1 Power method and Krylov subspaces

When estimating an eigenvalue of a matrix A with the power method, one starts with an initial random vector b and then computes iteratively the sequence $Ab, A^2b, \ldots, A^{n-1}b$ normalising and storing the result in b on each iteration. The sequence converges to the eigenvector of the largest eigenvalue of the $N \times N$ matrix A.

The set of vectors

$$\mathcal{K}_n = \left\{b, Ab, A^2b, \ldots, A^{n-1}b\right\} \,, \tag{1}$$

where $n < N$, is called the order-n *Krylov matrix*, and the subspace spanned by these vectors is called the order-n *Krylov subspace*. The vectors are not orthogonal but can be made so by e.g. Gram-Schmdt orthogonalisation.

For the same reason that $A^{n-1}b$ approximates the dominant eigenvector one can expect that the other orthogonalised vectors approximate the eigenvectors of the n largest eigenvalues.

Krylov subspaces are the basis of several successful iterative methods in numerical linear algebra, in particular: Arnoldi and Lanczos methods for finding one (or a few) eigenvalues of a matrix; and GMRES (Generalised Minimum RESidual) method for solving systems of linear equations.

These methods are particularly suitable for large sparse matrices as they avoid matrix-matrix operations but rather multiply vectors by the matrices and work with the resulting vectors and matrices in Krylov subspaces of modest sizes.

1.1 Arnoldi iteration

Arnoldi iteration is an algorithm where the order-n orthogonalised Krylov matrix Q_n of an $N \times N$ matrix A is build using stabilised Gram-Schmidt process:

- start with a set $Q = \{q_1\}$ of one random normalised vector q_1
- repeat for $k = 2$ to n:
  - make a new vector $q_k = Aq_{k-1}$
  - orthogonalise q_k to all vectors $q_i \in Q$ storing $q_i^\dagger q_k \to h_{i,k-1}$.
  - normalise q_k storing $\|q_k\| \to h_{k,k-1}$;
  - add q_k to the set Q

By construction the upper Hessenberg matrix H_n made of the elements h_{jk},

$$H_n = \begin{bmatrix} h_{1,1} & h_{1,2} & h_{1,3} & \cdots & h_{1,n} \\ h_{2,1} & h_{2,2} & h_{2,3} & \cdots & h_{2,n} \\ 0 & h_{3,2} & h_{3,3} & \cdots & h_{3,n} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & h_{n,n-1} & h_{n,n} \end{bmatrix} \,, \tag{2}$$

is a partial orthogonal reduction of A into Hessenberg form,

$$H_n = Q_n^\dagger A Q_n \,. \tag{3}$$

The matrix H_n can be viewed as a representation of A in the Krylov subspace $\mathcal{K}_n$. The eigenvalues and eigenvectors of the matrix H_n approximate the largest eigenvalues of matrix A.

Since H_n is a Hessenberg matrix of modest size its eigenvalues can be relatively easily computed with e.g. the QR-algorithm.

In practice if the size n of the Krylov subspace becomes too large the method is restarted.

1.2 Lanczos iteration

Lanczos iteration is Arnoldi iteration for Hermitian matrices in which case the Hessenberg matrix H_n of Arnoldi method becomes a tridiagonal matrix T_n.

Thus the Lanczos algorithm reduces the original hermitian $N \times N$ matrix A into a smaller $n \times n$ tridiagonal matrix T_n by an orthogonal projection onto the order-n Krylov subspace. The eigenvalues and eigenvectors of a tridiagonal matrix of a modest size can be easily found by e.g. the QR-diagonalisation method.

In practice the Lanczos method is not very stable due to round-off errors leading to quick loss of orthogonality. The eigenvalues of the resulting tridiagonal matrix may then not be a good approximation to the original matrix. Library implementations fight the stability issues by trying to prevent the loss of orthogonality and/or to recover the orthogonality after the basis is generated.

1.3 Generalised minimum residual (GMRES)

GMRES is an iterative method for the numerical solution of a system of linear equations,

$$Ax = b \,, \tag{4}$$

where the exact solution x is approximated by the vector $x_n \in \mathcal{K}_n$ that minimises the residual $Ax_n - b$,

$$x \approx x_n = \min_{x_n \in \mathcal{K}_n} \|Ax_n - b\| \,, \tag{5}$$

in the Krylov subspace $\mathcal{K}_n$.