1 Arnoldi and Lanczos Iteration

Let $A \in \mathrm{GL}_n(\mathbb{R})$ and $b \in \mathbb{R}^n \setminus \{0\}$. Then consider the Arnoldi iteration as sketched below (1) to produce an orthonormal basis $q_1, \ldots, q_r$ of the r-th Krylov subspace $K_r(A, b)$ with $r \leq \max_{s \leq n} \dim(K_s(A, b))$. Further let $Q_r := [q_1, \ldots, q_r] \in \mathbb{R}^{n \times r}$ and $H_r := Q_r^T A Q_r \in \mathbb{R}^{r \times r}$.

1. In the j-th step: Assume $q_1, \ldots, q_j$ have been computed according to the Arnoldi iteration 1 and assume that $q_1, \ldots, q_{j-1}$ are mutually orthonormal. Show that q_j is orthogonal to all $q_1, \ldots, q_{j-1}$.

2. Derive an expression for the (ℓ, k)-th entries of H_r and find these numbers in the Arnoldi iteration. What structure does H_r have?

3. Now assume A is symmetric. How does H_r look in this case? How can you simplify the Arnoldi iteration?

4. What can you say about the eigenvalues of H_n and A? Explain your answer.

INPUT: $A \in GL_n(\mathbb{R})$, $b \in \mathbb{R}^n$, $r \leq n$
OUTPUT: orthonormal basis $q_1, \ldots, q_r$ of the r-th Krylov subspace $K_r(A, b)$

$q_1 := \frac{b}{\|b\|_2}$
for $j = 2, \ldots, r$ **do**
    $\widehat{q}_j := Aq_{j-1} - \sum_{\ell=1}^{j-1} q_\ell^\top (Aq_{j-1}) \cdot q_\ell$
    if $\|\widehat{q}_j\|_2 = 0$ **then**
        break
    end
    $q_j := \frac{\widehat{q}_j}{\|\widehat{q}_j\|_2}$
end

Algorithm 1: Arnoldi Iteration

Solution:

1. Let $k < j$. Since $q_k^\top q_j = \frac{1}{\|\widehat{q}_j\|_2} q_k^\top \widehat{q}_j$ it suffices to show that $q_k^\top \widehat{q}_j = 0$. Now let $v := Aq_{j-1}$, then

$$\begin{aligned} q_k^\top \widehat{q}_j = q_k^\top \left(v - \sum_{\ell=1}^{j-1} q_\ell^\top v \cdot q_\ell \right) &= q_k^\top v - \sum_{\ell=1}^{j-1} q_\ell^\top v \cdot \underbrace{q_k^\top q_\ell}_{=\delta_{k\ell}} \\ &= q_k^\top v - q_k^\top v \cdot 1 \\ &= 0. \end{aligned}$$

2. By definition of the matrix product we obtain, for $1 \leq \ell, j \leq r$,

$$H_r^{\ell k} = (Q_r^\top A Q_r)_{\ell k} = q_\ell^\top A q_k.$$

   These are precisely the projection lengths that are computed during the Arnoldi iteration. Since by definition Aq_j can be uniquely generated by $q_1, \ldots, q_{j+1}$, we have that $h_{ij} = 0$ for all $i > j + 1$. In particular, H_r is an upper *Hessenberg* matrix (having precisely one subdiagonal).

3. If A is symmetric, then $H_r = Q_r^\top A Q_r$ is symmetric, so that it simplifies to a tridiagonal matrix. In particular $h_{ij} = (Aq_j)^\top q_i = 0$ for all i, j with $|i-j| > 2$ and Arnoldi becomes Lanczos by accounting for the simplification

$$\widehat{q}_j = Aq_{j-1} - \sum_{\ell=1}^{j-1} q_\ell^\top (Aq_{j-1}) \cdot q_\ell = Aq_{j-1} - q_{j-2}^\top (Aq_{j-1}) \cdot q_{j-2} - q_{j-1}^\top (Aq_{j-1}) \cdot q_{j-1}.$$

4. Since $Q_n^T A Q_n \in \mathbb{R}^{n\times n}$ is orthogonally similar to A, it has the same eigenvalues as A.