Lecture Note #7 **MTH652: Advanced Numerical Analysis**
Winter 2025 Instructor: Will Pazner

Krylov Methods for Non-SPD Linear Systems

We considered previously the finite element discretization of PDEs that lead to non-symmetric variational problems of the form: find $u \in V$ such that, for all $v \in V$,

$$a(u, v) = F(v),$$

where $a(\cdot, \cdot)$ is a **non-symmetric** bilinear form, and F is a bounded linear functional. After discretization and choice of basis for the finite-dimensional space V_h, we obtain the linear system

$$A\boldsymbol{x} = \boldsymbol{b}.$$

Since $a(\cdot, \cdot)$ is not symmetric, the $N \times N$ matrix A will also not be symmetric. This means that we cannot use methods like the conjugate gradient method, which only applied to matrices that are symmetric and positive definite. It is one example of a family of iterative methods for linear systems called **Krylov methods**. The following table summarizes the most commonly used Krylov methods

A **is...**	**Krylov Method**
Symmetric and positive-definite	Conjugate Gradient (CG)
Symmetric but indefinite	Minimum Residual (MINRES)
Non-symmetric (general)	Generalized Minimum Residual (GMRES)

1 What is a Krylov method?

We have already learned how the conjugate gradient method works, and claim that it is an example of a "Krylov method", but we have not yet defined what a Krylov method is. Krylov methods are iterative methods that are based on the idea of looking for solutions in **Krylov subspaces**. Given an $N \times N$ matrix A and a vector $\boldsymbol{u} \in \mathbb{R}^N$, the mth associated **Krylov matrix** $K_m(A, \boldsymbol{u})$ (abbreviated K_m when A and $\boldsymbol{u}$ are clear) is the $N \times m$ matrix

$$K_m(A, \boldsymbol{u}) := \begin{pmatrix} \boldsymbol{u} & A\boldsymbol{u} & A^2\boldsymbol{u} & \cdots & A^{m-1}\boldsymbol{u} \end{pmatrix}.$$

The mth associated **Krylov subspace** $\mathcal{K}_m(A, \boldsymbol{u})$ is the *column space* of K_m, that is, the subspace of $\mathbb{R}^n$ spanned by the columns of K_m,

$$\mathcal{K}_m(A, \boldsymbol{u}) := \text{span}\left\{\boldsymbol{u}, A\boldsymbol{u}, A^2\boldsymbol{u}, \cdots, A^{m-1}\boldsymbol{u}\right\}.$$

The dimension of $\mathcal{K}_m$ (the rank of K_m) is *at most* m. Note that the Krylov subspaces are nested ($\mathcal{K}_m \subseteq \mathcal{K}_{m+1}$).

How does this relate to the conjugate gradient method? Recall that the CG method proceeds by performing line-search in A-orthogonal search directions, minimizing the error in the A-norm at each step. Given an initial guess $\boldsymbol{x}^{(0)}$, the first search direction $\boldsymbol{d}^{(0)}$ is the residual $\boldsymbol{r}^{(0)} = \boldsymbol{b} - A\boldsymbol{x}^{(0)}$. Note that we clearly have $\boldsymbol{d}^{(0)}, \boldsymbol{r}^{(0)} \in \mathcal{K}_1(A, \boldsymbol{r}^{(0)})$.

The line search results in $\boldsymbol{x}^{(1)} = \boldsymbol{x}^{(0)} + \alpha \boldsymbol{d}^{(0)}$. The new residual is

$$\begin{aligned}
\boldsymbol{r}^{(1)} &= \boldsymbol{b} - A\boldsymbol{x}^{(1)} \\
&= \boldsymbol{b} - A(\boldsymbol{x}^0 + \alpha \boldsymbol{d}^0) \\
&= \boldsymbol{b} - A(\boldsymbol{x}^0 + \alpha \boldsymbol{r}^0) \\
&= \boldsymbol{r}^{(0)} - \alpha A \boldsymbol{r}^0,
\end{aligned}$$

From this, we see that $\boldsymbol{r}^{(1)} \in \operatorname{span}\{\boldsymbol{r}^{(0)}, A\boldsymbol{r}^{(0)}\} = \mathcal{K}_2(A, \boldsymbol{r}^{(0)})$. Since $\boldsymbol{d}^{(1)}$ is obtained from $\boldsymbol{r}^{(1)}$ through a Gram–Schmidt process, we also have $\boldsymbol{d}^{(1)} \in \mathcal{K}_2(A, \boldsymbol{r}^{(0)})$. Repeating this argument (i.e. arguing by induction), we see that

$$\boldsymbol{d}^{(i)}, \boldsymbol{r}^{(i)} \in \mathcal{K}_{i+1}(A, \boldsymbol{r}^{(0)}).$$

Since $\boldsymbol{x}^{(i)}$ is obtained by minimizing the error in the A-norm, we have that

$$\|\boldsymbol{x} - \boldsymbol{x}^{(i)}\|_A = \inf_{\boldsymbol{y} \in \mathcal{K}_i(A, \boldsymbol{r}^{(0)})} \|\boldsymbol{x} - (\boldsymbol{x}^{(0)} + \boldsymbol{y})\|_A.$$

Note that if the initial guess is zero, then this takes the simpler form

$$\|\boldsymbol{x} - \boldsymbol{x}^{(i)}\|_A = \inf_{\boldsymbol{y} \in \mathcal{K}_i(A, \boldsymbol{b})} \|\boldsymbol{x} - \boldsymbol{y}\|_A,$$

which means that $\boldsymbol{x}^{(i)}$ is the *best approximation* to the true solution $\boldsymbol{x}$ (measured in the A-norm) taken from the subspace $\mathcal{K}_i(A, \boldsymbol{b})$.

The other Krylov methods (MINRES and GMRES) also look for solutions from the Krylov subspaces, but since in the more general cases the matrix A does not induce a norm, then the procedure is slightly different.

2 Krylov subspaces

Suppose we want to approximate the solution to

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

in the subspace $\mathcal{K}_m(A, \boldsymbol{b})$. One idea is simply to do least squares, i.e. find $\boldsymbol{x}_m \in \mathcal{K}_m$ that minimizes

$$\|\boldsymbol{b} - A\boldsymbol{x}_m\|.$$

This is equivalent to finding $\boldsymbol{y}_m \in \mathbb{R}^m$ such that $\boldsymbol{x}_m = K_m \boldsymbol{y}_m$, i.e. minimizing

$$\|\boldsymbol{b} - AK_m \boldsymbol{y}_m\|.$$

This is solving a least-squares problem with the matrix AK_m. We can see that as m increases, the residual starts to stagnate (see Jupyter notebook). This is because the columns of K_m become close to parallel. To understand why that happens, we will briefly explain the **power method**.

2.1 Power Method

Suppose A is a diagonalizable matrix whose largest (in magnitude) eigenvalue is simple (not repeated), i.e.

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_N|.$$

The eigenvalue λ_1 is called the **dominant eigenvalue**. The associated eigenvectors are $\boldsymbol{v}_i$, satisfying $A\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$, or

$$AV = V\Lambda,$$

where $V = \begin{pmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \cdots & \boldsymbol{v}_N \end{pmatrix}$ and Λ is diagonal with $\Lambda_{ii} = \lambda_i$. The eigenvector $\boldsymbol{v}_1$ is called the **dominant eigenvector**. Let $\boldsymbol{x} \in \mathbb{R}^N$ be arbitrary. Set

$$\boldsymbol{z} = V^{-1}\boldsymbol{x}.$$

(In other words, since the eigenvectors span $\mathbb{R}^N$, the entries of $\boldsymbol{z}$ are the coefficients of $\boldsymbol{x}$ expanded in the basis of eigenvectors).

Then,

$$A^k\boldsymbol{x} = A^k V\boldsymbol{z} = V\Lambda^k\boldsymbol{z} = V\begin{pmatrix} \lambda_1^k z_1 \\ \lambda_2^k z_2 \\ \vdots \\ \lambda_N^k z_N \end{pmatrix}$$

Notice that

$$\begin{cases} \lambda_i^k/\lambda_1^k = 1, & i = 1 \\ \lambda_i^k/\lambda_1^k \to 0, & i \neq 1 \end{cases}$$

and so $A^k\boldsymbol{x}/\lambda_1^k \to \boldsymbol{v}_1$ as $k \to \infty$ (unless $z_1 = 0$). This means that repeated application of A makes vectors close to parallel to the dominant eigenvector. This iteration gives a method for approximating the dominant eigenvalue and eigenvector of a matrix, by repeated application of the matrix A (followed by normalization of the vector).

2.2 Arnolidi Iteration

As a consequence of the above reasoning, the columns of the Krylov matrix K_m become closer to the dominant eigenvector, and so they each become very close to parallel to each other. If a matrix has two parallel columns then it is singular, so for large m, K_m becomes "almost singular". This is the cause of the stagnation in the residual (it is purely numerical; if we were computing in exact arithmetic, it wouldn't stagnate).

We would like to find a basis for the space $\mathcal{K}_m$ that is *better conditioned* than the columns of K_m, i.e. a basis whose vectors are not almost parallel. The best we could hope to do is find a basis that is **orthogonal**. This can be achieved using the *QR factorization* (essentially Gram–Schmidt applied to the columns of K_m), giving

$$K_m = Q_m R_m,$$

where R_m is upper triangular and

$$Q_m^T Q_m = I.$$

The matrix Q_m can be written

$$Q_m = \begin{pmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_m \end{pmatrix},$$

and $\{\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_m\}$ forms an orthonormal basis for $\mathcal{K}_m$. We would like to build this basis step-by-step. In other words, given $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m$, find $\boldsymbol{q}_{m+1}$ that is orthonormal to the previous vectors and such that $\text{span}\{\boldsymbol{q}_1, \ldots, \boldsymbol{q}_{m+1}\} = \mathcal{K}_{m+1}$. Notice that

$$A\boldsymbol{q}_m \in \mathcal{K}_{m+1},$$

and so $A\boldsymbol{q}_m$ is in $\text{span}\{\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_m, \boldsymbol{q}_{m+1}\}$, i.e.

$$A\boldsymbol{q}_m = H_{1m}\boldsymbol{q}_1 + H_{2m}\boldsymbol{q}_2 + \cdots + H_{mm}\boldsymbol{q}_m + H_{m+1,m}\boldsymbol{q}_{m+1} \tag{1}$$

for some coefficients H_{ij}. Rearranging,

$$H_{m+1,m}\boldsymbol{q}_{m+1} = A\boldsymbol{q}_m - H_{1m}\boldsymbol{q}_1 - H_{2m}\boldsymbol{q}_2 - \cdots - H_{mm}\boldsymbol{q}_m.$$

Since the basis is orthonormal, we have

$$\boldsymbol{q}_i^T A\boldsymbol{q}_m = H_{im},$$

so all the terms on the right-hand side can be computed easily, so we can solve for the product $H_{m+1,m}\boldsymbol{q}_{m+1}$. Since the basis must be orthonormal, we can find $\boldsymbol{q}_{m+1}$ by normalizing.

The following algorithm computes an **orthonormal basis** for the Krylov subspace $\mathcal{K}_m(A, \boldsymbol{u})$.

Algorithm 1 Arnoldi Iteration

$\boldsymbol{q}_1 \leftarrow \boldsymbol{u}/\|\boldsymbol{u}\|$
for $k = 1, 2, \ldots, m-1$ **do**
    $\boldsymbol{z} \leftarrow A\boldsymbol{q}_k$
    $H_{ik} \leftarrow \boldsymbol{q}_i^T \boldsymbol{z}$ for $i = 1, \ldots, k$
    $\boldsymbol{z} \leftarrow \boldsymbol{z} - H_{1k}\boldsymbol{q}_1 - \cdots - H_{kk}\boldsymbol{q}_k$
    $H_{k+1,k} \leftarrow \|\boldsymbol{z}\|$
    $\boldsymbol{q}_{k+1} \leftarrow \boldsymbol{z}/H_{k+1,k}$
end for

Let Q_m be the matrix whose columns are the orthogonal basis for $\mathcal{K}_m$. Notice that

$$AQ_m = \begin{pmatrix} A\boldsymbol{q}_1 & A\boldsymbol{q}_1 & \cdots & A\boldsymbol{q}_m \end{pmatrix},$$

and recalling (1),

$$A\boldsymbol{q}_j = H_{1j}\boldsymbol{q}_1 + H_{2j}\boldsymbol{q}_2 + \cdots + H_{jj}\boldsymbol{q}_m + H_{j+1,j}\boldsymbol{q}_{j+1}$$

it holds that

$$\begin{pmatrix} A\boldsymbol{q}_1 & A\boldsymbol{q}_2 & \cdots & A\boldsymbol{q}_m \end{pmatrix} = \begin{pmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_{m+1} \end{pmatrix} \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1m} \\ H_{21} & H_{22} & \cdots & H_{2m} \\ 0 & H_{32} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & H_{m+1,m} \end{pmatrix}.$$

Here, we have a coefficient matrix H of size $(m+1) \times m$. This matrix is "almost upper-triangular"; there is one entry below the diagonal in each column. This kind of matrix (where $H_{ij} = 0$ for $i > j+1$) is called an **upper Hessenberg matrix**. The previous equation can be written in the form

$$AQ_m = Q_{m+1}H_m. \tag{2}$$

2.3 GMRES

Since K_m and Q_m have the same column spaces (their columns both span the Krylov subspace $\mathcal{K}_m$), the least-squares problem

$$\|\boldsymbol{b} - AK_m\boldsymbol{y}_m\| \to \min$$

is equivalent to the least-squares problem

$$\|\boldsymbol{b} - AQ_m\boldsymbol{y}_m\| \to \min.$$

Replacing K_m with Q_m is important because it fixes the issue of stagnation we observed with the standard least-squares approach. It is also important because we can use the key identity (2). Since $AQ_m = Q_{m+1}H_m$, we have the equivalent minimization problem

$$\|\boldsymbol{b} - Q_{m+1}H_m\boldsymbol{y}_m\| \to \min.$$

Since $\boldsymbol{q}_1 = \boldsymbol{b}/\|\boldsymbol{b}\|$, we have $\boldsymbol{b} = \|\boldsymbol{b}\|Q_{m+1}\boldsymbol{e}_1$ (where $\boldsymbol{e}_1$ is the standard basis vector). We can then write the problem as (writing $\alpha = \|\boldsymbol{b}\|$),

$$\|Q_{m+1}(\alpha\boldsymbol{e}_1 - H_m\boldsymbol{y}_m)\| \to \min.$$

Since Q_{m+1} is an orthogonal matrix, it is an **isometry** ($\|Q_{m+1}\boldsymbol{z}\| = \|\boldsymbol{z}\|$ for all $\boldsymbol{z}$). This means that

$$\|Q_{m+1}(\alpha\boldsymbol{e}_1 - H_m\boldsymbol{y}_m)\| = \|\alpha\boldsymbol{e}_1 - H_m\boldsymbol{y}_m\|,$$

and the minimization problem is equivalent to

$$\|\alpha\boldsymbol{e}_1 - H_m\boldsymbol{y}_m\| \to \min, \tag{3}$$

which is posed over the space $\mathbb{R}^m$ instead of the much larger space $\mathbb{R}^N$.

Each iteration of the GMRES method constructs the Arnoldi matrices Q_m and H_m, and solves the size-m least squares problem (3). The approximate solution is given by $\boldsymbol{x}_m = Q_m\boldsymbol{y}_m$. This minimizes the residual in the Krylov subspace $\mathcal{K}_m$.