Functions of large-scale matrices

How do we compute $f(A)$ if A is large and sparse? Huge recent research topic.

Most of the time, one wants $f(A)b$ rather than $f(A)$, because $f(A)$ is full (unless there is special structure in $f(A)$, e.g., it's a banded matrix).
The main techniques are those we have seen in the beginning.

- Replace f with an approximating polynomial (or rational function) on a region U that includes the spectrum of A (how?).
- Contour integration.
- Ad-hoc methods, involving e.g. discretization of differential equations: for instance, $\exp(A)b = v(1)$ where $\dot{v}(t) = Av(t)$, $v(0) = b$.

Arnoldi for matrix functions

Another possibility with the "Swiss-army knife algorithm" for large matrices: Arnoldi.

Recap: Arnoldi iteration

- Constructs a "partial Hessenberg reduction", i.e., gives the leading columns $Q_k = Q(:, 1:k)$ of Q and the leading block $H_k = H(1:k, 1:k)$ of H such that $A = QHQ^*$.
- Idea: (modified) Gram-Schmidt orthogonalization of $K_k(A, b) = \mathrm{span}(b, Ab, \ldots, A^{k-1}b)$.
- Start from $q_1 = b/\|b\|$; at each step j take Aq_j and orthogonalize it against all previous vectors q_i.
- $AQ_k = Q_k H_k + Q(:, k+1)H(k+1, k)e_k^T$

Arnoldi, matrix functions, and polynomial approximations

Arnoldi (with k steps) computes the action of A exactly on $K_{k-1}(A, b)$, i.e., all polynomials of degree $k-1$. In particular,

$$p(A)b = Q_k p(H_k) e_1.$$

Idea: let's compute $f(A)b \approx Q_k f(H_k) e_1$. This approximation is exact for polynomials of degree $\leq k-1$.

Moreover,

$$Q_k f(H_k) e_1 = Q_k p(H_k) e_1 = p(A)b,$$

where p is the interpolating polynomial on the spectrum of H_k (not that of A!)

Known behaviour from Arnoldi theory: for many matrices, the eigenvalues of H_k approximate the extremal eigenvalues of A.

Arnoldi variants

We expect good results if (1) enough steps are taken, and (2) the function f takes its larger values in the extremal eigenvalues of A.

What if f takes its larger values at some internal point of the spectrum of A, e.g., $f(x) = \frac{1}{x}$ and A has both positive and negative eigenvalues (or complex values not all in the same half-plane)?

Variants with better approximation spaces can be constructed, e.g., extended Krylov, i.e., Krylov on A and A^{-1} 'at the same time', or rational Krylov, which takes poles $\mu_1, \mu_2, \dots, \mu_k \in \mathbb{C}$ as input and constructs a basis of

$$\{\sum_{j=1}^{k} \alpha_j (A - \mu_j)^{-1} b \colon \alpha_1, \alpha_2, \dots, \alpha_k \in \mathbb{C}\},$$

i.e., all vectors of the form $r(A)b$, where $r(x)$ is a rational function with poles $\mu_1, \dots, \mu_k$.