2 Additional notes for GMRES

2.1 Derivation of GMRES

The GMRES method is a method for linear systems of equations $Ax = b$. It is based on the idea that if the residual

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

is small, $\tilde{x}$ is probably a good approximation to x. We try to minimize the norm of the residual, over an appropriate space. It turns out that if we minimize over a Krylov subspace, the minimizer can be elegantly and efficiently computed from the Arnoldi method, and convergence theory shows us that it can under certain conditions indeed provide good approximations. We define the approximation x_n generated after n steps of GMRES as minimizers of the residual norm (with respect to the 2-norm) over the Krylov subspace associated with A and the right-hand side of b:

$$\min_{x \in \mathcal{K}_n(A,b)} \|Ax - b\|_2 = \|Ax_n - b\|_2.$$

The minimization problem can be explicitly solved in terms of the Arnoldi factorization

$$AQ_n = Q_{n+1}\underline{H}_n. \tag{2.1}$$

where Q_n and $\underline{H}_n$ are generated by the Arnoldi method.

Lemma 2.1.1 (Minimization definition of GMRES iterates)**.** *Suppose Q_n and $\underline{H}_n$ satisfy the Arnoldi relation and $q_1 = b/\|b\|$. Then,*

$$\min_{x \in \mathcal{K}_n(A,b)} \|Ax - b\|_2 = \min_{z \in \mathbb{C}^n} \|\underline{H}_n z - \|b\| e_1\|_2. \tag{2.2}$$

Proof. During the proof we need the following property of orthogonal matrices. If $Q \in \mathbb{R}^{m \times k}$ with $m \geq k$ is an orthogonal matrix, then,

$$\|Qz\|_2^2 = z^T Q^T Qz = z^T z = \|z\|_2^2. \tag{2.3}$$

Since $\mathcal{K}_n(A,b) = \text{span}(q_1,\dots,q_n)$ we can reparameterize the set over which we minimize. The conclusion of the theorem follows from (2.1) and (2.3):

$$\begin{aligned}
\min_{x\in\mathcal{K}_n(A,b)} \|Ax-b\|_2 &= \min_{z\in\mathbb{C}^n} \|AQ_n z - b\|_2 \\
&= \min_{z\in\mathbb{C}^n} \|AQ_n z - \|b\|q_1\|_2 \\
&= \min_{z\in\mathbb{C}^n} \|Q_{n+1}\underline{H}_n z - \|b\|Q_{n+1}e_1\|_2 \\
&= \min_{z\in\mathbb{C}^n} \|Q_{n+1}(\underline{H}_n z - \|b\|e_1)\|_2 \\
&= \min_{z\in\mathbb{C}^n} \|\underline{H}_n z - \|b\|e_1\|_2
\end{aligned}$$

We start iteration with $q_1 = b/\|b\|$

Use the Arnoldi relation (2.1) and that $q_1 = Q_{n+1}e_1$.

Use (2.3) with $Q = Q_{n+1}$.

□

The approximations x_n are computed by solving the linear least-squares problem in the right-hand side of (2.2) and setting $x_n = Q_n z$.

2.2 *Convergence theory*

Due to the definition of GMRES-approximations as solution to the left-hand side of (2.2) we have a nice property that the solution can in a certain sense not become worse by further iteration. The sequence of Krylov subspaces correspond to an expanding set $\mathcal{K}_n(A,b) \subseteq \mathcal{K}_{n+1}(A,b)$, for any n. Therefore, the norm of the residual is not increasing:

$$\|r_{n+1}\| = \min_{x\in\mathcal{K}_{n+1}(A,b)} \|Ax-b\| \le \min_{x\in\mathcal{K}_n(A,b)} \|Ax-b\| = \|r_n\|.$$

Further analysis of convergence is simplified by the use polymomial sets.

Definition 2.2.1 (Polynomials and 0-normalized polynomials)**.**

$$P_n := \{\textit{polynomials of degree at most } n\} \quad (2.4a)$$
$$P_n^0 := \{p \in P_n : p(0) = 1\} \quad (2.4b)$$

Lemma 2.2.2 (Krylov subspace equivalence)**.** *Suppose $A \in \mathbb{C}^{m\times m}$ is invertible. Let $x \in \mathbb{C}^n$. The following statements are equivalent*

(i) $x \in \mathcal{K}_n(A,b)$

(ii) There exists $p \in P_n^0$ such that

$$b - Ax = p(A)b. \quad (2.5)$$

Proof. (i)⇒(ii): Suppose $x \in \mathcal{K}_n(A,b) = \text{span}(b, Ab, \dots, A^{n-1}b)$. From the definition of the Krylov subspace we have

$$x = \alpha_0 b + \cdots + \alpha_{k-1}A^{k-1}b = q(A)b$$

where $q(z) = q_0 + \cdots + q_n z^{n-1}$ and $q \in P_{n-1}$. In order to show (2.5), we note that

$$b - Ax = b - Aq(A)b = p(A)b,$$

if we define $p(z) = 1 - zq(z)$. The polynomial p is normalized since $p(0) = 1$ and we have shown (ii).

(ii)⇒(i): Suppose (2.5) is satisfied. Any normalized polynomial $p \in P_n^0$ of degree k satisfies

$$p(z) = 1 + zq(z)$$

for some polynomial $q \in P_{k-1}$. Hence, (2.5) implies that

$$b - Ax = p(A)b = (I + Aq(A))b$$

and $-Ax = Aq(A)b$. Since A is invertible by assumption

$$x = -q(A)b$$

and $x \in \mathcal{K}_n(A, b)$. □

Theorem 2.2.3 (Main convergence theorem of GMRES)**.** *Suppose $A \in \mathbb{C}^{m\times m}$ is an invertible and diagonalizable matrix. Let $A = V\Lambda V^{-1}$ be the Jordan decomposition of A, where Λ is a diagonal matrix. Let x_n, $n = 1, \ldots$ be iterates generated by GMRES. Then,*

$$\frac{\|Ax_n - b\|}{\|b\|} \le \|V\|\|V^{-1}\| \min_{p\in P_n^0} \max_{i=1,\ldots,m} |p(\lambda_i)|.$$

Proof.

$$\begin{aligned}
\|r_n\| &= \min_{x\in\mathcal{K}_n(A,b)} \|b - Ax\| \\
&= \min_{p\in P_n^0} \|p(A)b\| \\
&= \min_{p\in P_n^0} \|p(V\Lambda V^{-1})b\| \\
&= \min_{p\in P_n^0} \|Vp(\Lambda)V^{-1}b\| \\
&\le \min_{p\in P_n^0} \|V\|\|V^{-1}\|\|p(\Lambda)\|\|b\|.
\end{aligned}$$

Use Lemma 2.2.2

Use Jordan decomposition

Use that for any polynomial $p(VBV^{-1}) = Vp(B)V^{-1}$.

Norm bounds

Since Λ is a diagonal matrix we

$$p\left(\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}\right) = \begin{pmatrix} p(\lambda_1) & & \\ & \ddots & \\ & & p(\lambda_m) \end{pmatrix}. \tag{2.6}$$

Moreover, the two-norm of a diagonal matrix can be expressed explicitly. Since

$$\left\|\begin{pmatrix} \gamma_1 & & \\ & \ddots & \\ & & \gamma_n \end{pmatrix}\right\|_2^2 = \lambda_{\max}\left(\begin{pmatrix} \gamma_1 & & \\ & \ddots & \\ & & \gamma_n \end{pmatrix}\begin{pmatrix} \gamma_1 & & \\ & \ddots & \\ & & \gamma_n \end{pmatrix}^T\right) = \left(\max_{i=1,\ldots,m} |\gamma_i|\right)^2. \tag{2.7}$$

If we combine (2.6) and (2.7) we have

$$\|r_n\| \leq \min_{p \in P_n^0} \max_{i=1,\ldots,m} \|V\|\|V^{-1}\||p(\lambda_i)|\|b\|,$$

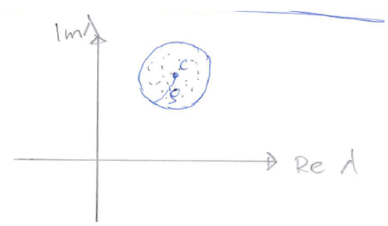
which concludes the proof. □

Corollary 2.2.4. *Suppose $A \in \mathbb{C}^{n\times n}$ satisfies the same conditions as in Theorem 2.2.3. Moreover, suppose all eigenvalues are contained in a disk of radius ρ centered at $c \in \mathbb{C}$,*

$$\lambda_i \in \bar{D}(c,\rho), \text{ for } i = 1,\ldots,n.$$

Then,

$$\frac{\|Ax_n - b\|}{\|b\|} \leq \|V\|\|V^{-1}\|\left(\frac{\rho}{|c|}\right)^n.$$



Proof. The result follows from Theorem 2.2.3 by considering the polynomial $q(z) := (c-z)^n/c^n$ since $q \in P_n^0$ and

$$\min_{p\in P_n^0}\max_{i=1,\ldots,m}|p(\lambda_i)| \leq \max_{i=1,\ldots,m}|q(\lambda_i)| = \max_{i=1,\ldots,m}\frac{|c-\lambda_i|^n}{|c|^n} \leq \frac{\rho^n}{|c|^n}.$$

□

