Krylov subspace methods (Continued)

- *Practical variants: restarting and truncating*
- *Symmetric case: The link with the Lanczos algorithm*
- *The Conjugate Gradient algorithm*
- *See Chapter 6 of text for details.*

Restarting and Truncating

Difficulty: As m increases, storage and work per step increase fast.

First remedy: Restart. Fix m (dim. of subspace)

ALGORITHM : 1. *Restarted GMRES (resp. Arnoldi)*

```
1. (Re)-Start: Compute $r_0 = b - Ax_0$, Set: $v_1 = r_0/(\beta := \|r_0\|_2)$.
2. Arnoldi Process: generate $\bar{H}_m$ and $V_m$.
3. Compute $y_m = H_m^{-1}\beta e_1$ (FOM), or
           $y_m = argmin\|\beta e_1 - \bar{H}_m y\|_2$ (GMRES)
4. $x_m = x_0 + V_m y_m$
5. If $\|r_m\|_2 \le \epsilon\|r_0\|_2$ stop
      else set $x_0 := x_m$ and go to 1.
```

Second remedy: Truncate the orthogonalization

Formula for v_{j+1} replaced by:

$$h_{j+1,j}v_{j+1} = Av_j - \sum_{i=j-k+1}^{j} h_{ij}v_i$$

- Each v_j is made orthogonal to the previous k v_i's.
- x_m still computed as $x_m = x_0 + V_m H_m^{-1}\beta e_1$.
- It can be shown that this is an oblique projection process.

- IOM (Incomplete Orthogonalization Method) = replace orthogonalization in FOM, by the above truncated (or 'incomplete') orthogonalization.

The direct version of IOM [DIOM]:

- Write the LU decomposition of H_m as $H_m = L_m U_m$

$$x_m = x_0 + \boxed{V_m U_m^{-1}}\ \boxed{L_m^{-1}\beta e_1} \equiv x_0 + P_m z_m$$

Structure of L_m, U_m when $k = 3$

$$L_m = \begin{bmatrix} 1 & & & & & \\ x & 1 & & & & \\ & x & 1 & & & \\ & & x & 1 & & \\ & & & x & 1 & \\ & & & & x & 1 \end{bmatrix} \qquad U_m = \begin{bmatrix} x & x & x & & & \\ & x & x & x & & \\ & & x & x & x & \\ & & & x & x & x \\ & & & & x & x \\ & & & & & x \end{bmatrix}$$

- $p_m = u_{mm}^{-1}[v_m - \sum_{i=m-k+1}^{m-1} u_{im}p_i]$ $\qquad z_m = \begin{bmatrix} z_{m-1} \\ \zeta_m \end{bmatrix}$

➤ Can update x_m at each step: $x_m = x_{m-1} + \zeta_m p_m$

Algorithm:

```
Until convergence do:
        Update LU factorization of $H_m \to H_m = L_m U_m$
        $p_m = u_{mm}^{-1}[v_m - \sum_{i=m-k+1}^{m-1} u_{im} p_i]$
        $x_m = x_{m-1} + \zeta_m p_m$
        $h_{m+1,m} v_{m+1} = A v_m - \sum_{i=m-k+1}^{m} h_{im} v_i$ (Arnoldi step)
Enddo
```

➤ Requires $2k+1$ vectors [in addition to solution]

Note: Several existing pairs of methods have a similar link: they are based on the LU, or other, factorizations of the H_m matrix

➤ CG-like formulation of IOM called DIOM [YS, 1982]

➤ ORTHORES(k) [Young & Jea '82] equivalent to DIOM(k)

➤ SYMMLQ [Paige and Saunders, '77] uses LQ factorization of H_m.

➤ Can incorporate partial pivoting in LU factorization of H_m

The symmetric case: Observation

Observe: When A is real symmetric then in Arnoldi's method:

$$\boxed{H_m = V_m^T A V_m}$$

must be symmetric. Therefore

Theorem. When Arnoldi's algorithm is applied to a (real) symmetric matrix then the matrix H_m is symmetric tridiagonal:

$$h_{ij} = 0 \quad 1 \le i < j-1; \quad \text{and}$$
$$h_{j,j+1} = h_{j+1,j}, \ j = 1, \ldots, m$$

➤ We can write

$$H_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & & \beta_m & \alpha_m \end{bmatrix} \qquad (1)$$

The v_i's satisfy a 3-term recurrence [Lanczos Algorithm]:

$$\beta_{j+1} v_{j+1} = A v_j - \alpha_j v_j - \beta_j v_{j-1}$$

➤ Simplified version of Arnoldi's algorithm for sym. systems.

Symmetric matrix + Arnoldi $\to$ Symmetric Lanczos

The Lanczos algorithm

ALGORITHM : 2. *Lanczos*

```
1.  Choose an initial vector $v_1$, s.t. $\|v_1\|_2 = 1$
        Set $\beta_1 \equiv 0, v_0 \equiv 0$
2.  For $j = 1, 2, \ldots, m$ Do:
3.      $w_j := Av_j - \beta_j v_{j-1}$
4.      $\alpha_j := (w_j, v_j)$
5.      $w_j := w_j - \alpha_j v_j$
6.      $\beta_{j+1} := \|w_j\|_2$. If $\beta_{j+1} = 0$ then Stop
7.      $v_{j+1} := w_j/\beta_{j+1}$
8.  EndDo
```

Lanczos algorithm for linear systems

➤ Usual orthogonal projection method setting:

- $L_m = K_m = span\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$
- Basis $V_m = [v_1, \ldots, v_m]$ of K_m generated by the Lanczos algorithm

➤ Three different possible implementations.

(1) Arnoldi-like;

(2) Exploit tridiagonal nature of H_m (DIOM);

(3) Conjugate gradient - derived from (2)

ALGORITHM : 3. *Lanczos Method for Linear Systems*

```
1.  Compute $r_0 = b - Ax_0$, $\beta := \|r_0\|_2$, and $v_1 := r_0/\beta$
2.  For $j = 1, 2, \ldots, m$ Do:
3.      $w_j = Av_j - \beta_j v_{j-1}$ (If $j = 1$ set $\beta_1 v_0 \equiv 0$)
4.      $\alpha_j = (w_j, v_j)$
5.      $w_j := w_j - \alpha_j v_j$
6.      $\beta_{j+1} = \|w_j\|_2$. If $\beta_{j+1} = 0$ set $m := j$ and go to 9
7.      $v_{j+1} = w_j/\beta_{j+1}$
8.  EndDo
9.  Set $T_m = tridiag(\beta_i, \alpha_i, \beta_{i+1})$, and $V_m = [v_1, \ldots, v_m]$.
10. Compute $y_m = T_m^{-1}(\beta e_1)$ and $x_m = x_0 + V_m y_m$
```

ALGORITHM : 4. *D-Lanczos*

```
1.  Compute $r_0 = b - Ax_0$, $\zeta_1 := \beta := \|r_0\|_2$, and $v_1 := \frac{r_0}{\beta}$
2.  Set $\lambda_1 = \beta_1 = 0$, $p_0 = 0$
3.  For $m = 1, 2, \ldots$, until convergence Do:
4.      Compute $w := Av_m - \beta_m v_{m-1}$ and $\alpha_m = (w, v_m)$
5.      If $m > 1$ compute $\lambda_m = \frac{\beta_m}{\eta_{m-1}}$ and $\zeta_m = -\lambda_m \zeta_{m-1}$
6.      $\eta_m = \alpha_m - \lambda_m \beta_m$
7.      $p_m = \eta_m^{-1}(v_m - \beta_m p_{m-1})$
8.      $x_m = x_{m-1} + \zeta_m p_m$
9.      If $x_m$ has converged then Stop
10.     $w := w - \alpha_m v_m$
11.     $\beta_{m+1} = \|w\|_2$, $v_{m+1} = w/\beta_{m+1}$
12. EndDo
```

The Conjugate Gradient Algorithm (A S.P.D.)

- In D-Lanczos, $r_m = scalar \times v_{m-1}$ and $p_m = scalar \times [v_m - \beta_m p_{m-1}]$
- And we have $x_m = x_{m-1} + \xi_m p_m$
- So there must exist an update of the form:

$$\boxed{\begin{array}{l} 1.\ p_{m+1} = r_m + \beta_m p_m \\ 2.\ x_{m+1} = x_m + \xi_{m+1} p_{m+1} \\ 3.\ r_{m+1} = r_m - \xi_{m+1} A p_{m+1} \end{array}}$$

- Note: p_m is scaled differently and β_m is not the same
- .. In CG, index of p_m aligned with that of r_m – so p_j replaced by p_{j-1}.
- Note: the p_i's are A-orthogonal
- The r_i''s are orthogonal.

The Conjugate Gradient Algorithm (A S.P.D.)

```
1. Start: $r_0 := b - Ax_0$, $p_0 := r_0$.
2. Iterate: Until convergence do,
   (a) $\alpha_j := (r_j, r_j)/(Ap_j, p_j)$
   (b) $x_{j+1} := x_j + \alpha_j p_j$
   (c) $r_{j+1} := r_j - \alpha_j Ap_j$
   (d) $\beta_j := (r_{j+1}, r_{j+1})/(r_j, r_j)$
   (e) $p_{j+1} := r_{j+1} + \beta_j p_j$
```

- $r_j = scaling \times v_{j+1}$. The r_j's are orthogonal.
- The p_j's are A-conjugate, i.e., $(Ap_i, p_j) = 0$ for $i \neq j$.

- Question: How to apply preconditioning?

A bit of history. From the 1952 CG article:

"The method of conjugate gradients was developed independently by E. Stiefel of the Institute of Applied Mathematics at Zurich and by M. R. Hestenes with the cooperation of J. B. Rosser, G. Forsythe, and L. Paige of the Institute for Numerical Analysis, National Bureau of Standards. The present account was prepared jointly by M. R. Hestenes and E. Stiefel during the latter' s stay at the National Bureau of Standards. The first papers on this method were given by E. Stiefel [1952] and by M. R. Hestenes [1951]. Reports on this method were given by E. Stiefel and J. B. Rosser at a Symposium on August 23-25, 1951. Recently, C. Lanczos [1952] developed a closely related routine based on his earlier paper on eigenvalue problem [1950]. Examples and numerical tests of the method have been by R. Hayes, U. Hoschstrasser, and M. Stein."