1 March 30th, 2021

1.1 Advanced Iterative Methods II

In this chapter, we consider:

$$Ax = b$$

where $A \in \mathbb{R}^{n\times n}$ is non-singular (no SPD constraint on A).

1.2 GMRES (Generalized Minimum Residual Method)

Recall that in the projection methods, we find:

$$\tilde{x} \in x_0 + K \text{ s.t. } b - A\tilde{x} \perp L$$

where K and L are two subspaces of $\mathbb{R}^n$ with the same dimension (in order to have $\tilde{x}$ be well-defined).

When A is SPD, we can choose $K = L$, so that:

$$\tilde{x} = \underset{x\in x_0+K}{\arg\min} \|x - x_*\|_A^2$$

However, when A is just a general non-singular matrix, we cannot follow this framework, as $\|A\|_A^2 = x^T Ax$ is not a norm on $\mathbb{R}^n$. Thus, we will not choose $K = L$. Instead, we choose $L = AK$. Doing so, the projection method becomes:

$$\begin{cases} \tilde{x} \in x_0 + K \\ b - A\tilde{x} \perp AK \end{cases} \iff \tilde{x} = \underset{x\in x_0+K}{\arg\min} \|b - Ax\|_2^2$$

Proof. Let $Ax = y$. We have:

$$\begin{aligned} \tilde{x} &= \underset{x\in x_0+K}{\arg\min} \|b - Ax\|_2^2 \\ \iff A\tilde{x} &= \underset{y\in Ax_0+AK}{\arg\min} \|b - y\|_2^2 \\ \iff &\begin{cases} b - A\tilde{x} \perp AK \\ \tilde{x} = x_0 + K \end{cases} \end{aligned}$$

□

In GMRES, given x_0, we generate x_k by projection with:

$$K = K_k = \text{span}\{r_0, Ar_0, A^2 r_0, \dots, A^{k-1} r_0\}$$

So:

$$x_k = \underset{x\in x_0+K_k}{\arg\min} \|b - Ax\|_2^2$$

Let V_k be a basis of K_k. Then $W_k = AV_k$ is a basis of AK_k. Then the minimization becomes:

$$\begin{aligned} \min_{x\in x_0+K_k} \|b - Ax\|_2^2 &\iff \min_{y\in\mathbb{R}^k} \|b - A(x_0 + V_k y)\|_2^2 \\ &\iff \min_{y\in\mathbb{R}^k} \|r_0 - AV_k y\|_2^2. \end{aligned}$$

Remark 1.1 — If $\dim(K_k) \neq k$ then the residue is 0, meaning we have already obtained the solution.

This is a typical least squares problem whose solution is given by:

$$V_k^T A^T A V_k y = V_k^T A^T r_0$$

Proof.

$$\begin{aligned}
\min_{y \in \mathbb{R}^k} \|r_0 - AV_k y\|_2^2 &\iff \begin{cases} \min_z \|r_0 - z\|_2^2 \\ \text{s.t. } z \in \operatorname{Ran}(AV_k) \end{cases} \\
&\iff r_0 - AV_k y \perp \operatorname{Ran}(AV_k) \\
&\iff \langle r_0 - AV_k y, AV_k u \rangle = 0 \quad \forall u \in \mathbb{R}^k \\
&\iff V_k^T A^T (r_0 - AV_k y) = 0.
\end{aligned}$$

□

However, we have two concerns if we solve $V_k^T A^T A V_k y = V_k^T A^T r_0$ directly to obtain $x_k = x_0 + V_k y$:

1. The condition number of $V_k^T A^T A V_k$ is the square of the condition number of AV_k. Thus, we lose some numerical stability.

   Remark 1.2 — Originally, we just need to solve the overdetermined linear system in $\min_{y \in \mathbb{R}^k} \|r_0 - AV_k y\|_2^2$. But if we want to solve $V_k^T A^T A V_k y = V_k^T A^T r_0$, then we are turning it into a square linear system.

2. The computation is not recursive, as we don't use x_{k-1} to obtain x_k. Therefore the computation per iteration is expensive (cost per step is $O(k^3)$ to solve).

As such, we need to consider how to solve a general least squares problem.

1.3 QR Decomposition

Let $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ satisfying $\operatorname{rank}(A) = n$, i.e. it is a tall, full rank matrix. Then we have the following decomposition $A = QR$:

Economic QR: where

$$\begin{aligned}
&Q \in \mathbb{R}^{m \times n} \text{ satisfying } Q^T Q = I \\
&R \in \mathbb{R}^{n \times n} \text{is upper triangular with non-zero diagonals.}
\end{aligned}$$

Full QR: where

$$\begin{aligned}
&Q \in \mathbb{R}^{m \times m} \text{ satisfying } Q^T Q = I \\
&R \in \mathbb{R}^{m \times n} \text{is upper triangular with non-zero diagonals.}
\end{aligned}$$

Remark 1.3 — Q in the economic QR is the first n columns of Q in the full QR. Similarly, R in the economic QR is the first n rows of R in the full QR.