Numerical Linear Algebra

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Plan

- Day 1: SVD and optimality
- Day 2: LU, QR and linear systems, least-squares
- Day 3: QR alg, SVD alg (and Krylov)
- Day 4: Krylov and RandSVD

References

- Golub-Van Loan (12): Matrix Computations
  - classic, encyclopedic
- Trefethen-Bau (97): Numerical Linear Algebra
  - covers essentials, beautiful exposition
- J. Demmel Applied (97): Numerical Linear Algebra
  - impressive content, some niche
- N. J. Higham (02), Accuracy and Stability of Algorithms
  - bible for stability, conditioning
- Horn and Johnson (12), Matrix Analysis (& topics (86))
  - amazing theoretical treatise, little numerical treatment

Linear algebra review

For $A \in \mathbb{R}^{n\times n}$, (or $\mathbb{C}^{n\times n}$; hardly makes difference)
The following are equivalent (how many can you name?):

1. A is nonsingular.

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The following are equivalent (how many can you name?):

1. A is nonsingular.
2. A is invertible: A^{-1} exists.
3. The map $A : \mathbb{R}^n \to \mathbb{R}^n$ is a bijection.
4. all n eigenvalues of A are nonzero.
5. all n singular values of A are positive.
6. $\mathrm{rank}(A) = n$.
7. the rows of A are linearly independent.
8. the columns of A are linearly independent.
9. $Ax = b$ has a solution for every $b \in \mathbb{C}^n$.
10. A has no nonzero null vector. Neither does A^T.
11. A^*A is positive definite (not just semidefinite).
12. $\det(A) \neq 0$.
13. A^{-1} exists such that $A^{-1}A = AA^{-1} = I_n$.
14. $\ldots$

Important matrices

For square matrices,

- Symmetric: $A_{ij} = A_{ji}$ (Hermitian: $A_{ij} = \bar{A}_{ji}$)
  - symmetric positive (semi)definite $A \succ (\succeq) 0$: symmetric and positive eigenvalues
- Orthogonal: $AA^T = A^T A = I$ (Unitary: $AA^* = A^* A = I$) $\rightarrow$ note $A^T A = I$ implies $AA^T = I$
- Skew-symmetric: $A_{ij} = -A_{ji}$ (skew-Hermitian: $A_{ij} = -\bar{A}_{ji}$)
- Normal: $A^T A = AA^T$
- Tridiagonal: $A_{ij} = 0$ if $|i - j| > 1$
- Triangular: $A_{ij} = 0$ if $i > j$

For (possibly nonsquare) matrices $A \in \mathbb{C}^{m \times n}$, $m \geq n$

- Hessenberg: $A_{ij} = 0$ if $i > j + 1$
- "orthonormal": $A^* A = I_n$,
- sparse: most elements are zero

other structures: Hankel, Toeplitz, circulant, symplectic, ...

SVD: the most important result in NLA

- **Symmetric eigenvalue decomposition**: $A = V\Lambda V^T$
  for symmetric $A \in \mathbb{R}^{n\times n}$, where $V^TV = I_n$, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$.
- **Singular Value Decomposition (SVD)**: $A = U\Sigma V^T$
  for any $A \in \mathbb{R}^{m\times n}$, $m \geq n$. Here $U^TU = V^TV = I_n$,
  $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_n$.

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SVD proof: Take Gram matrix A^TA and its eigendecomposition $A^TA = V\Lambda V^T$. Λ is nonnegative, and $(AV)^T(AV)$ is diagonal, so $AV = U\Sigma$ for some orthonormal U. Right-multiply V^T.

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SVD proof: Take Gram matrix $A^T A$ and its eigendecomposition $A^T A = V\Lambda V^T$. Λ is nonnegative, and $(AV)^T(AV)$ is diagonal, so $AV = U\Sigma$ for some orthonormal U. Right-multiply V^T.

SVD and eigendecomposition

- V eigvecs of $A^T A$
- U eigvecs (for nonzero eigvals) of AA^T (up to sign)
- $\sigma_i = \sqrt{\lambda_i(A^T A)}$
- Jordan-Wieldant matrix $\begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}$: eigvals $\pm\sigma_i(A)$, and $m-n$ copies of 0. Eigvec matrix is $\begin{bmatrix} U & U & U_0 \\ V & -V & 0 \end{bmatrix}$, $A^T U_0 = 0$

Vector norms

For vectors $x = [x_1, \dots, x_n]^T \in \mathbb{C}^n$

- p-norm $\|x\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{1/p}$
  - Euclidean norm=2-norm $\|x\|_2 = \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2}$
  - 1-norm $\|x\|_1 = |x_1| + |x_2| + \cdots + |x_n|$
  - ∞-norm $\|x\|_\infty = \max_i |x_i|$

Inequalities: For $x \in \mathbb{C}^n$,

- $\frac{1}{\sqrt{n}}\|x\|_2 \le \|x\|_\infty \le \|x\|_2$
- $\frac{1}{\sqrt{n}}\|x\|_1 \le \|x\|_2 \le \|x\|_1$
- $\frac{1}{n}\|x\|_1 \le \|x\|_\infty \le \|x\|_1$

$\|\cdot\|_2$ is **unitarily invariant** as $\|Ux\|_2 = \|x\|_2$ for any unitary U and any $x \in \mathbb{C}^n$.

Matrix norms

For matrices $A \in \mathbb{C}^{m\times n}$,

- p-norm $\|A\|_p = \max_x \frac{\|Ax\|_p}{\|x\|_p}$
  - 2-norm=spectral norm(=Euclidean norm) $\|A\|_2 = \sigma_{\max}(A)$ (largest singular value)
  - 1-norm $\|A\|_1 = \max_i \sum_{j=1}^{n} |A_{ji}|$
  - ∞-norm $\|A\|_\infty = \max_i \sum_{j=1}^{n} |A_{ij}|$
- Frobenius norm $\|A\|_F = \sqrt{\sum_i \sum_j |A_{ij}|^2}$ (2-norm of vectorization)
- trace norm=nuclear norm $\|A\|_* = \sum_{i=1}^{\min(m,n)} \sigma_i(A)$

Red: **unitarily invariant** norms $\|A\|_* = \|UA\|_*$

Inequalities: For $A \in \mathbb{C}^{m\times n}$,

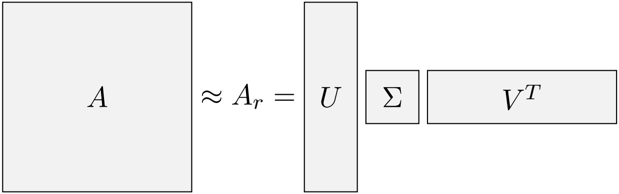
- $\frac{1}{\sqrt{n}}\|A\|_\infty \leq \|A\|_2 \leq \sqrt{m}\|A\|_\infty$
- $\frac{1}{\sqrt{m}}\|A\|_1 \leq \|A\|_2 \leq \sqrt{n}\|A\|_1$
- $\|A\|_2 \leq \|A\|_F \leq \sqrt{\min(m,n)}\|A\|_2$

Optimal low-rank approximation by SVD

Truncated SVD: $A_r = U_r \Sigma_r V_r^T$, $\Sigma_r = \mathrm{diag}(\sigma_1, \ldots, \sigma_r)$

$$\|A - A_r\|_2 = \sigma_{r+1} = \min_{\mathrm{rank}(B)=r} \|A - B\|_2$$

- Storage savings: if $\sigma_{r+1} \ll \sigma_1$, $A \approx A_r$ with



- Optimality holds for any unitarily invariant norm

SVD optimality proof in 2-norm

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- There exists orthogonal $W \in \mathbb{C}^{n\times(n-r)}$ s.t. $BW = 0$. Then $\|A - B\|_2 \ge \|(A-B)W\|_2 = \|AW\|_2 = \|U\Sigma(V^*W)\|_2$.

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- Now since W is $(n-r)$-dimensional, there is is an interesection between W and $[v_1, \ldots, v_{r+1}]$, the $(r+1)$-dimensional subspace spanned by the leading $r+1$ left singular vectors ($[W, v_1, \ldots, v_{r+1}]\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right] = 0$ has a solution; then Wx_1 is such a vector).

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- Then scale x_1 to have unit norm, and $\|U\Sigma V^* W x_1\|_2 = \|U\Sigma_{r+1} y_1\|_2$, where $\|y_1\|_2 = 1$ and Σ_{r+1} is the leading $r+1$ part of Σ. Then $\|U\Sigma_{r+1} y_1\|_2 \geq \sigma_{r+1}$ can be verified directly.

Matrix decompositions

- SVD $A = U\Sigma V^T$
- Eigenvalue decomposition $A = X\Lambda X^{-1}$
  - Normal: X unitary $X^*X = I$
  - Symmetric: X unitary and Λ real
- Jordan decomposition: $A = XJX^{-1}$,
  $J = \text{diag}(\begin{bmatrix} \lambda_i & 1 & & \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix})$
- Schur decomposition $A = QTQ^*$: T upper triangular
- QR: orthonormal, U: upper triangular
- LU: L: lower triangular, U: upper triangular

Red: Orthogonal decompositions, stable computation available

Numerical stability

For computational task $Y = f(X)$ and computed approximant $\hat{Y}$,

- Ideally, error $\|Y - \hat{Y}\|/\|Y\| = O(u)$: seldom true
  (u: unit roundoff, $\approx 10^{-16}$ in standard double precision)
- Good alg. has Backward stability $\hat{Y} = f(X + \Delta X)$, $\frac{\|X - \hat{X}\|}{\|X\|} = O(u)$ "exact solution of slightly wrong input"
- Forward stability $\|Y - \hat{Y}\|/\|Y\| = O(\kappa(f)u)$ "error is as small as backward stable alg." (sometimes used to mean small error; we follow Higham's book [2002])
- Most important condition number:

$$\kappa_2(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)} (\geq 1)$$

  e.g. for linear systems. A backward stable soln for $Ax = b$, i.e., $(A + \Delta A)\hat{x} = (b + \Delta b)$ satisfies

$$\frac{\|\hat{x} - x\|}{\|x\|} \lesssim u\kappa_2(A)$$

LU decomposition

$$A = LU \in \mathbb{R}^{n\times n}$$

L: lower triangular, U: upper triangular

- Cost $\frac{2}{3}n^3$ flops
- For $Ax = b$,
  - first solve $Ly = b$, then $Ux = y$.
  - triangular solve is always backward stable: e.g. $(L + \Delta L)\hat{y} = b$ (see Higham's book)
- Pivoting crucial for numerical stability: $PA = LU$, where P: permutation matrix. Then stability means $\hat{L}\hat{U} = PA + \Delta A$
  - Even with pivoting, unstable examples exist, but still always stable in practice and used everywhere!
- Special case where $A \succ 0$ positive definite: $A = R^T R$, Cholesky factorization, ALWAYS stable, $\frac{1}{3}n^3$ flops

QR decomposition

$$A = QR \in \mathbb{R}^{m \times n}$$

$Q \in \mathbb{R}^{m \times n}$: orthonormal, $R \in \mathbb{R}^{n \times n}$: upper triangular

- Many algorithms available: Gram-Schmidt, Householder, CholeskyQR, ...
- For $Ax = b$,
  - solve $Rx = Q^T b$: always stable! But LU used for speed, as QR needs $\frac{4}{3}n^3$ flops
- Pivoting $A = QRP$ not needed for numerical stability
  - but pivoting gives rank-revealing QR

Householder QR factorization

Householder reflectors:

$$Q = I - 2vv^T, \qquad v = \frac{x - \|x\|_2 e}{\|x - \|x\|_2 e\|_2}$$

satisfies $Qv = e$

$\Rightarrow$ find Q_1 s.t. $Q_1 A(:,1) = e = [1, 0, \ldots,]^T \|A(:,1)\|_2$, repeat to get $Q_n \cdots Q_2 Q_1 A = R$ upper triangular, then $A = (Q_1^T \cdots Q_{n-1}^T Q_n^T) R = QR$

Properties

- Cost $\frac{4}{3}n^3$ flops with Householder-QR (twice that of LU)
- Unconditionally backward stable: $\hat{Q}\hat{R} = A + \Delta A$, $\|\hat{Q}^T \hat{Q} - I\|_2 = O(u)$
- Q_i orthogonal+symmetric, eigvals 1 ($n-1$ copies) and -1

Least-squares problem

$$\min_x \|Ax - b\|_2, \qquad A \in \mathbb{R}^{m\times n}, m \geq n$$

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Let $A = [Q\ Q_\perp]\left[\begin{smallmatrix} R \\ 0 \end{smallmatrix}\right]$ be 'full' QR factorization (useful for theory, seldom used in computation). Then

$$\|Ax - b\|_2 = \|Q^T(Ax - b)\|_2 = \left\| \begin{bmatrix} R \\ 0 \end{bmatrix} x - \begin{bmatrix} Q^T b \\ Q_\perp^T b \end{bmatrix} \right\|_2$$

so $x = R^{-1}Q^T b$ is solution. This also gives algorithm:

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1. Compute (thin) QR factorization $A = QR$
2. Solve linear system $Rx = Q^T b$.

- This is backward stable: computed $\hat{x}$ solution for $\min_x \|(A + \Delta A)x + (b + \Delta b)\|_2$ (see Higham's book Ch.20)
- Mathematically, x satisfies normal equation $(A^T A)x = A^T b$, but this is NOT backward stable

Power method for eigenproblems

$x :=$random vector, $x = Ax$, $x = \frac{x}{\|x\|}$, $\lambda = x^T Ax$, repeat

- Basis for QR algorithm, Krylov methods (Lanczos, Arnoldi,...)
- Convergence analysis: let $x_0 = \sum_{i=1}^n c_i v_i$, $Av_i = \lambda_i v_i$ with $|\lambda_1| > |\lambda_2| > \cdots$. Then after k iterations,

$$x = C \sum_{i=1}^{n} \left(\frac{\lambda_i}{\lambda_1} \right)^k c_i v_i \to C c_1 v_1 \quad \text{as } k \to \infty$$

- Converges geometrically $(\lambda, x) \to (\lambda_1, x_1)$ with **linear rate** $\frac{|\lambda_2|}{|\lambda_1|}$
- What does this imply about $A^n = QR$ as $n \to \infty$?

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Inverse power method: $x := (A - \mu I)x$, $x = x/\|x\|$

- Converges with improved **linear rate** $\frac{|\lambda_{\sigma(2)} - \mu|}{|\lambda_{\sigma(1)} - \mu|}$ to eigval closest to μ (σ: permutation)
- μ can change adaptively with the iterations. The choice $\mu := x^T Ax$ gives Rayleigh quotient iteration, with **quadratic** convergence (cubic if A symmetric)

QR algorithm for eigenproblems

$$A_1 = Q_1 R_1, A_2 = R_1 Q_1, A_2 = Q_2 R_2, A_3 = R_2 Q_2, \ldots$$

- Basically: $QR \to RQ \to QR \to RQ \to \cdots$ **triangular**
- Fundamental work by Francis (61,62) and Kublanovskaya (63)
- Truely Magical algorithm!
  - backward stable, as based on orthogonal transforms
  - always converges, but global proof unavailable(!)
  - uses 'inverse power method' (rational funcs) without inversions

Two techniques to speed up from $> O(n^4)$ to $O(n^3)$

- Initial reduction to Hessenberg form via Unitary transform

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{Q_1}{\to} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix} \overset{Q_2}{\to} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix} \overset{Q_3}{\to} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix}$$

- shift $A_k - s_k I = Q_k R_k$, $A_{k+1} = R_k Q_k + s_k I$, repeat
  (effective choice: $s_k = A_k(n, n)$)

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QR algorithm and power method

QR algorithm: $A_k = Q_k R_k$, $A_{k+1} = R_k Q_k$

$$A^k = (Q_1 \cdots Q_k)(R_k \cdots R_1) = Q^{(k)} R^{(k)}.$$

Proof by induction: Suppose $A^{k-1} = Q^{(k-1)} R^{(k-1)}$. Then $A_k = R_{k-1} Q_{k-1} = (Q^{(k-1)})^* A Q^{(k-1)}$, and

$$(Q^{(k-1)})^* A Q^{(k-1)} = Q_k R_k.$$

Then $AQ^{(k-1)} = Q^{(k-1)} Q_k R_k$, and so

$$A^k = AQ^{(k-1)} R^{(k-1)} = Q^{(k-1)} Q_k R_k R^{(k-1)} = Q^{(k)} R^{(k)} \square$$

Now take inverse: $A^{-k} = (R^{(k)})^{-1} (Q^{(k)})^*$,

Conjugate transpose: $(A^{-k})^* = Q^{(k)} (R^{(k)})^{-*}$

$\Rightarrow$ QR factorization of matrix with eigvals $r(\lambda_i) = \lambda_i^{-k}$

$\Rightarrow$ Connection also with (unshifted) inverse power method

NB no matrix inverse performed

QR algorithm with shifts and shifted inverse power method

1. $A_k - s_k I = Q_k R_k$ (QR factorization)
2. $A_{k+1} = R_k Q_k + s_k I, \quad k \leftarrow k+1$, repeat.

QR algorithm with shifts and shifted inverse power method

1. $A_k - s_k I = Q_k R_k$ (QR factorization)
2. $A_{k+1} = R_k Q_k + s_k I$, $\quad k \leftarrow k+1$, repeat.

$$\prod_{i=1}^{k}(A - s_i I) = Q^{(k)} R^{(k)} \,(= (Q_1 \cdots Q_k)(R_k \cdots R_1))$$

Proof: Suppose true for $k-1$. Then QR alg. computes
$(Q^{(k-1)})^*(A - s_k I)Q^{(k-1)} = Q_k R_k$, so
$(A - s_k I)Q^{(k-1)} = Q^{(k-1)} Q_k R_k$, hence

$$\prod_{i=1}^{k}(A - s_i I) = (A - s_k I)Q^{(k-1)} R^{(k-1)} = Q^{(k-1)} Q_k R_k R^{(k-1)} = Q^{(k)} R^{(k)}.$$

Inverse conjugate transpose: $\prod_{i=1}^{k}(A - s_i I)^{-*} = Q^{(k)}(R^{(k)})^{-*}$

$\Rightarrow$ QR factorization of matrix with eigvals $r(\lambda_j) = \prod_{i=1}^{k} \frac{1}{\bar{\lambda}_j - s_i}$

$\Rightarrow$ Connection with shifted inverse power method, hence

rational approximation

QR algorithm for symmetric A

- Initial reduction to Hessenberg form $\rightarrow$ tridiagonal

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{Q_1}{\rightarrow} \begin{bmatrix} * & * & & & \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix} \overset{Q_2}{\rightarrow} \begin{bmatrix} * & * & & & \\ * & * & * & & \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix} \overset{Q_3}{\rightarrow} \begin{bmatrix} * & * & & & \\ * & * & * & & \\ & * & * & * & \\ & & * & * & * \\ & & & * & * \end{bmatrix}$$

- QR steps for tridiagonal: $O(n)$ instead of $O(n^2)$
- powerful alternatives available for tridiagonal eigenproblem (QR, divide-conquer ([Gu-Eisenstat 95]), HODLR ([Kressner-Susnjara 19], exploit low-rank structure),...)
- Cost: $\frac{4}{3}n^3$ flops for eigvals, $\approx 10n^3$ for eigvecs
- Since I am speaking, also mention spectral divide-and-conquer (w/ Freund, Higham): all about rational approximation

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{V_1}{\rightarrow} \begin{bmatrix} * & * & * & & \\ * & * & * & & \\ * & * & * & & \\ & & & * & * \\ & & & * & * \end{bmatrix} \overset{V_2}{\rightarrow} \begin{bmatrix} * & & & & \\ & * & * & & \\ & * & * & & \\ & & & * & \\ & & & & * \end{bmatrix} \overset{V_3}{\rightarrow} \begin{bmatrix} * & & & & \\ & * & & & \\ & & * & & \\ & & & * & \\ & & & & * \end{bmatrix} = \Lambda.$$

Golub-Kahan for SVD

Apply Householder reflectors from left and right (different ones) to **bidiagonalize**

$$A \to B$$

$$A \overset{H_{L,1}}{\to} \begin{bmatrix} \star & \star & \star & \star \\ & \star & \star & \star \\ & \star & \star & \star \\ & \star & \star & \star \\ & \star & \star & \star \end{bmatrix} \overset{H_{R,1}}{\to} \begin{bmatrix} \star & \star & & \\ & \star & \star & \star \\ & \star & \star & \star \\ & \star & \star & \star \\ & \star & \star & \star \end{bmatrix} \overset{H_{L,2}}{\to} \begin{bmatrix} \star & \star & & \\ & \star & \star & \star \\ & & \star & \star \\ & & \star & \star \\ & & \star & \star \end{bmatrix} \overset{H_{R,2}}{\to} \begin{bmatrix} \star & \star & & \\ & \star & \star & \\ & & \star & \star \\ & & \star & \star \\ & & \star & \star \end{bmatrix} \overset{H_{L,3}}{\to} \begin{bmatrix} \star & \star & & \\ & \star & \star & \\ & & \star & \star \\ & & & \star \\ & & & \star \end{bmatrix} \overset{H_{L,4}}{\to} B,$$

- Once bidiagonalized,
  - Mathematically, QR on $B^T B$
  - More elegant: dqds algorithm [Fernando-Parlett 1994]
- Cost: $\approx 4mn^2$ flops for singvals Σ, $\approx 20mn^2$ flops for singvecs U, V

Polynomial rootfinding $p(x) = 0$ via eigenvalues

- $p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$
  $p(\lambda) = 0 \Leftrightarrow \lambda$ eigenvalue of

$$C = \begin{bmatrix} -a_{n-1} & -a_{n-2} & \dots & -a_1 & -a_0 \\ 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & 0 \end{bmatrix} \in \mathbb{C}^{n \times n}$$

- $\tilde{p}(x) = T_n(x) + a_{n-1}T_{n-1}(x) + \cdots + a_1 T_1(x) + a_0 T_0(x)$,
  $T_i(x)$: Chebyshev polynomial. $\tilde{p}(\lambda) = 0 \Leftrightarrow \lambda$ eigenvalue of

$$\tilde{C} = \frac{1}{2} \begin{bmatrix} -a_{n-1} & 1 - a_{n-2} & -a_{n-3} & \cdots & -a_0 \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 2 & 0 \end{bmatrix} \in \mathbb{C}^{n \times n}$$

Powerful approach for nonlinear problems: **approximate with polynomial, and solve eigenproblem**

Exotic but tractable eigenvalue problems

- Standard eigenvalue problem $Ax = \lambda x$
  - A symmetric: tridiagonal QR algorithm
  - nonsymmetric: Hessenberg QR algorithm
  - QZ algorithm: QR applied to $B^{-1}A$ implicitly
- Polynomial eigenvalue problem $P(\lambda)x = 0$, e.g. $P(\lambda) = \lambda^2 A + \lambda B + C$
  - usually linearization + QZ
    $$\begin{bmatrix} -B & -C \\ I & 0 \end{bmatrix} \begin{bmatrix} \lambda x \\ x \end{bmatrix} = \lambda \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \lambda x \\ x \end{bmatrix}$$

All these are tractable! $O(n^3)$ cost (or $O((nd)^3)$, d: degree) or less

- Nonlinear eigenvalue problem: $F(\lambda)x = 0$, e.g. $F(\lambda) = \exp(\lambda)A + \log(\lambda)B + C$
  - usually: local approximation $F(\lambda) \approx P(\lambda)$ +linearization+QZ

Krylov subspace methods

Idea: find solution $\hat{x}$ in subspace

$$\mathcal{K}_k(A,b) := \text{span}([b, Ab, A^2b, \ldots, A^{k-1}b]).$$

equivalent to $\hat{x} = p_{k-1}(A)b$, p_{k-1} : polynomial of degree $k-1$

Why should it work?

- For eigenproblems $Ax = \lambda x$, when looking for dominant eigvals
  - or better yet, work with $(A-\mu I)^{-1}$: shift-invert Arnoldi
- For linear systems $Ax = b$, fast convergence roughly when $\kappa_2(A) = O(1)$
- Very useful to understand from polynomial(/rational) approximation viewpoint: $x \approx \hat{x} = p_{k-1}(A)b$

Arnoldi process

Denote by $Q \in \mathbb{C}^{n\times k}$ orthonormal that spans $(k = 1, 2, \ldots)$

$$\mathcal{K}_k(A, b) := \mathrm{span}([b, Ab, A^2b, \ldots, A^{k-1}b])$$

(note $Q(:, 1) = b/\|b\|_2$). Then consider matrix AQ. Careful consideration reveals identity

$$AQ = QH + q_{k+1}[0, \ldots, 0, h_{k+1,k}],$$

where H is upper Hessenberg

- ith column yields $Aq_i = \sum_{j=1}^{i} H_{ji}q_j + H_{i+1,i}q_{j+1}$: obtain H_{ji} by orthogonalization (Householder or Gram-Schmidt)
- far superior (in stability) to forming matrix $[b, Ab, A^2b, \ldots, A^{k-1}b]$ then computing QR

Lanczos

When A symmetric, Arnoldi simplifies to

$$AQ = QT + q_{k+1}[0, \ldots, 0, h_{k+1,k}],$$

where T is tridiagonal

- three-term recurrence, orthogonalize necessary only against past two vecs q_i, q_{i-1}

Lanczos' algorithm for symmetric eigenproblem:

- Conceptually, find Q and do **Rayleigh-Ritz**: compute eigvals of $Q^T AQ$: projection method
- We actually have $Q^T AQ = T$, tridiagonal eigenproblem

GMRES for $Ax = b$

Conceptually, solve

$$\min_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

Given $AQ = QH + q_{k+1} h_{k+1,k} e_{k+1}$ where $e_{k+1} := [0, \ldots, 0, h_{k+1,k}]$, equivalent to (same trick as in least-squares)

$$\begin{aligned} \min_y \|AQy - b\|_2 &= \min_y \|(QH + q_{k+1} h_{k+1,k} e_{k+1})y - b\|_2 \\ &= \min_y \left\| \begin{bmatrix} H \\ h_{k+1,k} e_{k+1} \end{bmatrix} y - \begin{bmatrix} Q^T \\ q_{k+1}^T \end{bmatrix} b \right\|_2 \end{aligned}$$

Solve final problem via QR (Givens rotations)+triangular solve, $O(n^2)$

GMRES convergence

Recall that $x \in \mathcal{K}_k(A, b) \Rightarrow x = p_{k-1}(A)b$. Hence GMRES solution is

$$\begin{aligned} \min_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2 &= \min_{p_{k-1} \in \mathcal{P}_{k-1}} \|Ap_{k-1}(A)b - b\|_2 \\ &= \min_{\tilde{p} \in \mathcal{P}_k, \tilde{p}(0)=0} \|(\tilde{p}(A) - I)b\|_2 \\ &= \min_{p \in \mathcal{P}_k, p(0)=1} \|p(A)b\|_2 \end{aligned}$$

If A diagonalizable $A = X\Lambda X^{-1}$,

$$\begin{aligned} \|p(A)\|_2 = \|Xp(\Lambda)X^{-1}\|_2 &\leq \|X\|_2\|X^{-1}\|_2\|p(\Lambda)\|_2 \\ &= \kappa_2(X) \max_{z \in \lambda(A)} |p(z)| \end{aligned}$$

Interpretation: find polynomial s.t. $p(0) = 1$ and $|p(\lambda_i)|$ small (demo)

CG, MINRES

When A symmetric, Lanczos gives $AQ = QT + q_{k+1}[0, \ldots, 0, 1]$,
T: tridiagonal

- CG: when $A \succ 0$, solve $Q^T(AQy - b) = 0, x = Qy$
  $\rightarrow$"Galerkin orthogonality": residual orthogonal to Q
  - three-term recurrence reduces cost to $O(k)$ A-matmuls
  - minimizes A-norm of error $x_k = \text{argmin}_{x \in Q} \|x - x_*\|_A$

  $$\begin{aligned}(x - x_*)^T A(x - x_*) &= (Qy - x_*)^T A(Qy - x_*) \\ &= y^T(Q^T AQ)y - 2b^T Qy + b^T x_*,\end{aligned}$$

  minimizer is $y = (Q^T AQ)^{-1} Q^T b$, so $Q^T(AQy - b) = 0$

- MINRES: symmetric (indefinite) version of GMRES
  - again, three-term recurrence, $O(k)$ A-matmuls

Preconditioning for GMRES, CG etc

$$Ax = b$$

Instead find $M \approx A^{-1}$ and solve

$$MAx = Mb$$

Desiderata of M:

- M simple enough s.t. lin. systems $Mx = b$ easy
- MA has clustered eigenvalues
- Finding effective preconditioners is never-ending research topic Andy Wathen is our Oxford expert!

Randomized SVD

[Halko, Martinsson, Tropp 2011]

(i) Generate a random matrix $\Omega \in \mathbb{R}^{n\times(r+\ell)}$, where ℓ is a small integer (say 5).
(ii) Compute $A\Omega$ and its QR factorization $A\Omega = QR$.
(iii) Compute Q^TA and its SVD $Q^TA = \tilde{U}\hat{\Sigma}\hat{V}^T$.
(iv) Take $\hat{U} = Q\tilde{U}$, and let $\hat{U}_r, \hat{\Sigma}_r, \hat{V}_r$ be the leading r parts of $\hat{U}, \hat{\Sigma}, \hat{V}_r$ respectively. Output $\hat{A}_r = \hat{U}_r\hat{\Sigma}_r\hat{V}_r^T$ as a rank-r approximant to A.

Approximation quality:

$$\mathbb{E}[\|A - \hat{A}_r\|_F] \leq \sqrt{1 + \frac{r}{\ell - 1}}\|A - A_r\|_F$$

Optimal up to $\sqrt{1 + \frac{r}{\ell-1}} = O(1)$

Understanding randomized SVD

Want $\|A - QQ^TA\|_F/\|A - A_r\|_F = O(1)$, where $A\Omega = QR$,

$$A\Omega = U\begin{bmatrix}\Sigma_1 V_1^T\Omega \\ \Sigma_2 V_2^T\Omega\end{bmatrix}, \qquad \Sigma_1 = \mathrm{diag}(\sigma_1, \dots, \sigma_r)$$

- $V_1^T\Omega$: $r \times (r+\ell)$ rectangular Gaussian, so *well-conditioned*, so w.h.p. $\|(V_1^T\Omega)^\dagger\| = O(1)$ ($X^\dagger$: pseudoinverse)
- Hence
$$A\Omega(\Sigma_1 V_1^T\Omega)^\dagger = U\begin{bmatrix} I \\ F\end{bmatrix}, \quad F = \Sigma_2 V_2^T\Omega(V_1^T\Omega)^\dagger\Sigma_1^{-1}$$
- Note $\|(I - QQ^T)A\|_F^2 = \|A\|_F^2 - \|Q^TA\|_F^2$
- Take $\tilde{Q} := A\Omega(\Sigma_1 V_1^T\Omega)^\dagger = U\begin{bmatrix} I \\ F\end{bmatrix}(I + F^TF)^{-1/2}$. Then

$$\begin{aligned}\|Q^TA\|_F^2 &\geq \|\tilde{Q}^TA\|_F^2 \geq \|(I+F^TF)^{-1/2}\Sigma_1\|_F^2 = \mathrm{Tr}(\Sigma_1(I+F^TF)^{-1}\Sigma_1) \\ &\geq \mathrm{Tr}(\Sigma_1(I - F^TF)\Sigma_1) = \|\Sigma_1\|_F^2 - \|\Sigma_2 V_2^T\Omega(V_1^T\Omega)^\dagger\|_F^2 \\ &= \|\Sigma_1\|_F^2 - \|\Sigma_2 M\|_F^2, \quad \|M\| = O(1)\end{aligned}$$

- Thus $\|(I - QQ^T)A\|_F^2 \leq \|\Sigma_2 M\|_F^2 = O(\|\Sigma_2\|_F^2)$

Important (N)LA topics not treated

- tensors
- FFT (values$\leftrightarrow$coefficients) for polynomials
- sparse direct solvers
- multigrid
- functions of matrices
- generalized, polynomial eigenvalue problems
- perturbation theory
- compressed sensing
- model order reduction
- communication-avoiding algorithms
- differential equations, optimisation, machine learning,... LA is everywhere in applied maths!

Eigenvalue perturbation theory

- first-order eigenvalue perturbation: $Ax = \lambda x$, $y^T A = \lambda y^T$, λ simple then

$$\lambda(A + \epsilon E) = \epsilon \frac{y^T E x}{y^T x} + O(\epsilon^2)$$

- Weyl's theorem: A, E symmetric then

$$\lambda_i(A) + \lambda_i(A + E) \leq \lambda_i(A) + \|E\|_2$$

- Davis-Kahan: A symmetric, $Ax_i = \lambda_i x_i$, $(A + E)\hat{x}_i = \hat{\lambda}_i \hat{x}_i$, $gap_i := \min_j |\lambda_i - \lambda_j|$

$$\sin \angle(x_i, \hat{x}_i) \leq \frac{\|E\|}{gap_i}$$

Sherman–Morrison(-Woodbury) formula

A: $n \times n$ invertible, U, V: $n \times k$, $k < (\ll) n$. Then

$$(A + UV^T)^{-1} = A^{-1} - A^{-1}U(I_k + V^T A^{-1} U)^{-1} V^T A^{-1}$$

- Low-rank update of A^{-1}

Similar updates possible for QR, (SVD), ...