

the tridiagonal matrix produced by the Lanczos algorithm, and (4.1) is identical to (2.30).

Algorithm 4.1: THE GMRES METHOD

Choose $\mathbf{u}^{(0)}$, compute $\mathbf{r}^{(0)} = \mathbf{f} - F\mathbf{u}^{(0)}$, $\beta_0 = \|\mathbf{r}^{(0)}\|$, $\mathbf{v}^{(1)} = \mathbf{r}^{(0)}/\beta_0$
 for $k = 1, 2, \dots$ until $\beta_k < \tau\beta_0$ do
 $\mathbf{w}_0^{(k+1)} = F\mathbf{v}^{(k)}$
 for $l = 1$ to k do
 $h_{lk} = \langle \mathbf{w}_l^{(k+1)}, \mathbf{v}^{(l)} \rangle$
 $\mathbf{w}_{l+1}^{(k+1)} = \mathbf{w}_l^{(k+1)} - h_{lk}\mathbf{v}^{(l)}$
 enddo
 $h_{k+1,k} = \|\mathbf{w}_{k+1}^{(k+1)}\|$
 $\mathbf{v}^{(k+1)} = \mathbf{w}_{k+1}^{(k+1)} / h_{k+1,k}$
 Compute $\mathbf{y}^{(k)}$ such that $\beta_k = \|\beta_0\mathbf{e}_1 - \hat{H}_k\mathbf{y}^{(k)}\|$ is minimized,
 where $\hat{H}_k = [h_{ij}]_{1 \leq i \leq k+1, 1 \leq j \leq k}$
 enddo
 $\mathbf{u}^{(k)} = \mathbf{u}^{(0)} + V_k\mathbf{y}^{(k)}$

To derive a Krylov subspace iteration for solving systems of equations, we let $\mathbf{u}^{(k)} \in \mathbf{u}^{(0)} + \mathcal{K}_k(F, \mathbf{r}^{(0)})$. For the choice $\mathbf{v}^{(1)} = \mathbf{r}^{(0)}/\beta_0$, with $\beta_0 = \|\mathbf{r}^{(0)}\|$ as in Algorithm 4.1, this is equivalent to

$$\mathbf{u}^{(k)} = \mathbf{u}^{(0)} + V_k\mathbf{y}^{(k)} \quad (4.2)$$

for some k -dimensional vector $\mathbf{y}^{(k)}$. But the first line of (4.1) can be rewritten as $FV_k = V_{k+1}\hat{H}_k$, and this implies that the residual satisfies

$$\mathbf{r}^{(k)} = \mathbf{r}^{(0)} - AV_k\mathbf{y}^{(k)} = V_{k+1}(\beta_0\mathbf{e}_1 - \hat{H}_k\mathbf{y}^{(k)}), \quad (4.3)$$

where $\mathbf{e}_1 = (1, 0, \dots, 0)^T$ is the unit vector of size k . The vectors $\{\mathbf{v}^{(j)}\}$ are pairwise mutually orthogonal, so that

$$\|\mathbf{r}^{(k)}\| = \beta_k = \|\beta_0\mathbf{e}_1 - \hat{H}_k\mathbf{y}^{(k)}\|. \quad (4.4)$$

In particular, the residual of the iterate (4.2) with smallest Euclidean norm is determined by the choice of $\mathbf{y}^{(k)}$ that minimizes the expression on the right side of (4.4).

This upper-Hessenberg least squares problem can be solved by transforming \hat{H}_k into upper triangular form $\begin{pmatrix} R_k \\ 0 \end{pmatrix}$, where R_k is upper triangular, using $k+1$ plane rotations (which are also applied to $\beta_0\mathbf{e}_1$). Here, \hat{H}_k contains \hat{H}_{k-1} as a submatrix, so that in a practical implementation, R_k can be updated from R_{k-1} . Moreover, by an analysis similar to that leading to (2.37), it can be shown that $\|\mathbf{r}^{(k)}\|$ is available at essentially no cost. Hence, a step of the GMRES algorithm