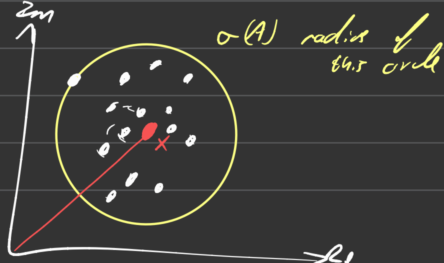
$$\rho(B) = \max\{ |\lambda| : \lambda \in \sigma(B) \}$$

where $\sigma(B)$ is the spectrum of B is the set of all eigen values

For some problem $Ax = b$

$0 \in \sigma(A)$

$\det(A - \lambda I) = 0$



~~Example~~

- $A = \begin{bmatrix} -3 & 5 & 7 \\ 2 & 6 & 4 \\ 0 & 2 & 8 \end{bmatrix}$

$\Rightarrow \|A\|_1 = 19$

$\Rightarrow \|A\|_\infty = 15$

$\Rightarrow \|A\|_2 \approx 13.347$

- $A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ has $\operatorname{rank}(A) = 1$

$\Rightarrow \|A\|_1 = \|A\|_\infty = 1$

$A^T A = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

$= \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$

$\Rightarrow \rho(A^T A) = 1$

Definition

The matrix condition number of a matrix is

$$\operatorname{cond}(A) = \|A\| \, \|A^{-1}\|$$

Clearly depends on the norm

eg $\|\cdot\|_2 \to \operatorname{cond}_2(\cdot)$

If A is singular : $\operatorname{cond}(A) = \infty$
$(\det(A) = 0)$

Definition

A is well posed problem $Ax = b$ fixed
The perturbed system $A(x+h) = b + d$
The condition number is the relative change in the solution. Divide by the relative change in the data

$$\frac{\|h\| / \|x\|}{\|d\| / \|b\|} = \frac{\|h\| \cdot \|b\|}{\|d\| \cdot \|x\|}$$

since $Ax = b$

$$\|b\| \leq \|A\| \cdot \|x\|$$

$$\leq \frac{\left(\|A^{-1}\| \|d\|\right)\left(\|A\| \cdot \|x\|\right)}{\|d\| \cdot \|x\|}$$

$$= \|A^{-1}\| \cdot \|A\| = \text{cond}(A)$$

Theorem Conditioning of linear systems

If $A(x + \Delta x) = b + \Delta b$

then
$$\frac{\|\Delta x\|}{\|x\|} \leq \text{cond}(A) \cdot \frac{\|\Delta b\|}{\|b\|}$$

If $(A + \Delta A)(x + \Delta x) = b$

then
$$\frac{\|\Delta x\|}{\|x\|} \leq \text{cond}(A) \frac{\|\Delta A\|}{\|A\|} \quad \text{for } \Delta A \to 0$$

Note For an induced matrix norm one has

$$1 = \|\mathbb{1}\| = \|A A^{-1}\| \leq \|A\| \|A^{-1}\| = \text{cond}(A) \leq \infty$$

So $1 \leq \text{cond}(A) < \infty$

for cond(A) large => ill posed problem!

Definition

Residual of linear system

For a problem $Ax = b$, the residual r at a solution estimate $\tilde{x}$ is

$$r = b - A \cdot \tilde{x}$$

Note

- $r = 0 \iff x - \tilde{x} = 0$

=> we have the solution

(within machine precision)

- $$\frac{\|x - \tilde{x}\|}{\|x\|} \leq \text{cond}(A) \cdot \frac{\|r\|}{\|b\|}$$

The gap between rel error and rel residual is the condition number

Example

$$A = \begin{bmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{bmatrix}$$

$$b = \begin{bmatrix} 0.8642 \\ 0.1440 \end{bmatrix}$$

$$A^{-1} = 10^8 \cdot \begin{bmatrix} 0.1441 & -0.8648 \\ -0.2161 & 1.2969 \end{bmatrix}$$

$$\text{Eigenvalues}(A) = \{1.441,\ 6.93 \cdot 10^{-8}\}$$

$$\text{Eigenvalues}(A^{-1}) = \{1.441 \cdot 10^8,\ 0.69\}$$

$$\text{Cond}_1(A) = 3.27 \cdot 10^8$$

$$\text{Cond}_2(A) = 2.49 \cdot 10^8$$

$$\text{Cond}_\infty(A) = 4.67 \cdot 10^8$$

Ill posed problem! $\tau = 10^{-8}$

$\Rightarrow$ have to choose $\tau \approx 10^{-12}$ for 3-4 sig digits

$\tau \approx 10^{-16}$

max and min eigenvalue

For some norm, $\operatorname{cond}(A) = \dfrac{\lambda_{max}(A)}{\lambda_{min}(A)}$

Iterative Methods

$$x_{k+1} = \Phi(x_k)$$

Definition

An iterative method is simply defined as

$$x_{k+1} = \Phi(x_k) \qquad k \geq 0$$

for a given linear system $Ax = b$ with exact solution x_* one defines the error as

$$e_k = x_k - x_*$$

the iterative method is linear if there exist a matrix C such that

$$e_{k+1} = C e_k$$

A basic iteration method splits A into

$$A = M - N$$

with matrix M being easily invertible
This leads to the recursive formula

$$M x_{n+1} = N x_n + b$$

$$x_{n+1} = x_n + M^{-1}(b - A x_n)$$

$$= M^{-1} b + (1 - M^{-1} A) x_n$$

What's C

Check

$$e_{n+1} = x_{n+1} - x_*$$

$$= M^{-1} b + (1 - M^{-1} A) x_n - x_*$$

$$= M^{-1}(b - A x_n) + \underbrace{(x_n - x_*)}_{= e_n}$$

$$= M^{-1} A \overbrace{(x_* - x_n)}^{= -e_n} + e_n$$

$$= (1 - M^{-1} A) e_n$$

$\Rightarrow \quad C = 1 - M^{-1}A = M^{-1}N$

$\Rightarrow \quad x_{k+1} = Cx_k + c$

where $C = 1 - M^{-1}A$, $c = M^{-1}b$

~~Recap~~

Iteration method

$x_{k+1} = \Phi(x_k)$ $\qquad Ax = b$

$x_{k+1} = Cx_k + c$ $\qquad A = M - N$

$C = 1 - M^{-1}A$

$c = M^{-1}b$

Note

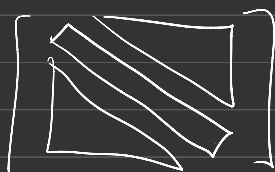
- We call an iteration method convergent if the iteration matrix C obeys

$$\lim_{k \to \infty} C^k = 0$$

That is the case iff $\rho(C) < 1$

- The splitting matrix M is chosen to reduce the condition number of the problem. Any method that improves the condition number significantly is referred to as <u>preconditioning</u> of the system.

<u>List of basic iterative methods</u>

$$A = D + L + U =$$ 

method	M
Jacobi	D
damped Jacobi	$\frac{1}{\omega} D$
Gauss Seidel	$D + L$
Richardson	$\frac{1}{\omega} \mathbb{1}$
Successive overrelaxation (SOR)	$\frac{1}{\omega} D + L$
symmetric SOR	$\frac{1}{\omega(2-\omega)}(D+\omega L)D^{-1}(D+\omega U)$

ω: relaxation parameter

Example

Jacobi

$Ax = b$, $\quad M = D \qquad C = I - D^{-1}A$

$$c = D^{-1}b$$

The convergence $x_k \to x_* \quad \forall x_0$

$$\iff \rho(C) < 1$$

is true for Jacobi iterate can be shown by considering powers of Jordan canonical form of C. This bound is sharp in the sense

$$\limsup_{k\to\infty} \|x_k - x_*\|^{1/k} \leq \rho(C) < 1$$

Unless a solution is known we cannot compute the error

$$e_k = x_k - x_*$$

For checking convergence we normally use the residual

$$r_k = b - Ax_k$$

$$= -A(x_k - x_*) = -A e_k$$

$$\tau_k = -A e_k$$

$$\underbrace{\Phi(x_k) - x_k}_{x_{k+1} - x_k} = C x_k + c - x_k = (C - I) x_k + c = -M^{-1}A x_k - M^{-1} b$$

$$= M^{-1}(-A x_k + b) = \underbrace{M^{-1} \tau_k}_{\text{transformed residual}}$$

Note my τ are actually supposed to be r

without loss of generality

$$x_{k+1} = x_k + r_k$$

$$= x_0 + \sum_{i=0}^{k} r_i$$

Left multiplication by $-A^{-1}$ and adding b

$$r_{k+1} = r_k - A r_k = (I - A) r_k$$

$$\Rightarrow r_k = (I - A)^k r_0 = p_k(A)\, r_0$$

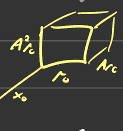
where $p_k(\xi) = (1 - \xi)^k$ is a polynomial of degree k

$\Rightarrow \quad r_n = p_n(A) r_0 \in \text{span}\{r_0, Ar_0, A^2 r_0, \dots, A^n r_0\}$

accordingly $\quad x_n = x_0 + q_{n-1}(A) r_0$

$\Rightarrow$ x_n lies in the affine space

$$x_0 + \underbrace{\text{span}\{r_0, Ar_0, \dots, A^{n-1} r_0\}}$$



obtained by shifting a subspace of r_{n-1}

Definition

The set of all linear combinations of a set of vectors $G = \{a_1, \dots, a_q\}$ of $\mathbb{C}^n$ is a vector subspace of $\mathbb{C}^n$, called the linear span of G

$$\text{span}\{G\} = \text{span}\{a_1, \dots, a_q\} = \{z \in \mathbb{C}^n \mid z = \sum_{i=1}^{q} \alpha_i a_i, \ \alpha_i \in \mathbb{C}\}$$

A matrix $A \in \mathbb{C}^{n \times m}$ is a linear map

$$T_A : \mathbb{C}^m \longrightarrow \mathbb{C}^n, \quad x \in \mathbb{C} \qquad T_A(x) = Ax \in \mathbb{C}^n$$

Definition

The range of $A \in \mathbb{C}^{m \times n}$ is denoted by $\text{range}(A) = \{Ax \mid x \in \mathbb{C}^n\}$ and is equal to the linear span of its columns

$$A = [a_1, \ldots, a_n]$$

The kernel of A is

$$\ker(A) = \{x \in \mathbb{C}^n \mid Ax = 0\}$$

The rank of A is

$$\text{rank}(A) = \dim(\text{range}(A))$$

Krylov Subspace

Definition

Given a non singular matrix $A \in \mathbb{C}^{n \times n}$ and $y \neq 0 \in \mathbb{C}^n$, the n^{th} Krylov subspace

$\mathcal{K}_n(A, y)$

generated by A from y is

$$\mathcal{K} = \mathcal{K}_n(A, y) = \text{span}\{y, Ay, \dots, A^{n-1}y\}$$

Comments

- $\mathcal{K}_1 \subseteq \mathcal{K}_2 \subseteq \mathcal{K}_3 \subseteq \dots$ and dimension increases at most by one
- The n^{th} approximate solution

  $x_n \in x + \mathcal{K}_n(A, r_0)$

- $\dim(\mathcal{K}_n(A, y)) \leq n$, i.e. Krylov subspace dim is at most n

Lemma

There is a positive integer

$$\nu = \nu(A, y)$$

called the grade of y wrt A such that

$$\dim(\mathcal{K}_n(A, y)) = \min(n, \nu)$$

$$\nu = \deg(p) \text{ st } p(A)y = 0$$

$\mathcal{K}_\nu(A, y)$ is the smallest A-invariant subspace containing y and $p \neq 0$ a polynomial of lowest degree

$$\Rightarrow \nu = \min\{ k \mid A^{-1} y \in \mathcal{K}_k(A, y) \}$$

Corollary

Let x_* be a solution of $Ax = b$ and let x_0 be an initial approximation of it and $r_0 = b - Ax$ the corresponding residual. Moreover, $\nu = \nu(A, r_0)$ then

$$x_* \in x_0 + \mathcal{K}_n(A, r_0)$$

$\rightarrow n$ or ν

Lemma

Let $Ax = b$ be well defined with regular $A \in \mathbb{C}^{n \times n}$ and $x_* = A^{-1}b$ the exact solution of ~~the~~ linear system. Then equivalence relation hold

(a) vectors $y, Ay, \dots, A^k y$ are lin independent

(b) $\mathcal{K}_k(A,y) = \mathcal{K}_{k+1}(A,y)$

(c) $A\mathcal{K}_k(A,y) \subseteq \mathcal{K}_k(A,y)$

$\iff \mathcal{K}_k(A,y)$ is A-inv subspace

(d) $x_* \in \mathcal{K}_k(A,y)$

Cayley-Hamilton Theorem

Every square matrix A over a commutative ring $(\mathbb{Z}, \mathbb{R}, \mathbb{C})$ satisfies its own characteristic equation

$$p_A(\lambda) = \det(\lambda \mathbb{I}_{n \times n} - A)$$

$$= \lambda^n + c_{n-1}\lambda^{n-1} + c_{n-2}\lambda^{n-2} + \dots + \lambda c_1 + c_0$$

$$\Rightarrow p_A(A) = 0$$

$$\stackrel{\mathbb{C}}{=} \prod_{k=1}^{n} (\lambda - \lambda_k) \quad , \quad \lambda_k \in \sigma(A)$$

- Since $p_A(A) = 0$

$$A^n = -(c_{n-1} A^{n-1} + c_{n-2} A^{n-2} + \dots + c_1 A + c_0 \mathbb{1})$$

- When ~~the~~ ring a is field $(\mathbb{R}, \mathbb{C})$ the CH-theorem states ~~the~~ minimal polynomial of a square matrix divides its characteristic polynomial

- $p_A(\lambda) = \prod_{n=1}^{n} (\lambda - \lambda_k)$ with $\{\lambda_k\} \Rightarrow c_k = c_k(\{\lambda_k\})$

- $$p_A(A) = A^n + c_{n-1} A^{n-1} + \dots + c_1 A + \underbrace{(-1)^n \det(A)}_{= c_0} \mathbb{1}$$

$$= 0$$

$$\Rightarrow A^{-1} = \frac{(-1)^{n-1}}{\det(A)} (A^{n-1} + c_{n-1} A^{n-2} + \dots + c_n \mathbb{1} \equiv g_{n-1}(A)$$

A (standard) Krylov subspace method for solving a lin system $Ax = b$ called a KRYLOV SUBSPACE SOLVER, is an iterative method starting from some initial approximation x_0 and corresponding residual $r_0 = b - Ax_0$. It iterates x_n st

$$x_n - x_0 = q_{n-1}(A) r_0 \in \mathcal{K}_n(A, r_0)$$

with polynomial q_{n-1} of degree $n-1$ until it possibly finds the exact solution. For some n, x_n may not exist or q_{n-1} may have lower degree

Lemma

The residuals of Krylov subspace solver satisfy

$$r_n = p_n(A) r_0 \in r_0 + A\mathcal{K}_n(A, r_0) \subseteq \mathcal{K}_{n+1}(A, r_0)$$

for some polynomial p_n of degree n. p_n is related to q_{n-1}. In particular $p_n(0) = 1$

$$p_n(\xi) = 1 - \xi q_{n-1}(\xi)$$

The following iterative methods are based on projecting an n dimensional problem onto a lower dimensional Krylov subspace. So specifically important algorithms are the following

Problem	$A \neq A^T$	$A = A^T$
$Ax = b$	GMRES, CGN BCG	CG
$(A - \lambda \mathbb{1})x = 0$ $\Leftrightarrow Ax = \lambda x$	Arnoldi	Lanczos

For hermitian matrices A, the reduced matrices are tridiagonal, whereas for non-hermitian A, they have Hessenberg form

How to solve linear systems using Krylov subspaces?

Method of Minimal Residuals

Let $\|\cdot\|$ be the euclidean norm in $\mathbb{R}^n$ and $B \in \mathbb{R}^{n\times n}$ a regular matrix. This induces the following vector and matrix norms

$$\|x\|_B = \|Bx\| \qquad x \in \mathbb{R}^n$$

$$\|A\|_B = \|BAB^{-1}\| \qquad A \in \mathbb{R}^{n\times n}$$

Solving a linear system becomes equivalent to minimizing the residuals

$$\min \tfrac{1}{2}\|b - Ax\|_B^2 \qquad x \in \mathbb{R}^n$$

For an initial vector $x_0 \in \mathbb{R}^n$ the starting residual $r_0 = Ax_0 - b$ defines the Krylov subspace

$$\mathcal{K}_k(A, r_0) = \operatorname{span}\{r_0, Ar_0, \dots, A^k r_0\}$$

replacing the n-dim problem to a k-dim in step k

$$\min \|b - Ax\|_B^2 \qquad x \in x_0 + \mathcal{K}_k(A, r_0)$$

Algorithm (Residual method)

- choose $x_0 \in \mathbb{R}^n$, $B \in \mathbb{R}^{n \times n}$ $\Rightarrow$ $r_0 = Ax_0 - b$

- for $k = 1, 2, \dots$

  determine $x_k \in \mathbb{R}^n$ as solution of
  $\min \|Ax - b\|^2$ for $x \in x_0 + \mathcal{K}_k(A, r_0)$

END

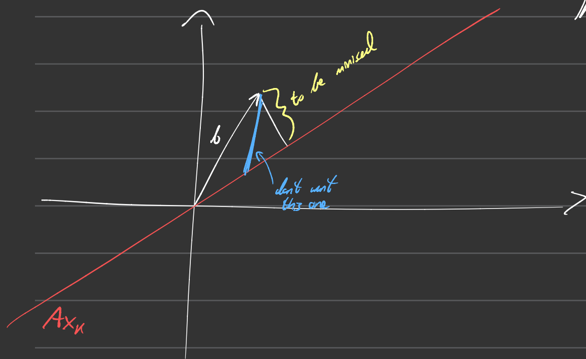
Note

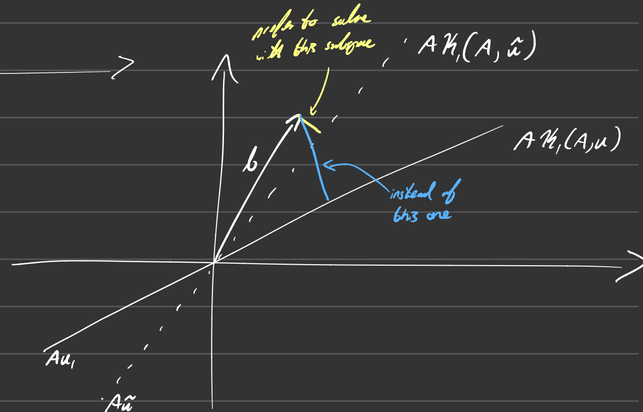
- After at most n steps we have $\mathcal{K}_n = \mathcal{K}_{n+1}$ in $\mathbb{R}^n$

- There are various algorithmic choices to implement minimization based on different factorization strategies

	$A = QR$	$A = QHQ^T$
orthogonal structuring	Householder	Householder
standard orthogonalization	Gram-Schmidt	Arnoldi

$\mathbb{R}^n$





$$x_* = A^{-1}b = q_{n-1}(A)b$$

$$x_k = p_{k-1}(A)\,b$$

Algorithm Arnoldi Iterations

- given some b, compute $q_1 = \frac{b}{\|b\|}$ $\qquad \|\cdot\| = \|\cdot\|_2$

For $n = 1, 2, 3, \ldots$

$\quad v = Aq_n$

$\quad$ For $j = 1, \ldots, n$

$\qquad h_{jn} = q_j^* v$

$\qquad v = v - h_{jn} q_j$

$\quad$ END

$\quad h_{n+1,n} = \|v\|$

$\quad q_{n+1} = \frac{v}{h_{n+1,n}}$

$A \in \mathbb{C}^{N \times N}$

END

Goal

reduce A to Hessenberg form through orthogonal similarity transformations like

$$A = QHQ^{+} \quad \text{or} \quad AQ = QH \qquad (Q = Q^{+})$$

To reduce the problem size we consider the first n columns of $AQ = QH$. Let $Q_n \in \mathbb{C}^{N\times n}$ be

$$Q_n = [q_1 / q_2 / \dots / q_n] \qquad \text{"partial reduction"}$$

column vector n

Arnoldi yields

$$AQ_n = Q_n H_n + q_{n+1} h_{n+1,n} \xi_n^T \equiv Q_{n+1} \tilde{H}_n$$

with $n\times n$ Hessenberg matrix

$$H_n = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \ddots & \vdots \\ & h_{32} & \ddots & \vdots \\ 0 & & \ddots & \\ & & h_{n,n-1} & h_{nn} \end{bmatrix}$$

$$\xi_n^T = (0, \dots, 0, 1)$$

$$\Rightarrow \tilde{H}_n = \begin{bmatrix} H_n \\ h_{n+1,n} \xi^T \end{bmatrix} \quad \Rightarrow \tilde{H}_n = \begin{bmatrix} H_n \\ \hline 0 \;\dots\; 0 \; h_{n+1,n} \end{bmatrix}$$

$\Rightarrow \; AQ_n = Q_{n+1} \tilde{H}_n$

or $[A][q_1 | \dots | q_n]$

$$= [q_1 | \dots | q_{n+1}] \begin{bmatrix} H_n \\ h_{n+1,1} \xi^T \end{bmatrix}$$

$\Rightarrow$ n th column

$$A q_{n+1} = h_{1n} q_1 + \dots h_{nn} q_n + h_{n+1,n} q_{n+1}$$

$$\Rightarrow \boxed{q_{n+1} = (A q_n - h_{1n} q_n - h_{2n} q_2 - \dots - h_{nn} q_n) / h_{n+1,n}}$$

satisfies a $(n+1)$ recurrence relation

$\Rightarrow$ inner loop

Apply Arnoldi to GMRES

- original problem: find $x_* \in \mathbb{R}^n$ st $Ax_* = b$
- minimising problem: find $x \in V$ with $\dim(V) = k \ll n$
  st $\|Ax - b\|^2$ is minimised

: find $y \in \mathbb{R}^k$ st $\|AQ_k y - b\|^2$ is minimised

$\Rightarrow x_k = Q_k y$ is best estimate of x_*

$\|AQ_k y - b\| = \|Q_{k+1} \hat{H}_k y - b\|$

since Q_n has orthogonal columns

$\Rightarrow Q_k^\dagger Q_k = P_k$ orthogonal projection

from $\mathbb{R}^n$ into column space of Q_k

$= \|Q_{k+1}^\dagger (Q_{k+1} \hat{H}_k y - b)\|$

$= \|Q_{k+1}^\dagger Q_{k+1} \hat{H}_k y - Q_{k+1}^\dagger b\|$

$= \|\hat{H}_k y - Q_{k+1}^\dagger b\|$

with $Q_{k+1}^\dagger q_1 = e_1 = (1, 0, .. 0)^T$

and $b = \|b\| \cdot q_1 = \beta \cdot q_1$

$= \|\hat{H}_k y - \beta \cdot e_1\|$

Minimizing Problem

Find $y \in \mathbb{R}^n$ st $\|\tilde{H}_n y - \beta e_1\|$ is minimum

Book

SAAD GMRES pg 158

Alg 6.9 Alg 6.10