Arnoldi & Lanczos A-orthogonalizations and their applications to Krylov subspace methods

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A. N. Krylov.
1861-1945

A.N.Krylov. On the numerical solution of the equation which define into the technical questions, the frequencies of small oscillations of material systems.

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CONTENTS

$$Au = f, \quad A = \{a_{i,j}\} \in \mathcal{C}^{N,N}(\mathcal{R}^{N,N}),$$

$$u = \{u_i\}, \ \ f = \{f_i\} \in \mathcal{C}^{N}(\mathcal{R}^{N}),$$

$$A \neq A^H, \ \ A = A^T, \ \ |A| \neq 0,$$

$$(Au, u) \leq 0, \ \ (u, v) = \sum_i \bar{u}_i v_i, \ \ (u, v)_0 = \sum_i u_i v_i,$$

$$normal \ \ A : AA^H = A^H A$$

MINIMAL AND A-MINIMAL ITERATIONS

$$u^n = u^0 + y_1 v^n + \ldots + y_n v^n, \quad (v^n, A^s v^k) = d_n^{(s)} \delta_{k,n},$$
$$d_n^{(s)} = (v^n, A^s v^n)$$

Arnoldi Orthogonalization ($s = 0, 1$):

$$v^{n+1} = Av^n - \sum_{k=1}^{n} h_{k,n}^{(s)} v^k, \quad v^1 = r^0 = f - Au^0,$$

$$h_{k,n}^{(s)} = \frac{(Av^n, A^s v^k)}{(A^s v^k, v^k)}, \quad k = 1, \ldots, n+1, \quad V_{n+1} = (v^1, \ldots, v^{n+1})$$

$$\bar{H}_n = \begin{bmatrix} H_n \\ e_n^t \end{bmatrix} \in \mathcal{R}^{n+1,n}, \quad H_n = \{h_{k,n}\} \in \mathcal{R}^{n,n}, \quad e_n^t = (0, \ldots, 0, 1)$$

$$\mathcal{K}_{n+1}(r^0, A) = \mathrm{span}\{v^1, v^{n+1}\} = \mathrm{span}\{r^0, Ar^0, \ldots, A^n r^0\}$$

$$V_n^t (A^s)^t V_n = D_n, \quad V_n^t (A^s)^t A V_n = D_n H_n, \quad D_n = diag\{d_i\},$$

$$u^n = u^0 + V_n y^n, \quad y^n = (y_1, ..., y_n)^t, \quad r^n = r^0 - A V_n y^n,$$

$$V_n^t (A^s)^t r^n = V_n^t (A^s)^t r^0 - V_n^t (A^s)^t A V_n y^n =$$

$$= d_1 e_1 - D_n H_n y^n = 0 \quad \textbf{for} \quad H_n y^n = e_1,$$

$$r^n = v^1 - V_{n+1} \bar{H}_n y^n = v^1 - V_n H_n y^n - v^{n+1} e_n^t y^n = -v^{n+1} y_n,$$

$$(r^n, r^n) = (v^{n+1}, v^{n+1}) y_n^2, \qquad H_n = L_n U_n,$$

$$L_n z^n = e_1, \qquad U_n y^n = z^n$$

GMRES ($s = 0$) and AGMRES (s=1)

$$r^n = V_{n+1}(\beta e_1 - \bar{H}_n y^n), \quad \beta = ||r^0||_2, \quad V_{n+1}^t (A^s)^t V_{n+1} = I_n,$$

$$(r^n, A^s r^n) = (V_{n+1}^t (A^s)^t V_{n+1}(\beta e_1 - \bar{H}_n y^n), (\beta e_1 - \bar{H}_n y^n)) =$$

$$= (Q_{n+1}^t Q_{n+1}(\beta e_1 - \bar{H}_n y^n), Q_{n+1}^t Q_{n+1}(\beta e_1 - \bar{H}_n y^n)) =$$

$$= (\bar{g} - \bar{R}_n y^n), (\bar{g} - \bar{R}_n y^n)) = (g^n - R_n y^n), (g^n - R_n y^n)) + g_{n+1}^2$$

$$\min_{y^n}(r^n, A^s r^n) = g_{n+1}^2, \quad R_n y^n = g^n, \quad R_n \in \mathcal{R}^{n,n}, \quad g^n \in \mathcal{R}^n,$$

$$\bar{g} = \beta Q_{n+1} e_1 = \begin{bmatrix} g^n \\ g_{n+1} \end{bmatrix}, \quad \bar{R}_n = Q_{n+1} \bar{H}_n = \begin{bmatrix} R_n \\ 0 \end{bmatrix},$$

$$u^n = u^0 + v^1 y^1 + v^2 y^2 + \ldots + v^n y^n$$

A^s-Quasi-Minimal Residual (A^s-QMR)

$$v^{n+1} = Av^n - \alpha_n^{(s)} v^n - \beta_n^{(s)} v^{n-1},$$

$$w^{n+1} = A^t w^n - \alpha_n^{(s)} w^n - \beta_n^{(s)} w^{n-1},$$

$$\beta_1^{(s)} = 0, \quad v^1 = w^1 = r^0 \equiv f - Au^0,$$

$$(v^n, A^s w^k) = d_n^{(s)} \delta_{n,k}, \, d_n^{(s)} = (v^n, A^s w^n),$$

$$\alpha_n^{(s)} = (Av^n, A^s w^n)/d_n^{(s)}, \quad \beta_n^{(s)} = (Av^n, A^s w^{n-1})/d_{n-1}^{(s)},$$

$$T_n = 3 - \textbf{diag}\{t_{k,n}\} \in \mathcal{R}^{n,n}, \quad t_{k+1,k} = 1, \quad t_{k,k} = \alpha_k, \quad t_{k,k+1} = \beta_k,$$

$$AV_n = V_n T_n + v^{n+1} e_n^t = V_{n+1} \bar{T}_n, \quad \bar{T}_n \in \mathcal{R}^{n+1,n},$$

$$A^t W_n = W_n T_n + w^{n+1} e_n^t = W_{n+1} \bar{T}_n, \quad W_n \in \mathcal{R}^{N,n},$$

$$\bar{T}_n = \left[\begin{array}{c} T_n \\ e_n^t \end{array} \right], \quad V_n = (v^1, ..., v^n), \quad W_n = (w^1, ..., w^n),$$

$$u^n = u^0 + V_n y^n, \quad W_n^t A^s A V_n = T_n, \quad W_n^t A^s V_n = D_n = \mathbf{diag}\{d_n^{(s)}\},$$

$$r^n = v^1 - V_{n+1} \bar{T}_n y^n = V_{n+1}(e_1 - \bar{T}_n y^n) \equiv V_{n+1} z^n,$$

$$y^n = \mathbf{arg}\{\min_y ||z^n||\},$$

A^s-BiConjugate Direction Methods

$$u^{n+1} = u_n + \alpha_n^{(s)} p^n, \quad r^0 = \tilde{r}^0 = p^0 = \tilde{p}^0 = f - Au^0,$$
$$r^{n+1} = r^n - \alpha_n^{(s)} A p^n, \quad \tilde{r}^{n+1} = \tilde{r}^n - \alpha_n^{(s)} A^t \tilde{p}^n,$$
$$p^{n+1} = r^{n+1} + \beta_n^{(s)} p^n, \quad \tilde{p}^{n+1} = \tilde{r}^{n+1} + \beta_n^{(s)} \tilde{p}^n,$$

$$(A^s p^n, A^t \tilde{p}^k) = \rho_n^{(s)} \delta_{k,n}, \quad \rho_n^{(s)} = (A^s p^n, A^t \tilde{p}^n),$$
$$(A^s r^n, \tilde{p}^k) = (A^s r^n, \tilde{p}^n)\delta_{k,n}, \quad (A^s p^k, \tilde{r}^n) = (A^s p^n, \tilde{r}^n)\delta_{k,n},$$
$$(A^s r^n, \tilde{r}^k) = \delta_{k,n}, \quad \sigma_n^{(s)} = (A^s r^n, \tilde{r}^n),$$

$$\alpha_n^{(s)} = \sigma_n^{(s)} / \rho_n^{(s)}, \quad \beta_n^{(s)} = \sigma_n^{(s)} / \sigma_n^{(s)},$$

BiCG, BiCR: $r^n = \varphi_n^{(s)}(A) r^0, \quad \tilde{r}^n = \varphi_n^{(s)}(A^t) \tilde{r}^0$

CGS, CRS: $r^n = \Phi_n^{(s)}(A) r^0, \quad \Phi_n^{(s)}(t) = (\varphi_n^{(s)}(t))$

Semi – Conjugate Direction Methods

$$r^0 = f - Au^0, \quad p^0 = B_0^{-1} r^0, \quad s = 0, 1:$$

$$r^{n+1} = r^n - \alpha_n^{(s)} A p^n, \quad u^{n+1} = u^n + \alpha_n^{(s)} p^n,$$

$$(A^s p^k, Ap^n) = \rho_n^{(s)} \delta_{k,n}, \quad \rho_n^{(s)} = (A^s p^n, Ap^n), \quad k = 0, 1, ..., n-1,$$

$$p^{n+1} = B_{n+1}^{-1} r^{n+1} + \sum_{k=0}^{n} \beta_{n,k}^{(s)} p^k,$$

$$(r^n, A^s p^k) = 0, \quad k = 0, 1, ..., n-1,$$

$$\alpha_n^{(s)} = (A^s B_n^{-1} r^n, r^n)/\rho_n^{(s)}, \quad \beta_{n,k}^{(s)} = -(A^s p^k, A B_{n+1}^{-1} r^{n+1})/\rho_n^{(s)},$$

$$s = 1 \ (SCR): \quad \partial(r^n, r^n)/\partial\alpha_k = 0, \quad k = 0, 1, ..., n-1,$$

$$(r^{n+1}, r^{n+1}) = (r^0, r^0) - \frac{(A B_0^{-1} r^0, r^0)^2}{\rho_0^{(1)}(r^0, r^0)} - ... - \frac{(A B_n^{-1} r^n, r^n)^2}{\rho_n^{(1)}(r^n, r^n)}$$

Preconditioning

- modified incomplete factorizations,
- projection algorithms (Kaczmarz, Cimmino),
- domain decomposition in subspaces,
- block preconditioning,
- user defined preconditioning

Krylov: the Library of Algorithms for Solving Sparse SLAEs

- types of original problems
  - fast solvers for separable variables,
  - universal solvers for conventional compessed formats,
  - block algorithms for special problems (algebraic saddle point, Maxwell, Lame, Navier–Stokes eqs),
- code optimization, using efficient tools (MKL, Sparse Blas),
- parallelization, algebraic domain decomposition, hybrid programming (MPI, OpenMP)

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