LARGE SPARSE EIGENVALUE PROBLEMS

- **Projection methods**
- **The subspace iteration**
- **Krylov subspace methods: Arnoldi and Lanczos**
- **Golub-Kahan-Lanczos bidiagonalization**

General Tools for Solving Large Eigen-Problems

➤ Projection techniques – Arnoldi, Lanczos, Subspace Iteration;

➤ Preconditionings: shift-and-invert, Polynomials, ...

➤ Deflation and restarting techniques

➤ Computational codes often combine these three ingredients

A few popular solution Methods

- Subspace Iteration [Now less popular – sometimes used for validation]
- Arnoldi's method (or Lanczos) with polynomial acceleration
- Shift-and-invert and other preconditioners. [Use Arnoldi or Lanczos for $(A - \sigma I)^{-1}$.]
- Davidson's method and variants, Jacobi-Davidson
- Specialized method: Automatic Multilevel Substructuring (AMLS).

Projection Methods for Eigenvalue Problems

Projection method onto K orthogonal to L

➤ Given: Two subspaces K and L of same dimension.

➤ Approximate eigenpairs $\tilde{\lambda}, \tilde{u}$, obtained by solving:

$$\text{Find: } \tilde{\lambda} \in \mathbb{C}, \tilde{u} \in K \quad \text{such that} (\tilde{\lambda} I - A)\tilde{u} \perp L$$

➤ Two types of methods:

Orthogonal projection methods: Situation when $L = K$.

Oblique projection methods: When $L \neq K$.

➤ First situation leads to Rayleigh-Ritz procedure

Rayleigh-Ritz projection

Given: a subspace X known to contain good approximations to eigenvectors of A.
Question: How to extract 'best' approximations to eigenvalues/ eigenvectors from this subspace?

Answer: Orthogonal projection method

➤ Let $Q = [q_1, \ldots, q_m]$ = orthonormal basis of X

➤ Orthogonal projection method onto X yields: $Q^H(A - \tilde{\lambda}I)\tilde{u} = 0 \;\rightarrow$

➤ $\boxed{Q^H AQy = \tilde{\lambda}y \text{ where } \tilde{u} = Qy}$ Known as Rayleigh Ritz process

Procedure:
1. Obtain an orthonormal basis of X
2. Compute $C = Q^H AQ$ (an $m \times m$ matrix)
3. Obtain Schur factorization of C, $C = YRY^H$
4. Compute $\tilde{U} = QY$

Property: if X is (exactly) invariant, then procedure will yield exact eigenvalues and eigenvectors.

Proof: Since X is invariant, $(A - \tilde{\lambda}I)u = Qz$ for a certain z. $Q^H Qz = 0$ implies $z = 0$ and therefore $(A - \tilde{\lambda}I)u = 0$.

➤ Can use this procedure in conjunction with the subspace obtained from subspace iteration algorithm

Subspace Iteration

Original idea: projection technique onto a subspace of the form $Y = A^k X$

Practically: A^k replaced by suitable polynomial

Advantages:
- Easy to implement (in symmetric case);
- Easy to analyze;

Disadvantage: Slow.

➤ Often used with polynomial acceleration: $A^k X$ replaced by $C_k(A)X$. Typically C_k = Chebyshev polynomial.

Algorithm: Subspace Iteration with Projection

1. Start: Choose an initial system of vectors $X = [x_0, \ldots, x_m]$ and an initial polynomial C_k.
2. Iterate: Until convergence do:
   (a) Compute $\hat{Z} = C_k(A)X$. [Simplest case: $\hat{Z} = AX$.]
   (b) Orthonormalize $\hat{Z}$: $[Z, R_Z] = qr(\hat{Z}, 0)$
   (c) Compute $B = Z^H AZ$
   (d) Compute the Schur factorization $B = YR_BY^H$ of B
   (e) Compute $X := ZY$.
   (f) Test for convergence. If satisfied stop. Else select a new polynomial $C'_{k'}$ and continue.

THEOREM: Let $S_0 = span\{x_1, x_2, \ldots, x_m\}$ and assume that S_0 is such that the vectors $\{Px_i\}_{i=1,...,m}$ are linearly independent where P is the spectral projector associated with $\lambda_1, \ldots, \lambda_m$. Let $\mathcal{P}_k$ the orthogonal projector onto the subspace $S_k = span\{X_k\}$. Then for each eigenvector u_i of A, $i = 1, \ldots, m$, there exists a unique vector s_i in the subspace S_0 such that $Ps_i = u_i$. Moreover, the following inequality is satisfied

$$\|(I - \mathcal{P}_k)u_i\|_2 \leq \|u_i - s_i\|_2 \left(\left| \frac{\lambda_{m+1}}{\lambda_i} \right| + \epsilon_k \right)^k, \qquad (1)$$

where ϵ_k tends to zero as k tends to infinity.

KRYLOV SUBSPACE METHODS

Krylov subspace methods

Principle: Projection methods on Krylov subspaces:

$$K_m(A, v_1) = \text{span}\{v_1, Av_1, \cdots, A^{m-1}v_1\}$$

- The most important class of projection methods [for linear systems and for eigenvalue problems]
- Variants depend on the subspace L

➤ Let $\mu =$ deg. of minimal polynom. of v_1. Then:

- $K_m = \{p(A)v_1 | p = \text{polynomial of degree} \leq m-1\}$
- $K_m = K_\mu$ for all $m \geq \mu$. Moreover, K_μ is invariant under A.
- $dim(K_m) = m$ iff $\mu \geq m$.

Arnoldi's algorithm

➤ Goal: to compute an orthogonal basis of K_m.

➤ Input: Initial vector v_1, with $\|v_1\|_2 = 1$ and m.

ALGORITHM : 1 . *Arnoldi's procedure*

For $j = 1, ..., m$ *do*
  Compute $w := Av_j$
  For $i = 1, \ldots, j$, *do* $\begin{cases} h_{i,j} := (w, v_i) \\ w := w - h_{i,j}v_i \end{cases}$
  $h_{j+1,j} = \|w\|_2$;
  $v_{j+1} = w/h_{j+1,j}$
End

➤ Based on Gram-Schmidt procedure

Result of Arnoldi's algorithm

Let: $\overline{H}_m = \begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \\ & x & x & x & x \\ & & x & x & x \\ & & & x & x \\ & & & & x \end{pmatrix}$, $H_m = \begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \\ & x & x & x & x \\ & & x & x & x \\ & & & x & x \end{pmatrix}$

Results:

1. $V_m = [v_1, v_2, ..., v_m]$ orthonormal basis of K_m.
2. $AV_m = V_{m+1}\overline{H}_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T$
3. $V_m^T A V_m = H_m \equiv \overline{H}_m -$ last row.

Application to eigenvalue problems

- Write approximate eigenvector as $\tilde{u} = V_m y$
- Galerkin condition:

$$(A - \tilde{\lambda} I) V_m y \perp \mathcal{K}_m \quad \rightarrow \quad V_m^H (A - \tilde{\lambda} I) V_m y = 0$$

- Approximate eigenvalues are eigenvalues of H_m

$$H_m y_j = \tilde{\lambda}_j y_j$$

- Associated approximate eigenvectors are

$$\tilde{u}_j = V_m y_j$$

- Typically a few of the outermost eigenvalues will converge first.

Hermitian case: The Lanczos Algorithm

- The Hessenberg matrix becomes tridiagonal :

$$A = A^H \quad \text{and} \quad V_m^H A V_m = H_m \quad \rightarrow H_m = H_m^H$$

- Denote H_m by T_m and $\bar{H}_m$ by $\bar{T}_m$. We can write

$$T_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & & \beta_m & \alpha_m \end{pmatrix}$$

- Relation $AV_m = V_{m+1}\overline{T_m}$

- Consequence: three term recurrence

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

ALGORITHM : 2. *Lanczos*

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

Hermitian matrix + Arnoldi $\rightarrow$ Hermitian Lanczos

- In theory v_i's defined by 3-term recurrence are orthogonal.
- However: in practice severe loss of orthogonality;

Observation [Paige, 1981]: Loss of orthogonality starts suddenly, when the first eigenpair has converged. It is a sign of loss of linear independence of the computed eigenvectors. When orthogonality is lost, then several the copies of the same eigenvalue start appearing.

Reorthogonalization

- Full reorthogonalization – reorthogonalize v_{j+1} against all previous v_i's every time.
- Partial reorthogonalization – reorthogonalize v_{j+1} against all previous v_i's only when needed [Parlett & Simon]
- Selective reorthogonalization – reorthogonalize v_{j+1} against computed eigenvectors [Parlett & Scott]
- No reorthogonalization – Do not reorthogonalize - but take measures to deal with 'spurious' eigenvalues. [Cullum & Willoughby]

Lanczos Bidiagonalization

- We now deal with rectangular matrices. Let $A \in \mathbb{R}^{m\times n}$.

ALGORITHM : 3 . *Golub-Kahan-Lanczos*

1. *Choose an initial* v_1 *with* $\|v_1\|_2 = 1$;
   Set $\beta_0 \equiv 0, u_0 \equiv 0$
2. *For* $k = 1, \ldots, p$ *Do:*
3. $\quad \hat{u} := Av_k - \beta_{k-1}u_{k-1}$
4. $\quad \alpha_k = \|\hat{u}\|_2 \,; \qquad u_k = \hat{u}/\alpha_k$
5. $\quad \hat{v} = A^T u_k - \alpha_k v_k$
6. $\quad \beta_k = \|\hat{v}\|_2 \,; \qquad v_{k+1} := \hat{v}/\beta_k$
7. *EndDo*

Let:
$$\begin{aligned} V_{p+1} &= [v_1, v_2, \cdots, v_{p+1}] \quad \in \mathbb{R}^{n\times(p+1)} \\ U_p &= [u_1, u_2, \cdots, u_p] \quad \in \mathbb{R}^{m\times p} \end{aligned}$$

Let:
$$B_p = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ & \alpha_2 & \beta_2 & & \\ & & \ddots & \ddots & \\ & & & \ddots & \ddots \\ & & & & \alpha_p \quad \beta_p \end{bmatrix};$$

- $\hat{B}_p = B_p(:, 1:p)$
- $V_p = [v_1, v_2, \cdots, v_p] \in \mathbb{R}^{n\times p}$

Result:

- $V_{p+1}^T V_{p+1} = I$
- $U_p^T U_p = I$
- $AV_p = U_p \hat{B}_p$
- $A^T U_p = V_{p+1} B_p^T$

- Observe that :

$$\begin{aligned} A^T(AV_p) &= A^T(U_p\hat{B}_p) \\ &= V_{p+1}B_p^T\hat{B}_p \end{aligned}$$

- $B_p^T\hat{B}_p$ is a (symmetric) tridiagonal matrix of size $(p+1) \times p$

- Call this matrix $\overline{T_k}$. Then:

$$(A^TA)V_p = V_{p+1}\overline{T_p}$$

- Standard Lanczos relation !
- Algorithm is equivalent to standard Lanczos applied to A^TA.
- Similar result for the u_i's [involves AA^T]

✍1 Work out the details: What are the entries of $\bar{T}_p$ relative to those of B_p?