Krylov Subspace Methods

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This document aims to describe Krylov subspace methods, one of the best options for solving linear systems of equations. Briefly, they have the following desirable properties:

- No explicit form of $\mathbf{A}$ is needed; only a matrix-vector product is required.
- Well-suited for large and sparse systems.
- Optimised variations of Krylov methods are available for specific matrix types.
- For approximate solutions, Krylov methods have good convergence/approximation properties.

This is based on MATH3204 lectures and notes, lectured by Fred Roosta. The lecure slides contain proofs of some theorems not proved here.

1 Motivation

The general form of a linear system is

$$\mathbf{A}\boldsymbol{v}^\star = \boldsymbol{b}$$

where $\mathbf{A} \in \mathbb{C}^{\times n}$ and $\mathbf{A}$ is invertible. Assume $\rho(\mathbf{I} - \mathbf{A}) < 1$. Then, we can write $\mathbf{A}^{-1}$ as a geometric series,

$$\mathbf{A}^{-1} = (\mathbf{I} - (\mathbf{I} - \mathbf{A}))^{-1} = \sum_{k=0}^{\infty} (\mathbf{I} - \mathbf{A})^k.$$

Suppose we have an initial guess $\boldsymbol{x}_0 \in \mathbb{C}^n$. Define the residual of this guess as $\boldsymbol{r}_0 = \mathbf{A}\boldsymbol{x}^\star - \mathbf{A}\boldsymbol{x}_0$. Then,

$$\begin{aligned}\boldsymbol{x}^\star &= \mathbf{A}^{-1}\boldsymbol{b} = \mathbf{A}^{-1}(\mathbf{A}\boldsymbol{x}^\star - \mathbf{A}\boldsymbol{x}_0 + \mathbf{A}\boldsymbol{x}_0) \\ &= \boldsymbol{x}_0 + \mathbf{A}^{-1}\boldsymbol{r}_0 = \boldsymbol{x}_0 + \sum_{k=0}^{\infty}(\mathbf{I} - \mathbf{A})^k \boldsymbol{r}_0\end{aligned}$$

This is great, but largely useless if we need to compute infinitely many vectors to find $\boldsymbol{x}^\star$. However it turns out that we actually don't need to.

Theorem (Cayley–Hamilton)**.** *Let $p_n(\lambda) = \sum_{i=0}^{n} c_i \lambda^i$ be the characteristic polynomial of the matrix $\mathbf{A}$. Then, $p_n(\mathbf{A}) = 0$.*

This implies that $\mathbf{A}^{-1}$ can be written as a finite sum of linear combinations of powers of $\mathbf{A}$. Specifically, it is a matrix polynomial of degree at most $n-1$. As a result,

$$\boldsymbol{x}^\star \in \boldsymbol{x}_0 + \operatorname{Span}\left\{\boldsymbol{r}_0, \mathbf{A}\boldsymbol{r}_0, \ldots, \mathbf{A}^{n-1}\mathrm{r}_0\right\}.$$

Suppose we only consider a subspace of this, so choose $k < n$

$$\boldsymbol{x}_k \in \boldsymbol{x}_0 + \operatorname{Span}\left\{\boldsymbol{r}_0, \mathbf{A}\boldsymbol{r}_0, \ldots, \mathbf{A}^{k-1}\mathrm{r}_0\right\}.$$

This is the central question of Kylov methods. How good is the approximation $\boldsymbol{x}_k$ to $\boldsymbol{x}^\star$? What does "good" even mean?

In fact, Richardson iterations is a case of these subspace approximations. In Richardson,

$$\boldsymbol{x}_k = \boldsymbol{x}_0 + \sum_{i=0}^{k-1} \alpha_i \prod_{j=0}^{i-1}(\mathbf{I} - \alpha_j \mathbf{A})\boldsymbol{r}_0$$

However, depending on our choice of α_k, we saw dramatically different convergence.

The great quest of Krylov subspace methods is to find the the "best" (in some sense) $\boldsymbol{x}_k \approx \boldsymbol{x}^\star$ for some $k \ll n$.

Definition (Krylov Subspace)**.** *The Krylov subspace of order k, generated by the matrix $\mathbf{A}$ and vector $\boldsymbol{v}$ is defined as*

$$\mathcal{K}_k(\mathbf{A}, \boldsymbol{v}) = \operatorname{Span}\left\{\boldsymbol{v}, \mathbf{A}\boldsymbol{v}, \ldots, \mathbf{A}^{k-1}\boldsymbol{v}\right\}$$

for $k \geq 1$ and $\mathcal{K}_0(\mathbf{A}, \boldsymbol{v}) = \{\mathbf{0}\}$.

Because these subspaces are nested, their dimensions cannot grow indefinitely. At some point, the Krylov subspace will be large enough that it "contains" all the information we can extract from $\mathbf{A}$ through its multiplication by $\boldsymbol{v}$. Consider the simplest case when $\boldsymbol{v}$ is an eigenvector, then the Kyrlov space just has dimension 1 for all k.

Theorem (Grade of $\boldsymbol{v}$ with respect to $\mathbf{A}$)**.** *There exists a positive integer $t = t(\boldsymbol{v}, \mathbf{A})$, the grade of $\boldsymbol{v}$ with respect to $\mathbf{A}$ such that*

$$\dim \mathcal{K}_k(\mathbf{A}, \boldsymbol{v}) = \min\{k, t\}.$$

This means that for any $k \leq t$, all the generated vectors are linearly independent. After t, the new vectors are linearly dependent on the previous ones. This means that for $k > t$, $\mathcal{K}_k(\mathbf{A}, \boldsymbol{v}) = \mathcal{K}_{k+1}(\mathbf{A}, \boldsymbol{v})$. As a direct corollary of this,

$$t = \min\left\{k \mid \mathbf{A}^{-1}\boldsymbol{v} \in \mathcal{K}_k(\mathbf{A}, \boldsymbol{v})\right\}.$$

Recall that initially we had $\boldsymbol{x}^\star \in \boldsymbol{x}_0 + \mathcal{K}_n(\mathbf{A}, \boldsymbol{r}_0)$. Now, we have a more specific result that

$$\boldsymbol{x}^\star \in \boldsymbol{x}_0 + \mathcal{K}_t(\mathbf{A}, \boldsymbol{r}_0)$$

where $\boldsymbol{r}_0 = \boldsymbol{b} - \mathbf{A} - \boldsymbol{x}_0$ and t is the grade of $\boldsymbol{r}_0$ with respect to $\mathbf{A}$.

To summarise, standard Krylov subspace solvers can be descibed as follows.

Definition (Standard Krylov Subspace Method)**.** *A standard Krylov subspace method is an iterative method, which starting from some $\boldsymbol{x}_0$, generates an appropriate sequence of iterates $\boldsymbol{x}_k \in \boldsymbol{x}_0 + \mathcal{K}_k(\mathbf{A}, \boldsymbol{r}_0)$, until it finds $\boldsymbol{x}^\star$ in exactly t steps.*

The iterates are chosen appropriately such that if we terminate early, we have still $\boldsymbol{x}_k \approx \boldsymbol{x}^\star$ in some sense.

Note that not all Krylov methods are of this form. Some are bulid upon different types of subspace or work with multiple subspaces (e.g. they also consider $\mathcal{K}_t(\mathbf{A}^*, \boldsymbol{w})$).

Many terms are intentionally left vague in the above definition, because Krylov subspace solders differ among themselves in many aspects, such as

- the underlying Krylov subspace,
- the method in which $\boldsymbol{x}_k$ is chosen, and
- the sense in which $\boldsymbol{x}_k \approx \boldsymbol{x}^\star$ is measured.

Additionally, in exact arithmetic, Krylov methods have finite termination property (i.e. they will always finish with an exact solution in finite iterations). Unfortunately, this does not hold in finite-precision arithmetic, such as on a computer.