C6.1 Numerical Linear Algebra

- **SVD** and its properties, applications
- **Direct methods** for linear systems and least-squares problems
- **Direct methods** for eigenvalue problems
- **Iterative** (Krylov subspace) methods for linear systems
- **Iterative** (Krylov subspace) methods for eigenvalue problems
- **Randomised algorithms** for SVD and least-squares

References

- Trefethen-Bau (97): Numerical Linear Algebra
  - covers essentials, beautiful exposition
- Golub-Van Loan (12): Matrix Computations
  - classic, encyclopedic
- Horn and Johnson (12): Matrix Analysis (& topics (86))
  - excellent theoretical treatise, little numerical treatment
- J. Demmel (97): Applied Numerical Linear Algebra
  - impressive content, some niche
- N. J. Higham (02): Accuracy and Stability of Algorithms
  - bible for stability, conditioning
- H. C. Elman, D. J. Silvester, A. J. Wathen (14): Finite elements and fast iterative solvers
  - PDE applications of linear systems, preconditioning

What is numerical linear algebra?

The study of numerical algorithms for problems involving matrices

Two main (only!?) problems:

1. Linear system

$$Ax = b$$

2. Eigenvalue problem

$$Ax = \lambda x$$

λ: eigenvalue (eigval), x: eigenvector (eigvec)

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1. Linear system

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2. Eigenvalue problem

$$Ax = \lambda x$$

λ: eigenvalue (eigval), x: eigenvector (eigvec)

3. SVD (singular value decomposition)

$$A = U\Sigma V^T$$

U, V: orthonormal/orthogonal, Σ diagonal

Why numerical linear algebra?

- Many (in fact most) problems in scientific computing (and even machine learning) boil down to a linear problem
  - Because that's often the only way to deal with the scale of problems we face today! (and in future)
  - For linear problems, so much is understood and reliable algorithms available
- $Ax = b$: e.g. Newton's method for $F(x) = 0$, $F : \mathbb{R}^n \to \mathbb{R}^n$ nonlinear
  1. start with initial guess $x^{(0)} \in \mathbb{R}^n$
  2. find Jacobian matrix $J \in \mathbb{R}^{n \times n}$, $J_{ij} = \frac{\partial F_i(x)}{\partial x_j}|_{x=x^{(0)}}$
  3. update $x^{(1)} := x^{(0)} - J^{-1}F(x^{(0)})$, repeat
- $Ax = \lambda x$: e.g. Principal component analysis (PCA), data compression, Schrödinger eqn., Google pagerank,
- Other sources: differential equations, optimisation, regression, data analysis, ...

Basic 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. ...

Structured matrices

For square matrices,

- Symmetric: $A = A^T$, i.e. $A_{ij} = A_{ji}$ (Hermitian: $A_{ij} = \bar{A_{ji}}$) has eigenvalue decomposition $A = V\Lambda V^T$, V orthogonal, $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$.
  - 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, ...

Vector norms

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

- 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 $\|x\|_\infty = \max_i |x_i|$

Norm axioms

- $\|\alpha x\| = |\alpha| \|x\|$ for any $\alpha \in \mathbb{C}$
- $\|x\| \geq 0$ and $\|x\| = 0 \Leftrightarrow x = 0$
- $\|x + y\| \leq \|x\| + \|y\|$

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

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

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

Cauchy-Schwarz inequality

For any $x, y \in \mathbb{R}^n$,

$$|x^T y| \leq \|x\|_2 \|y\|_2$$

Proof:

- For any scalar c, $\|x - cy\|^2 = \|x\|^2 - 2cx^T y + c^2 \|y\|^2$.
- This is minimised w.r.t. c at $c = \frac{x^T y}{\|y\|^2}$ with minimiser $\|x\|^2 - \frac{(x^T y)^2}{\|y\|^2}$.
- Since the minimal value must be ≥ 0, the CS inequality follows.

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 (=operator norm) $\|A\|_2 = \sigma_{\max}(A)$ (largest singular value)
  - 1-norm $\|A\|_1 = \max_i \sum_{j=1}^{m} |A_{ji}|$
  - ∞-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 $\|A\| = \|UAV\|$ for any unitary (or orthogonal) U, V

Norm axioms hold for each. Inequalities: For $A \in \mathbb{C}^{m\times n}$, (exercise)

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

Subspaces and orthonormal matrices

Subspace $\mathcal{S}$ of $\mathbb{R}^n$: vectors of form $\sum_{i=1}^{d} c_i v_i$, $c_i \in \mathbb{R}$

- $v_1, \ldots, v_d$ are **basis vectors**, linearly independent
- $x \in \mathcal{S} \Leftrightarrow \sum_{i=1}^{d} c_i v_i$
- d is the *dimension* of $\mathcal{S}$

Representation: $\mathcal{S} = \text{span}(V)$ (i.e., $x \in \mathcal{S} \Leftrightarrow x = Vc$), or just V; often convenient if $V (= Q)$ is orthonormal

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Lemma

$\mathcal{S}_1 = \text{span}(V_1)$ and $\mathcal{S}_2 = \text{span}(V_2)$ where $V_1 \in \mathbb{R}^{n \times d_1}$ and $V_2 \in \mathbb{R}^{n \times d_2}$, with $d_1 + d_2 > n$. Then $\exists x \neq 0$ in $\mathcal{S}_1 \cap \mathcal{S}_2$, i.e., $x = V_1 c_1 = V_2 c_2$ for some vectors c_1, c_2.

Proof: Let $M := [V_1, V_2]$, of size $n \times (d_1 + d_2)$. Since $d_1 + d_2 > n$ by assumption, M has a right null vector. $Mc = 0$. Write $c = \begin{bmatrix} c_1 \\ -c_2 \end{bmatrix}$.

Some useful results

- $(AB)^T = B^T A^T$
- If A, B invertible, $(AB)^{-1} = B^{-1}A^{-1}$
- If A, B square and $AB = I$, then $BA = I$
- $\begin{bmatrix} I_m & X \\ 0 & I_n \end{bmatrix}^{-1} = \begin{bmatrix} I_m & -X \\ 0 & I_n \end{bmatrix}$
- Neumann series: if $\|X\| < 1$ in any norm,

$$(I - X)^{-1} = I + X + X^2 + X^3 + \cdots$$

- Trace $\mathrm{Trace}(A) = \sum_{i=1}^{n} A_{i,i}$ (sum of diagonals, $A \in \mathbb{R}^{m \times n}$). For any X, Y s.t. $\mathrm{Trace}(XY) = \mathrm{Trace}(YX)$. For $B \in \mathbb{R}^{m \times n}$, we have $\|B\|_F^2 = \sum_i \sum_j |B_{ij}|^2 = \mathrm{Trace}(B^T B)$.
- Triangular structure is invariant under addition, multiplication, and inversion
- Symmetry is invariant under addition and inversion, *but not multiplication*; AB usually not symmetric even if A, B are

SVD: the most important matrix decomposition

- **Symmetric eigenvalue decomposition**: $A = V\Lambda V^T$
  for symmetric $A \in \mathbb{R}^{n\times n}$, where $V^TV = I_n$, $\Lambda = \mathsf{diag}(\lambda_1, \ldots, \lambda_n)$.
- **Singular Value Decomposition (SVD)**: $A = U\Sigma V^T$
  for any $A \in \mathbb{R}^{m\times n}$, $m \geq n$. Here $U^TU = V^TV = I_n$, $\Sigma = \mathsf{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

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Terminologies:

- σ_i: *singular values* of A.
- *rank*(A): number of positive singular values.
- The columns of U: the *left singular vectors*, columns of V: *right singular vectors*

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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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Full SVD: $A = U \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} V^T$ where $U \in \mathbb{R}^{m\times m}$ orthogonal

Example: computation

Let $A = \begin{bmatrix} -1 & -2 \\ 2 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$. To compute the SVD,

1. Compute the Gram matrix $A^TA = \begin{bmatrix} 6 & 4 \\ 4 & 6 \end{bmatrix}$.
2. $\lambda(A^TA) = \{10, 2\}$ (e.g. via characteristic polynomial). The eigvec matrix is $V = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$ (e.g. via the null vectors of $A - \lambda I$). So $A^TA = V\Sigma^2V^T$ where $\Sigma = \begin{bmatrix} \sqrt{10} & \\ & \sqrt{2} \end{bmatrix}$.
3. Let $U = AV\Sigma^{-1} = \begin{bmatrix} -3/\sqrt{20} & -1/2 \\ 3/\sqrt{20} & -1/2 \\ 1/\sqrt{20} & -1/2 \\ 1/\sqrt{20} & 1/2 \end{bmatrix}$, which is orthonormal. Thus $A = U\Sigma V^T$.

rank, column/row space, etc

From the SVD one gets

- rank r of $A \in \mathbb{R}^{m \times n}$: number of nonzero singular values $\sigma_i(A)$ (=# linearly indep. columns, rows)
  - We can always write $A = \sum_{i=1}^{\text{rank}(A)} \sigma_i u_i v_i^T$.
- column space (linear subspace spanned by vectors Ax): span of $U = [u_1, \ldots, u_r]$
- row space: row span of $v_1^T, \ldots, v_r^T$
- null space: $v_{r+1}, \ldots, v_n$

SVD and eigenvalue decomposition

- V eigvecs of $A^T A$
- U eigvecs (for nonzero eigvals) of AA^T (up to sign)
- $\sigma_i = \sqrt{\lambda_i(A^T A)}$
- Think of eigenvalues vs. SVD of symmetric matrices, unitary, skew-symmetric, normal matrices, triangular,...
- Jordan-Wieldant matrix $\left[\begin{smallmatrix} 0 & A \\ A^T & 0 \end{smallmatrix}\right]$: eigvals $\pm\sigma_i(A)$, and $m - n$ copies of 0. Eigvec matrix is $\left[\begin{smallmatrix} U & U & U_\perp \\ V & -V & 0 \end{smallmatrix}\right]$, $A^T U_\perp = 0$

Uniqueness etc

- U, V (clearly) not unique: ± 1 multiplication possible (but be careful—not arbitarily)
- When multiple singvals exist $\sigma_i = \sigma_{i+1}$, more degrees of freedom
- Extreme example: what is the SVD(s) of an orthogonal matrix?

Recap: spectral norm of matrix

$$\|A\|_2 = \max_x \frac{\|Ax\|_2}{\|x\|_2} = \max_{\|x\|_2=1} \|Ax\|_2 = \sigma_1(A)$$

Proof: Use SVD

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Proof: Use SVD

$$\begin{aligned}
\|Ax\|_2 &= \|U\Sigma V^T x\|_2 \\
&= \|\Sigma V^T x\|_2 \quad \text{by unitary invariance} \\
&= \|\Sigma y\|_2 \quad \text{with } \|y\|_2 = 1 \\
&= \sqrt{\sum_{i=1}^n \sigma_i^2 y_i^2} \\
&\leq \sqrt{\sum_{i=1}^n \sigma_1^2 y_i^2} = \sigma_1 \|y\|_2^2 = \sigma_1.
\end{aligned}$$

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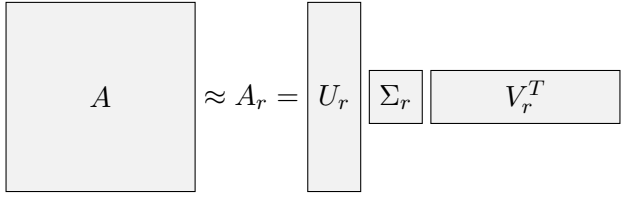
\end{aligned}$$

Frobenius norm: $\|A\|_F = \sqrt{\sum_i \sum_j |A_{ij}|^2} = \sqrt{\sum_{i=1}^n (\sigma_i(A))^2}$ (exercise)

Low-rank approximation of a matrix

Given $A \in \mathbb{R}^{m \times n}$, find A_r such that



- Storage savings (data compression)

Optimal low-rank approximation by SVD

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

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

$$A = \underbrace{\begin{bmatrix} * \\ * \\ \vdots \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & \cdots & * & * \end{bmatrix}}_{\sigma_1 u_1 v_1} + \underbrace{\begin{bmatrix} * \\ * \\ \vdots \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & \cdots & * & * \end{bmatrix}}_{\sigma_2 u_2 v_2} + \cdots + \underbrace{\begin{bmatrix} * \\ * \\ \vdots \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & \cdots & * & * \end{bmatrix}}_{\sigma_n u_n v_n},$$

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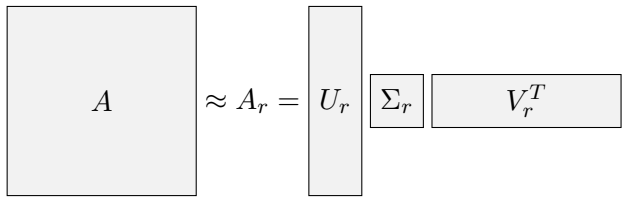
- Good approximation if $\sigma_{r+1} \ll \sigma_1$:



- Optimality holds for any unitarily invariant norm
- Prominent application: PCA
- Many matrices have explicit or hidden low-rank structure (nonexaminable)

SVD optimality proof in spectral norm

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

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- Now since W is $(n-r)$-dimensional, there is an intersection 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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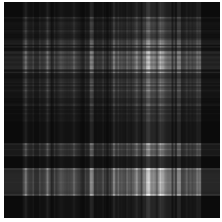
- Then scale x_1, x_2 to have unit norm, and $\|U\Sigma V^T W x_1\|_2 = \|U_{r+1}\Sigma_{r+1} x_2\|_2$, Where U_{r+1}, Σ_{r+1} are leading $r+1$ parts of U, Σ. Then $\|U_{r+1}\Sigma_{r+1} y_1\|_2 \geq \sigma_{r+1}$ can be verified directly.

Low-rank approximation: image compression

grayscale image=matrix

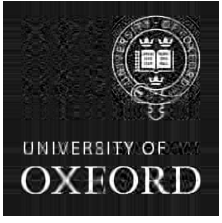
original



rank 1

rank 5

rank 10



rank 20

rank 50

Courant-Fischer minmax theorem

ith largest eigval λ_i of symmetric/Hermitian A is (below $x \neq 0$)

$$\lambda_i(A) = \max_{\dim \mathcal{S}=i} \min_{x \in \mathcal{S}} \frac{x^T A x}{x^T x} \quad \left(= \min_{\dim \mathcal{S}=n-i+1} \max_{x \in \mathcal{S}} \frac{x^T A x}{x^T x} \right)$$

Analogously, for any rectangular $A \in \mathbb{C}^{m \times n} (m \geq n)$, we have

$$\sigma_i(A) = \max_{\dim \mathcal{S}=i} \min_{x \in \mathcal{S}} \frac{\|Ax\|_2}{\|x\|_2} \quad \left(= \min_{\dim \mathcal{S}=n-i+1} \max_{x \in \mathcal{S}} \frac{\|Ax\|_2}{\|x\|_2} \right).$$

- $\min_{x \in \mathcal{S}, \|x\|_2=1} \|Ax\|_2 = \min_{Q^T Q = I_i, \|y\|_2=1} \|AQy\|_2 = \sigma_{\min}(AQ) = \sigma_i(AQ)$, where $\text{span}(Q) = \mathcal{S}$.
- C-F says $\sigma_i(A)$ is maximum possible value over all subspaces $\mathcal{S}$ of dimension i.

Courant-Fischer minmax theorem

ith largest eigval λ_i of symmetric/Hermitian A is (below $x \neq 0$)

$$\lambda_i(A) = \max_{\dim \mathcal{S}=i} \min_{x \in \mathcal{S}} \frac{x^T A x}{x^T x} \quad \left(= \min_{\dim \mathcal{S}=n-i+1} \max_{x \in \mathcal{S}} \frac{x^T A x}{x^T x} \right) \tag{1}$$

Analogously, for any rectangular $A \in \mathbb{C}^{m \times n} (m \geq n)$, we have

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Proof for (2):

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ith largest eigval λ_i of symmetric/Hermitian A is (below $x \neq 0$)

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Proof for (2):

1. Fix S and let $V_i = [v_i, \ldots, v_n]$. We have $\dim(\mathcal{S}) + \dim(\text{span}(V_i)) = i + (n - i + 1) = n + 1$, so $\exists$intersection $w \in S \cap V_i$, $\|w\|_2 = 1$.

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2. For this w, $\|Aw\|_2 = \|\text{diag}(\sigma_i, \ldots, \sigma_n)(V_i^T w)\|_2 \leq \sigma_i$; thus $\sigma_i(A) \geq \min_{x \in \mathcal{S}} \frac{\|Ax\|_2}{\|x\|_2}$.

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2. For this w, $\|Aw\|_2 = \|\text{diag}(\sigma_i, \ldots, \sigma_n)(V_i^T w)\|_2 \leq \sigma_i$; thus $\sigma_i(A) \geq \min_{x \in \mathcal{S}} \frac{\|Ax\|_2}{\|x\|_2}$.
3. For the reverse inequaltiy, take $S = [v_1, \ldots, v_i]$, for which $w = v_i$.

Weyl's inequality

ith largest eigval λ_i of symmetric/Hermitian A is (below $x \neq 0$)

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Analogously, for any rectangular $A \in \mathbb{C}^{m \times n} (m \geq n)$, we have

$$\sigma_i(A) = \max_{\dim \mathcal{S}=i} \min_{x \in \mathcal{S}} \frac{\|Ax\|_2}{\|x\|_2} \quad \left(= \min_{\dim \mathcal{S}=n-i+1} \max_{x \in \mathcal{S}} \frac{\|Ax\|_2}{\|x\|_2} \right).$$

Corollary: Weyl's inequality (Proof: exercise)

- for singular values
  - $\sigma_i(A + E) \in \sigma_i(A) + [-\|E\|_2, \|E\|_2]$
  - Special case: $\|A\|_2 - \|E\|_2 \leq \|A + E\|_2 \leq \|A\|_2 + \|E\|_2$
- for symmetric eigenvalues $\lambda_i(A + E) \in \lambda_i(A) + [-\|E\|_2, \|E\|_2]$

Singvals and symmetric eigvals are insensitive to perturbation (well conditioned).

Nonsymmetric eigvals are different!

Eigenvalues of nonsymmetric matrices are sensitive

Consider eigenvalues of a Jordan block and its perturbation

$$J = \begin{bmatrix} 1 & 1 & & \\ & 1 & \ddots & \\ & & \ddots & 1 \\ & & & 1 \end{bmatrix} \in \mathbb{R}^{n \times n}, \quad J + E = \begin{bmatrix} 1 & 1 & & \\ & 1 & \ddots & \\ & & \ddots & 1 \\ \epsilon & & & 1 \end{bmatrix}$$

$\lambda(J) = 1$ (n copies), but $|\lambda(J + E) - 1| \approx \epsilon^{1/n}$

More applications of C-F

- $\sigma_i \left(\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \right) \geq \max(\sigma_i(A_1), \sigma_i(A_2))$

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  Proof (sketch): LHS $= \max_{\dim \mathcal{S}=i} \min_{x\in\mathcal{S}, \|x\|_2=1} \left\| \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} x \right\|_2$, and for any x,

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- $\sigma_i(\begin{bmatrix} A_1 & A_2 \end{bmatrix}) \geq \max(\sigma_i(A_1), \sigma_i(A_2))$

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  $\left\| \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} x \right\|_2 \geq \max(\|A_1 x\|_2, \|A_2 x\|_2)$.

- $\sigma_i(\begin{bmatrix} A_1 & A_2 \end{bmatrix}) \geq \max(\sigma_i(A_1), \sigma_i(A_2))$

  Proof: LHS $= \max_{\dim \mathcal{S}=i} \min_{\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]\in\mathcal{S}, \left\|\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]\right\|_2=1} \left\| \begin{bmatrix} A_1 & A_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|_2$, while

  $\sigma_i(A_1) =$

  $\max_{\dim \mathcal{S}=i, \text{range}(\mathcal{S})\in\text{range}(\begin{bmatrix} I_n \\ 0 \end{bmatrix})} \min_{\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]\in\mathcal{S}, \left\|\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]\right\|_2=1} \left\| \begin{bmatrix} A_1 & A_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|_2$.

  Since the latter maximises over a smaller $\mathcal{S}$, the former is at least as big.

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 $A = QTQ^*$: Q orthogonal, T upper triangular
- QR: Q orthonormal, U upper triangular
- LU: L lower triangular, U upper triangular

Red: Orthogonal decompositions, stable computation available

Solving $Ax = b$ via LU decomposition

If $A = LU$ is available

solving $Ax = b$ can be done as follows:

1. Solve $Ly = b$ for y,
2. solve $Ux = y$ for x.

Each is a **triangular** system, which is easy to solve via forward (or backward) substitution for $Ly = b$ ($Ux = y$).

LU decomposition

Let $A \in \mathbb{R}^{n \times n}$. Suppose we can decompose (or factorise)

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = \begin{bmatrix} * & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & \\ * & * & * & * & * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & & * \end{bmatrix} = LU$$

L: lower triangular, U: upper triangular. How to find L, U?

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L: lower triangular, U: upper triangular. How to find L, U?

$$A = \begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix} + \begin{bmatrix} & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{L_1 U_1} + \underbrace{\begin{bmatrix} 0 \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} 0 & * & * & * & * \end{bmatrix}}_{L_2 U_2} + \begin{bmatrix} & & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix} = \cdots$$

LU decomposition cont'd

First step:

$$A = \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{L_1 U_1} + \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}$$

algorithm:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & & & & \\ A_{31} & & & & \\ A_{41} & & & & \\ A_{51} & & & & \end{bmatrix} = \begin{bmatrix} L_{11} & & & & \\ L_{21} & & & & \\ L_{31} & & & & \\ L_{41} & & & & \\ L_{51} & & & & \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} & U_{14} & U_{15} \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} + \begin{bmatrix} & & & & \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 1 & & & & \\ A_{21}/a & & & & \\ A_{31}/a & & & & \\ A_{41}/a & & & & \\ A_{51}/a & & & & \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}}_{=L_1 U_1 \quad (a=A_{11})} + \begin{bmatrix} & & & & \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$$

LU decomposition cont'd 2

$$A = \begin{bmatrix}*\\*\\*\\*\\*\end{bmatrix}\begin{bmatrix}* & * & * & * & *\end{bmatrix} + \begin{bmatrix}0\\*\\*\\*\\*\end{bmatrix}\begin{bmatrix}0 & * & * & * & *\end{bmatrix} + \begin{bmatrix}0\\0\\*\\*\\*\end{bmatrix}\begin{bmatrix}0 & 0 & * & * & *\end{bmatrix} + \begin{bmatrix}0\\0\\0\\*\\*\end{bmatrix}\begin{bmatrix}0 & 0 & 0 & * & *\end{bmatrix} + \begin{bmatrix}0\\0\\0\\0\\*\end{bmatrix}\begin{bmatrix}0 & 0 & 0 & 0 & *\end{bmatrix}$$

$$= \quad L_1U_1 \quad + \quad L_2U_2 \quad + \quad L_3U_3 \quad + \quad L_4U_4 \quad + \quad L_5U_5$$

$$= [L_1, L_2, \ldots, L_5]\begin{bmatrix}U_1\\U_2\\\vdots\\U_5\end{bmatrix} = \begin{bmatrix}* & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & \\ * & * & * & * & *\end{bmatrix}\begin{bmatrix}* & * & * & * & *\\ & * & * & * & *\\ & & * & * & *\\ & & & * & *\\ & & & & *\end{bmatrix}$$

(note: nonzero structure crucial in final equality)

Solving $Ax = b$ via LU

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

L: lower triangular, U: upper triangular

- Cost $\frac{2}{3}n^3$ flops (floating-point operations)
- For $Ax = b$,
  - *first solve* $Ly = b$, *then* $Ux = y$. Then $b = Ly = LUx = Ax$.
  - 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

LU decomposition with pivots

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & & & & \\ A_{31} & & & & \\ A_{41} & & & & \\ A_{51} & & & & \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ A_{21}/a & & & & \\ A_{31}/a & & & & \\ A_{41}/a & & & & \\ A_{51}/a & & & & \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} + \begin{bmatrix} & & & & \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$$

Trouble if $a = A_{11} = 0$! e.g. no LU for $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ solution: pivot, permute rows s.t. largest entry of first (active) column is at top. $\Rightarrow PA = LU$, P: permutation matrix

- $PA = LU$ exists for any nonsingular A (exercise)
- for $Ax = b$, solve $LUx = P^T b$
- the nonzero structure of L_i, U_i is preserved under P
- cost still $\frac{2}{3}n^3 + O(n^2)$

Cholesky factorisation for $A \succ 0$

If $A \succ 0$ (symmetric positive definite (S)PD$\Leftrightarrow \lambda_i(A) > 0$), two simplifications:

- We can take $U_i = L_i^T =: R_i$ by symmetry $\Rightarrow \frac{1}{3}n^3$ flops
- No pivot needed

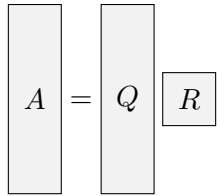
$$A = \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{R_1 R_1^T} + \underbrace{\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}}_{\text{also PD}}$$

Notes:

- diag(R) no longer 1's
- A can be written as $A = R^T R$ for some $R \in \mathbb{R}^{n \times n}$ iff $A \succeq 0$ ($\lambda_i(A) \geq 0$)
- Indefinite case: when $A = A^*$ but A not PD, $\exists\ A = LDL^*$ where D diagonal (when $A \in \mathbb{R}^{n \times n}$, D can have 2×2 diagonal blocks), L has 1's on diagonal

QR factorisation

For any $A \in \mathbb{C}^{m \times n}$, $\exists$ factorisation



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

- Many algorithms available: Gram-Schmidt, Householder, CholeskyQR, ...
- various applications: least-squares, orthogonalisation, computing SVD, manifold retraction...
- With Householder, pivoting $A = QRP$ not needed for numerical stability
  - but pivoting gives rank-revealing QR (nonexaminable)

QR via Gram-Schmidt

Gram-Schmidt: Given $A = [a_1, a_2, \ldots, a_n] \in \mathbb{R}^{m \times n}$ (assume full rank $\text{rank}(A) = n$), find orthonormal $[q_1, \ldots, q_n]$ s.t. $\text{span}(q_1, \ldots, q_n) = \text{span}(a_1, \ldots, a_n)$

G-S process: $q_1 = \frac{a_1}{\|a_1\|}$, then $\tilde{q}_2 = a_2 - q_1 q_1^T a_2$, $q_2 = \frac{\tilde{q}_2}{\|\tilde{q}_2\|}$,
repeat for $j = 3, \ldots, n$: $\tilde{q}_j = a_j - \sum_{i=1}^{j-1} q_i q_i^T a_j$, $q_j = \frac{\tilde{q}_j}{\|\tilde{q}_j\|}$.

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This gives QR! Let $r_{ij} = q_i^T a_j$ $(i \neq j)$ and $r_{jj} = \|a_j - \sum_{i=1}^{j-1} r_{ij} q_i\|$,

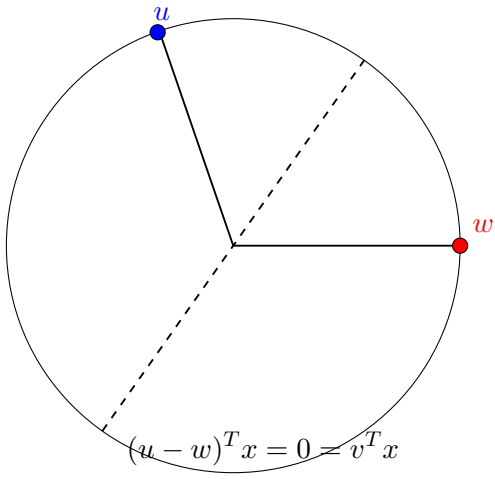
$$
\begin{aligned}
q_1 &= \frac{a_1}{r_{11}} \\
q_2 &= \frac{a_2 - r_{12} q_1}{r_{22}} \\
q_j &= \frac{a_j - \sum_{i=1}^{j-1} r_{ij} q_i}{r_{jj}}
\end{aligned}
\quad \Leftrightarrow \quad
\begin{aligned}
a_1 &= r_{11} q_1 \\
a_2 &= r_{12} q_1 + r_{22} q_2 \\
a_j &= r_{1j} q_1 + r_{2j} q_2 + \cdots + r_{jj} q_j
\end{aligned}
\quad \Leftrightarrow \quad
\boxed{A} = \boxed{Q}\,\boxed{R}
$$

- But this isn't the recommended way to do QR; numerically unstable

Householder reflectors

$$H = I - 2vv^T, \qquad \|v\| = 1$$

- H orthogonal and symmetric: $H^T H = H^2 = I$, eigvals 1 ($n-1$ copies) and -1 (1 copy)
- For any given $u, w \in \mathbb{R}^n$ s.t. $\|u\| = \|w\|$ and $u \neq v$, $H = I - 2vv^T$ with $v = \frac{w-u}{\|w-u\|}$ gives $Hu = w$ ($\Leftrightarrow u = Hw$, thus 'reflector')
- We'll use this mostly for $w = [*, 0, 0, \ldots, 0]^T$



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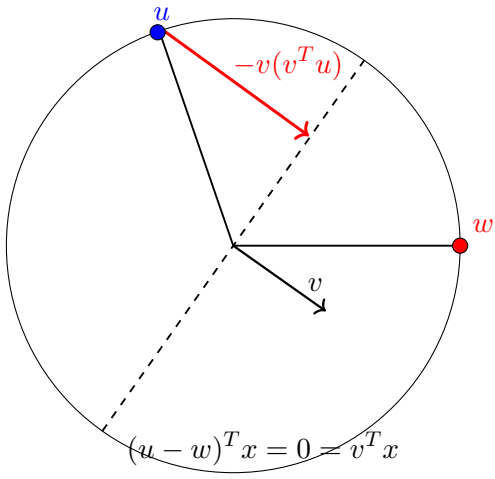


Householder reflectors for QR

Householder reflectors:

$$H = I - 2vv^T, \qquad v = \frac{x - \|x\|_2 e}{\|x - \|x\|_2 e\|_2}, \qquad e = [1, 0, \ldots, 0]^T$$

satisfies $Hx = [\|x\|, 0, \ldots, 0]^T$

Householder reflectors for QR

Householder reflectors:

$$H = I - 2vv^T, \qquad v = \frac{x - \|x\|_2 e}{\|x - \|x\|_2 e\|_2}, \qquad e = [1, 0, \ldots, 0]^T$$

satisfies $Hx = [\|x\|, 0, \ldots, 0]^T$

$\Rightarrow$ To do QR, find H_1 s.t. $H_1 a_1 = \begin{bmatrix} \|a_1\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$,

repeat to get $H_n \cdots H_2 H_1 A = R$ upper triangular, then
$A = (H_1 \cdots H_{n-1} H_n) R = QR$

Householder QR factorisation, diagram

$$A = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}$$

Apply sequence of Householder reflectors

$$H_1 A = (I - 2v_1 v_1^T)A = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \end{bmatrix}, \qquad H_2 H_1 A = (I - 2v_2 v_2^T)H_1 A = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & * & * \\ & & * & * \end{bmatrix},$$

$$H_3 H_2 H_1 A = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \\ & & & * \end{bmatrix}, \qquad H_n \cdots H_3 H_2 H_1 A = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \\ & & & \end{bmatrix},$$

Note $v_k = [\underbrace{0, 0, \ldots, 0}_{k-1 \text{ 0's}}, *, *, \ldots, *]^T$

Householder QR factorisation, example

$$A = \begin{bmatrix} 0.302 & -0.629 & 2.178 & 0.164 \\ 0.400 & -1.204 & 1.138 & 0.748 \\ -0.930 & -0.254 & -2.497 & -0.273 \\ -0.177 & -1.429 & 0.441 & 1.576 \\ -2.132 & -0.021 & -1.398 & -0.481 \\ 1.145 & -0.561 & -0.255 & 0.328 \end{bmatrix}$$

Householder QR factorisation, example

$$H_1 A = \begin{bmatrix} 2.647 & -0.295 & 2.284 & 0.652 \\ 0 & -1.261 & 1.120 & 0.665 \\ 0 & -0.121 & -2.455 & -0.080 \\ 0 & -1.403 & 0.449 & 1.613 \\ 0 & 0.283 & -1.301 & -0.038 \\ 0 & -0.724 & -0.307 & 0.090 \end{bmatrix}$$

Householder QR factorisation, example

$$H_2 H_1 A = \begin{bmatrix} 2.647 & -0.295 & 2.284 & 0.652 \\ 0 & 2.044 & -0.925 & -1.550 \\ 0 & 0 & -2.530 & -0.161 \\ 0 & 0 & -0.419 & 0.673 \\ 0 & 0 & -1.126 & 0.152 \\ 0 & 0 & -0.755 & -0.395 \end{bmatrix}$$

Householder QR factorisation, example

$$H_3H_2H_1A = \begin{bmatrix} 2.647 & -0.295 & 2.284 & 0.652 \\ 0 & 2.044 & -0.925 & -1.550 \\ 0 & 0 & 2.901 & 0.087 \\ 0 & 0 & 0 & 0.692 \\ 0 & 0 & 0 & 0.203 \\ 0 & 0 & 0 & -0.361 \end{bmatrix}$$

Householder QR factorisation, example

$$H_4H_3H_2H_1A = \begin{bmatrix} 2.647 & -0.295 & 2.284 & 0.652 \\ 0 & 2.044 & -0.925 & -1.550 \\ 0 & 0 & 2.901 & 0.087 \\ 0 & 0 & 0 & 0.806 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} R \\ 0 \end{bmatrix}$$

Householder QR factorisation

$$H_n \cdots H_2 H_1 A = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \\ & & & \end{bmatrix} = \begin{bmatrix} R \\ 0 \end{bmatrix}$$

$\Leftrightarrow A = (H_1^T \cdots H_{n-1}^T H_n^T) \begin{bmatrix} R \\ 0 \end{bmatrix} =: Q_F \begin{bmatrix} R \\ 0 \end{bmatrix}$ (**full** QR; Q_F is square orthogonal)

Writing $Q_F = [Q\ Q_\perp]$ where $Q \in \mathbb{R}^{m \times n}$ orthonormal, $A = QR$ (**'thin'** QR or just QR)

Properties

- Cost $\frac{4}{3}n^3$ flops with Householder-QR (twice that of LU)
- Unconditionally backward stable: $\hat{Q}\hat{R} = A + \Delta A$, $\|\hat{Q}^T\hat{Q} - I\|_2 = \epsilon$ (next lec)
- Constructive proof for $A = QR$ existence
- To solve $Ax = b$, solve $Rx = Q^T b$ via triangle solve.
  $\rightarrow$ Excellent method, but twice slower than LU (so rarely used)

Givens rotation

$$G = \begin{bmatrix} c & s \\ -s & c \end{bmatrix}, \quad c^2 + s^2 = 1$$

Designed to 'zero' one element at a time. E.g. QR for upper Hessenberg matrix

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix}, \quad G_1 A = \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix}, \quad G_2 G_1 A = \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix},$$

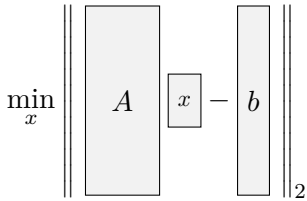
$$G_3 G_2 G_1 A = \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & * & * \end{bmatrix}, \quad G_4 G_3 G_2 G_1 A = \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & & * \end{bmatrix} =: R$$

$\Leftrightarrow A = G_1^T G_2^T G_3^T G_4^T R$ is the QR factorisation.

- G acts locally on two rows (two columns if right-multiplied)
- Non-neighboring rows/cols allowed

Least-squares problem

Given $A \in \mathbb{R}^{m \times n}, m \geq n$ and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ s.t.



- More data than degrees of freedom
- 'Overdetermined' linear system; $Ax = b$ usually impossible
- Thus minimise $\|Ax - b\|$; usually $\|Ax - b\|_2$ but sometimes e.g. $\|Ax - b\|_1$ of interest (we focus on $\|Ax - b\|_2$)
- Assume full rank $\text{rank}(A) = n$; this makes solution unique

Least-squares problem via QR

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

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Let $A = [Q\ Q_\perp]\begin{bmatrix} R \\ 0 \end{bmatrix} = Q_F \begin{bmatrix} R \\ 0 \end{bmatrix}$ be 'full' QR factorization. Then

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

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

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1. Compute **thin** QR factorization $A = QR$
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so $x = R^{-1}Q^T b$ is the solution. This also gives algorithm:

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)
- Unlike square system $Ax = b$, one really needs QR: LU won't do the job

Normal equation: Cholesky-based least-squares solver

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

$x = R^{-1}Q^T b$ is the solution $\Leftrightarrow$ x solution for $n \times n$ **normal equation**

$$(A^T A)x = A^T b$$

- $A^T A \succeq 0$ (always) and $A^T A \succ 0$ if rank$(A) = n$; then PD linear system; use Cholesky to solve.
- Fast! but NOT backward stable; $\kappa_2(A^T A) = (\kappa_2(A))^2$ where $\kappa_2(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$ **condition number** (next lecture)

Application: regression/function approximation

Given function $f : [-1, 1] \to \mathbb{R}$,

Consider approximating via polynomial $f(x) \approx p(x) = \sum_{i=0} c_i x^i$.

Very common technique: **Regression**

1. Sample f at points $\{z_i\}_{i=1}^m$, and
2. Find coefficients c defined by Vandermonde system $Ac \approx f$,

$$\begin{bmatrix} 1 & z_1 & \cdots & z_1^n \\ 1 & z_2 & \cdots & z_2^n \\ \vdots & \vdots & & \vdots \\ 1 & z_m & \cdots & z_m^n \end{bmatrix} \begin{bmatrix} c_0 \\ \vdots \\ c_n \end{bmatrix} \approx \begin{bmatrix} f(z_1) \\ f(z_2) \\ \vdots \\ f(z_m) \end{bmatrix}.$$

- Numerous applications, e.g. in statistics, numerical analysis, approximation theory, data analysis!

Numerical stability

Question: Can a computed result trusted?

e.g. is $Ax = b$ always solved correctly via the LU algorithm?

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- The situation is complicated. For example, let $A = U\Sigma V^T$, where $U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$, $\Sigma = \begin{bmatrix} 1 & \\ & 10^{-15} \end{bmatrix}$, $V = I$, and let $b = A\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ (i.e., $x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$).

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  In MATLAB, $\texttt{x} = \texttt{A}\backslash\texttt{b}$ outputs $\begin{bmatrix} 1.0000 \\ 0.94206 \end{bmatrix}$

- Did something go wrong?

  NO—this is a ramification of ill-conditioning, not instability
- In fact, $\|\texttt{Ax} - \texttt{b}\|_2 (= \|A\hat{x} - b\|_2) \approx 10^{-16}$

(After this section, make sure you can explain what happened above!)

Floating-point arithmetic

- Computers store number in base 2 with finite/fixed memory (bits)
- Irrational numbers are stored inexactly, e.g. $1/3 \approx 0.333...$
- Calculations are rounded to nearest floating-point number (rounding error)
- Thus the accuracy of the final error is nontrivial

Two examples with MATLAB

- $((\texttt{sqrt}(2))^2 - 2) * \texttt{1e15} = 0.4441$ (should be 0..)
- $\sum_{n=1}^{\infty} \frac{1}{n} \approx 30$ (should be ∞..)

An important (but not main) part of numerical analysis/NLA is to study the effect of rounding errors

Best reference: Higham's book (2002)

Conditioning and stability

- Conditioning is the sensitivity of a problem (e.g. of finding $y = f(x)$ given x) to perturbation in inputs, i.e., how large $\kappa := \sup_{\delta x} \|f(x + \delta x) - f(x)\|/\|\delta x\|$ is in the limit $\delta x \to 0$.
  (this is *absolute* condition number; equally important is *relative* condition number $\kappa_r := \lim_{\|\delta x\|_2 \to 0} \sup_{\delta x} \frac{\|f(x+\delta x)-f(x)\|}{\|f(x)\|} / \frac{\|\delta x\|}{\|x\|}$)

- (Backward) Stability is a property of an algorithm, which describes if the computed solution $\hat{y}$ is a 'good' solution, in that it is an exact solution of a nearby input, that is, $\hat{y} = f(x + \Delta x)$ for a small Δx.

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If problem is ill-conditioned $\kappa \gg 1$, then blame the problem not the algorithm

Notation/convention: $\hat{x}$ denotes a computed approximation to x (e.g. of $x = A^{-1}b$)
ϵ denotes a small term $O(u)$, on the order of unit roundoff/working precision; so we write e.g. $u, 10u, (m + n)u, mnu$ all as ϵ

- Consequently (in this lecture/discussion) norm choice does not matter today

Numerical stability: backward stability

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

- Ideally, error $\|Y - \hat{Y}\|/\|Y\| = \epsilon$: seldom true
  (u: unit roundoff, $\approx 10^{-16}$ in standard double precision)
- Good alg. has Backward stability $\hat{Y} = f(X + \Delta X)$, $\frac{\|\Delta X\|}{\|X\|} = \epsilon$ "exact solution of slightly wrong input "

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- Justification: **Input (matrix) is usually inexact anyway!** $f(X + \Delta X)$ is just as good at $f(X)$ at approximating $f(X_*)$ where $\|\Delta X\| = O(\|X - X_*\|)$
  We shall 'settle with' such solution, though it may not mean $\hat{Y} - Y$ is small

- 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])

Backward stable+well conditioned=accurate solution

Suppose

- $Y = f(X)$ computed backward stably i.e., $\hat{Y} = f(X + \Delta X)$, $\|\Delta X\| = \epsilon$.

Then with conditioning $\kappa = \lim_{\|\delta x\|_2 \to 0} \sup_{\delta x} \frac{\|f(X) - f(X+\Delta X)\|}{\|\Delta X\|}$,

$$\|\hat{Y} - Y\| \lesssim \kappa\epsilon$$

(relative version possible)

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(relative version possible) 'proof':

$$\|\hat{Y} - Y\| = \|f(X + \Delta X) - f(X)\| \lesssim \kappa\|\Delta X\|\|f(X)\| = \kappa\epsilon$$

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If well-conditioned $\kappa = O(1)$, good accuracy! Important examples:

- Well-conditioned linear system $Ax = b$, $\kappa_2(A) \approx 1$
- Eigenvalues of symmetric matrices (via Weyl's bound $\lambda_i(A + E) \in \lambda_i(A) + [-\|E\|_2, \|E\|_2]$)
- Singular values of any matrix $\sigma_i(A + E) \in \sigma_i(A) + [-\|E\|_2, \|E\|_2]$

Note: eigvecs/singvecs can be highly ill-conditioned

Matrix condition number

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

e.g. for linear systems. (when A is $m \times n (m > n)$, $\kappa_2(A) = \frac{\sigma_1(A)}{\sigma_n(A)}$) A backward stable soln for $Ax = b$, s.t. $(A + \Delta A)\hat{x} = b$ satisfies, assuming backward stability $\|\Delta A\| \leq \epsilon \|A\|$ and $\kappa_2(A) \ll \epsilon^{-1}$ (so $\|A^{-1}\Delta A\| \ll 1$),

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

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'proof': By Neumann series

$$(A + \Delta A)^{-1} = (A(I + A^{-1}\Delta A))^{-1} = (I - A^{-1}\Delta A + O(\|A^{-1}\Delta A\|^2))A^{-1}$$

So $\hat{x} = (A + \Delta A)^{-1}b = A^{-1}b - A^{-1}\Delta A A^{-1}b + O(\|A^{-1}\Delta A\|^2) =$
$x - A^{-1}\Delta A x + O(\|A^{-1}\Delta A\|^2)$, Hence

$$\|x - \hat{x}\| \lesssim \|A^{-1}\Delta A x\| \leq \|A^{-1}\|\|\Delta A\|\|x\| \leq \epsilon \|A\|\|A^{-1}\|\|x\| = \epsilon \kappa_2(A)\|x\|$$

Backward stability of triangular systems

Recall $Ax = b$ via $Ly = b$, $Ux = y$ (triangular systems).

The computed solution $\hat{x}$ for a (upper/lower) triangular linear system $Rx = b$ solved via back/forward substitution is backward stable, i.e., it satisfies

$$(R + \Delta R)\hat{x} = b, \qquad \|\Delta R\| = O(\epsilon\|R\|).$$

Proof: Trefethen-Bau or Higham (nonexaminable but interesting)

- backward error can be bounded componentwise
- this means $\|\hat{x} - x\|/\|x\| \leq \epsilon\kappa_2(R)$
  - (unavoidably) poor worst-case (and attainable) bound when ill-conditioned
  - often better with triangular systems

(In)stability of $Ax = b$ via LU with pivots

Fact (proof nonexaminable): Computed $\hat{L}\hat{U}$ satisfies $\frac{\|\hat{L}\hat{U}-A\|}{\|L\|\|U\|} = \epsilon$

(note: not $\frac{\|\hat{L}\hat{U}-A\|}{\|A\|} = \epsilon$)

- If $\|L\|\|U\| = O(\|A\|)$, then $(L + \Delta L)(U + \Delta U)\hat{x} = b$
  $\Rightarrow \hat{x}$ backward stable solution (exercise)

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Question: Does $LU = A + \Delta A$ or $LU = PA + \Delta A$ with $\|\Delta A\| = \epsilon\|A\|$ hold?

Without pivot ($P = I$): $\|L\|\|U\| \gg \|A\|$ unboundedly (e.g. $\left[\begin{smallmatrix} \epsilon & 1 \\ 1 & 1 \end{smallmatrix}\right]$) unstable

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With pivots:

- Worst-case: $\|L\|\|U\| \gg \|A\|$ grows exponentially with n, unstable
  - growth governed by that of $\|L\|\|U\|/\|A\| \Rightarrow \|U\|/\|A\|$
- In practice (average case): perfectly stable
  - Hence this is how $Ax = b$ is solved, despite alternatives with guaranteed stability exist (but slower; e.g. via SVD, or QR (next))

Resolution/explanation: among biggest open problems in numerical linear algebra!

Examples of stability and instability

Forthcoming examples: nonexaminable

Stability of Cholesky for $A \succ 0$

Cholesky $A = R^T R$ for $A \succ 0$

- succeeds without pivot (active matrix is always positive definite)
- R never contains entries $> \sqrt{\|A\|_2}$

$$A = \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{R_1 R_1^T} + \underbrace{\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}}_{\text{also PSD}}$$

(exercise: show $\|R_1\|_2 \leq \sqrt{\|A\|_2}$)

$\Rightarrow$ backward stable! Hence positive definite linear system $Ax = b$ stable via Cholesky

(In)stability of Gram-Schmidt

- Gram-Schmidt is subtle
  - plain (classical) version: $\|\hat{Q}^T\hat{Q} - I\| \leq \epsilon(\kappa_2(A))^2$
  - modified Gram-Schmidt (orthogonalise 'one vector at a time'): $\|\hat{Q}^T\hat{Q} - I\| \leq \epsilon\kappa_2(A)$
  - Gram-Schmidt twice (G-S again on computed $\hat{Q}$): $\|\hat{Q}^T\hat{Q} - I\| \leq \epsilon$

Matrix multiplication is not backward stable

Shock! It is not always true that $fl(AB)$ equal to $(A + \Delta A)(B + \Delta B)$ for small $\Delta A, \Delta B$

- Vec-vec mult. backward stable: $fl(y^T x) = (y + \Delta y)(x + \Delta x)$; in fact $fl(y^T x) = (y + \Delta y)x$.
- Hence mat-vec also backward stable: $fl(Ax) = (A + \Delta A)x$.
- Still mat-mat is not backward stable.

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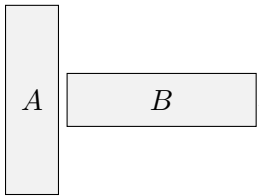
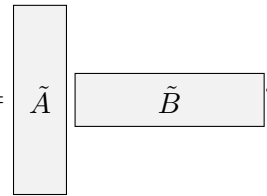
$AB =$  $fl(AB) = AB + \epsilon =$ 

??

with $\tilde{A} = A + \epsilon\|A\|$, $\tilde{B} = B + \epsilon\|B\|$? No—e.g., $fl(AB)$ is usually not low rank

Matrix multiplication is not backward stable

Shock! It is not always true that $fl(AB)$ equal to $(A + \Delta A)(B + \Delta B)$ for small $\Delta A, \Delta B$

- Vec-vec mult. backward stable: $fl(y^T x) = (y + \Delta y)(x + \Delta x)$; in fact $fl(y^T x) = (y + \Delta y)x$.
- Hence mat-vec also backward stable: $fl(Ax) = (A + \Delta A)x$.
- Still mat-mat is not backward stable.

What **is** true: $\|fl(AB) - AB\| \leq \epsilon \|A\| \|B\|$, so $\|fl(AB) - AB\|/\|AB\| \leq \epsilon \min(\kappa_2(A), \kappa_2(B))$.

- Great when A or B orthogonal (or square well-conditioned): say if $A = Q$ orthogonal,

$$\|fl(QB) - QB\| \leq \epsilon \|B\|,$$

so $fl(QB) = QB + \epsilon \|B\|$, hence $fl(QB) = Q(B + \Delta B)$ where $\Delta B = Q^T \epsilon \|B\|$

orthogonal multiplication is backward stable

Stability of Householder QR

With Householder QR, the computed $\hat{Q}, \hat{R}$ satisfy

$$\|\hat{Q}^T\hat{Q} - I\| = O(\epsilon), \quad \|A - \hat{Q}\hat{R}\| = O(\epsilon\|A\|),$$

and (of course) R upper triangular.

Rough proof

- Each reflector orthogonal, so satisfies $fl(H_iA) = H_iA + \epsilon_i\|A\|$
- Hence $(\hat{R} =) fl(H_n \cdots H_1 A) = H_n \cdots H_1 A + \epsilon\|A\|$
- $fl(H_n \cdots H_1) =: \hat{Q}^T = H_n \cdots H_1 + \epsilon$,
- Thus $\hat{Q}\hat{R} = A + \epsilon\|A\|$

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- $fl(H_n \cdots H_1) =: \hat{Q}^T = H_n \cdots H_1 + \epsilon$,
- Thus $\hat{Q}\hat{R} = A + \epsilon\|A\|$

Notes:

- This doesn't mean $\|\hat{Q} - Q\|, \|\hat{R} - R\|$ are small at all! Indeed Q, R are as ill-conditioned as A
- QR for $Ax = b$, least-squares are stable (NB normal eqn $A^TAx =$ is NOT)

Orthogonal Linear Algebra

With orthogonal matrices Q,

$$\frac{\|fl(QA) - QA\|}{\|QA\|} \leq \epsilon, \qquad \frac{\|fl(AQ) - AQ\|}{\|AQ\|} \leq \epsilon$$

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$\|fl(AB) - AB\| / \|AB\| \leq \epsilon \min(\kappa_2(A), \kappa_2(B))$

Hence algorithms involving ill-conditioned matrices are unstable (e.g. eigenvalue decomposition of non-normal matrices, Jordan form, etc), whereas those based on orthogonal matrices are stable, e.g.

- Householder QR factorisation
- **QR algorithm** for $Ax = \lambda x$
- **Golub-Kahan** algorithm for $A = U \Sigma V^T$
- **QZ algorithm** for $Ax = \lambda B x$

We next turn to the algorithms in boldface

Key points on stability

- Definition: (backward) stability vs. conditioning
- Orthogonal linear algebra is backward stable

- Significance of $\kappa_2(A) = \|A\|_2\|A^{-1}\|$
- Stable operations: triangular systems, Cholesky,...

Eigenvalue problem $Ax = \lambda x$

First of all, $Ax = \lambda x$ no explicit solution (neither λ nor x); huge difference from $Ax = b$ for which $x = A^{-1}b$

- Eigenvalues are roots of characteristic polynomial
- For any polynomial p, $\exists$ (infinitely many) matrices whose eigvals are roots of p

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- Eigenvalues are roots of characteristic polynomial
- For any polynomial p, $\exists$ (infinitely many) matrices whose eigvals are roots of p
- Let $p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$, $a_i \in \mathbb{C}$. Then $p(\lambda) = 0 \Leftrightarrow \lambda$ eigenvalue of

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

Eigenvalue problem $Ax = \lambda x$

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- Eigenvalues are roots of characteristic polynomial
- For any polynomial p, $\exists$ (infinitely many) matrices whose eigvals are roots of p
- So no finite-step algorithm exists for $Ax = \lambda x$

Eigenvalue algorithms are necessarily iterative and approximate

- Same for SVD, as $\sigma_i(A) = \sqrt{\lambda_i(A^T A)}$
- But this doesn't mean they're inaccurate!

Usual goal: compute the Schur decomposition $A = UTU^*$: U unitary, T upper triangular

- For normal matrices $A^*A = AA^*$, automatically diagonalised (T diagonal)
- For nonnormal A, if diagonalisation $A = X\Lambda X^{-1}$ really necessary, done via Sylvester equations but nonorthogonal/unstable (nonexaminable)

Schur decomposition

Let $A \in \mathbb{C}^{n \times n}$ (square arbitrary matrix). Then $\exists$ unitary $U \in \mathbb{C}^{n \times n}$ s.t.

$$A = UTU^*,$$

with T upper triangular.

- $\text{eig}(A) = \text{eig}(T) = \text{diag}(T)$
- T diagonal iff A normal $A^*A = AA^*$

Proof:

Schur decomposition

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- T diagonal iff A normal $A^*A = AA^*$

Proof: Let $Av = \lambda_1 v$ and find $U_1 = [v_1, V_\perp]$ unitary. Then

$AU_1 = U_1 \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix} \Leftrightarrow U_1^* A U_1 = \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$. Repeat on the lower-right $(n-1)\times(n-1)$ part to get $U_{n-1}^* U_{n-2}^* \dots U_1^* A U_1 U_2 \dots U_{n-1} = T$.

Recap: 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** $A = QTQ^*$: Q orthogonal, T upper triangular
- QR: Q orthonormal, U upper triangular
- LU: L lower triangular, U upper triangular

Red: Orthogonal decompositions, stable computation available

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- **Schur decomposition** $A = QTQ^*$: Q orthogonal, T upper triangular
- QR: Q orthonormal, U upper triangular
- LU: L lower triangular, U upper triangular
- QZ for $Ax = \lambda Bx$: (genearlised eigenvalue problem) Q, Z orthogonal s.t. QAZ, QBZ are both upper triangular

Red: Orthogonal decompositions, stable computation available

Power method for $Ax = \lambda x$

$x \in \mathbb{R}^n$:=random vector, $x = Ax$, $x = \frac{x}{\|x\|}$, $\hat{\lambda} = x^T Ax$, repeat

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- Convergence analysis: suppose A is diagonalisable (generic assumption). We can write $x_0 = \sum_{i=1}^n c_i v_i$, $Av_i = \lambda_i v_i$ 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 $(\lambda, x) \to (\lambda_1, v_1)$ with **linear rate** $\frac{|\lambda_2|}{|\lambda_1|}$
- What does this imply about $A^k = QR$ as $k \to \infty$? First vector of $Q \to v_1$

Power method for $Ax = \lambda x$

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Notes:

- Google pagerank & Markov chain linked to power method
- As we'll see, power method is basis for refined algs (QR algorithm, Krylov methods (Lanczos, Arnoldi,...))

Why compute eigenvalues? Google PageRank

'Importance' of websites via dominant eigenvector of column-stochastic matrix

$$A = \alpha P + (1-\alpha)\begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix}$$

P: adjacency matrix, $\alpha \in (0,1)$

image from wikipedia

Google does (did) a few steps of Power method: with initial guess x_0, $k = 0, 1, \ldots$

1. $x_{k+1} = Ax_k$
2. $x_{k+1} = x_{k+1}/\|x_{k+1}\|_2, \quad k \leftarrow k+1$, repeat.

- $x_k \to$ PageRank vector $v_1 : Av_1 = \lambda_1 v_1$

Inverse power method

Inverse (shift-and-invert) power method: $x := (A - \mu I)^{-1} x$, $x = x/\|x\|$

- Converges with improved **linear rate** $\frac{|\lambda_{\sigma(2)} - \mu|}{|\lambda_{\sigma(1)} - \mu|}$ to eigval closest to μ (σ: permutation)

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- μ can change adaptively with the iterations. The choice $\mu := x^T A x$ gives Rayleigh quotient iteration, with **quadratic** convergence $\|Ax^{(k+1)} - \lambda^{(k+1)} x^{(k+1)}\| = O(\|Ax^{(k)} - \lambda^{(k)} x^{(k)}\|^2)$ (cubic if A symmetric)

Solving an eigenvalue problem

Given $A \in \mathbb{R}^{n \times n}$ or $\mathbb{C}^{n \times n}$,

$$Ax = \lambda x$$

Goal: find *all* eigenvalues (and eigenvectors) of a matrix

- Look for Schur form $A = UTU^*$

We'll describe an algorithm called the QR algorithm that is used universally, e.g. by MATLAB's `eig`. It

- finds all eigenvalues (approximately but reliably) in $O(n^3)$ flops,
- is backward stable.

Sister problem: Given $A \in \mathbb{R}^{m \times n}$ or $\mathbb{C}^{m \times n}$, compute SVD $A = U\Sigma V^*$

- 'ok' algorithm: eig$(A^T A)$ to find V, then normalise AV
- there's a better algorithm: Golub-Kahan bidiagonalisation

QR algorithm for eigenproblems

Set $A_1 = A$, and

$$A_1 = Q_1 R_1, \quad A_2 = R_1 Q_1, \quad A_2 = Q_2 R_2, \quad A_3 = R_2 Q_2, \quad \dots$$

- A_k are all similar: $A_{k+1} = Q_k^T A_k Q_k$
- We shall 'show' that $A \to$ **triangular** (diagonal if A normal)
- Basically: QR(factorise)$\to RQ$(swap)$\to QR \to RQ \to \cdots$

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- We shall 'show' that $A \to$ **triangular** (diagonal if A normal)
- Basically: QR(factorise)$\to RQ$(swap)$\to QR \to RQ \to \cdots$
- Fundamental work by Francis (61,62) and Kublanovskaya (63)
- Truly Magical algorithm!
  - backward stable, as based on orthogonal transforms
  - always converges (with shifts), but global proof unavailable(!)
  - uses 'shifted inverse power method' (rational functions) without inversions

QR algorithm and power method

QR algorithm: $A_k = Q_k R_k$, $A_{k+1} = R_k Q_k$, repeat. Claims: for $k \geq 1$,

$$A^k = (Q_1 \cdots Q_k)(R_k \cdots R_1) =: Q^{(k)} R^{(k)}, \qquad A_{k+1} = (Q^{(k)})^T A Q^{(k)}.$$

Proof: recall $A_{k+1} = Q_k^T A_k Q_k$, repeat.

Proof by induction: $k = 1$ trivial.
Suppose $A^{k-1} = Q^{(k-1)} R^{(k-1)}$. We have

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

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

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

QR algorithm and power method

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$$A^k = (Q_1 \cdots Q_k)(R_k \cdots R_1) =: Q^{(k)} R^{(k)}, \qquad A_{k+1} = (Q^{(k)})^T A Q^{(k)}.$$

QR factorisation of A^k: 'dominated by leading eigenvector' x_1,
where $Ax_1 = \lambda_1 x_1$ (recall power method)

In particular, consider $A^k[1, 0, \ldots, 0]^T = A^k e_n$:

- $A^k e_n = R^{(k)}(1,1)Q^{(k)}(:, 1)$, parallel to 1st column of $Q^{(k)}$
- By power method, this implies $Q^{(k)}(:, 1) \to x_1$
- Hence by $A_{k+1} = (Q^{(k)})^T A Q^{(k)}$, $A_k(:, 1) \to [\lambda_1, 0, \ldots, 0]^T$

Progress! But there is much better news

QR algorithm and inverse power method

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

$$A^k = (Q_1 \cdots Q_k)(R_k \cdots R_1) =: Q^{(k)} R^{(k)}, \qquad A_{k+1} = (Q^{(k)})^T A Q^{(k)}.$$

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

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

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

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

NB no matrix inverse performed

- This means final column of $Q^{(k)}$ converges to minimum left eigenvector x_n with factor $\frac{|\lambda_n|}{|\lambda_{n-1}|}$, hence $A_k(n,:) \to [0, \ldots, 0, \lambda_n]$
- (Very) fast convergence if $|\lambda_n| \ll |\lambda_{n-1}|$
- Can we force this situation? **Yes by shifts**

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.

Roughly, if $s_k \approx \lambda_n$, then $A_{k+1} \approx \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ & & & & \lambda_n \end{bmatrix}$ by argument just made.

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

- QR factorization of matrix with eigvals $r(\lambda_j) = \prod_{i=1}^{k} \frac{1}{\lambda_j - s_i}$
- Converges like ratio of $\prod_{i=1}^{k} (\bar{\lambda}_j - s_i)$; very fast if $s_i \approx \lambda_j$. Ideally, choose $s_k \approx \lambda_n$
- Connection with shifted inverse power method, hence rational approximation

QR algorithm preprocessing

We've seen the QR iterations drives colored entries to 0 (esp. red ones)

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}$$

- Hence $A_{n,n} \to \lambda_n$, so choosing $s_k = A_{n,n}$ is sensible
- This reduces #QR iterations to $O(n)$ (empirical but reliable estimate)
- But each iteration is $O(n^3)$ for QR, overall $O(n^4)$
- We next discuss a preprocessing technique to reduce to $O(n^3)$

QR algorithm preprocessing: Hessenberg reduction

To improve cost of QR factorisation, first reduce via orthogonal Householder transformations

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}, \quad H_1 A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}, \quad H_1 = I - 2v_1 v_1^T,\ v_1 = \begin{bmatrix} 0 \\ * \\ * \\ * \\ * \end{bmatrix}$$

Then $H_1 A H_1 = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$. Repeat with $H_2 = I - 2v_2 v_2^T, v_2 = [0, 0, *, *, *]^T$, ...:

$$H_2 H_1 A H_1 H_2 = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}, \qquad H_3 H_2 H_1 A H_1 H_2 H_3 = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix},$$

Hessenberg reduction continued

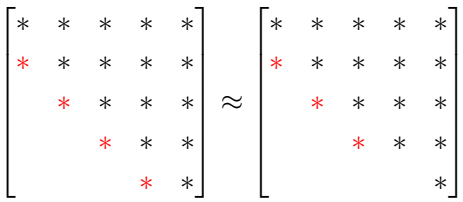
$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{H_1}{\to} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix} \overset{H_2}{\to} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix} \overset{H_3}{\to} \cdots \overset{H_{n-2}}{\to} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix}.$$

- QR iterations preserve structure: if $A_1 = QR$ Hessenberg, then so is $A_2 = RQ$
- using Givens rotations, each QR iter is $O(n^2)$ (not $O(n^3)$)
- overall shifted QR algorithm cost is $O(n^3), \approx 25n^3$ flops

- Remaining task (done by shifted QR): drive subdiagonal $*$ to 0
- bottom-right $* \to \lambda_n$, can be used for shift s_k

Deflation

Once bottom-right $|*| < \epsilon$,

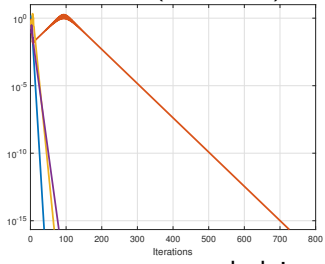


and continue with shifted QR on $(n-1) \times (n-1)$ block, repeat

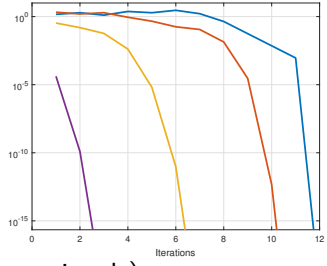
QR algorithm in action

Convergence of $|A_{i+1,i}|$

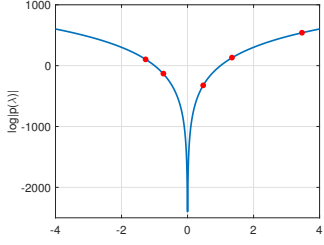
No shift (plain QR)

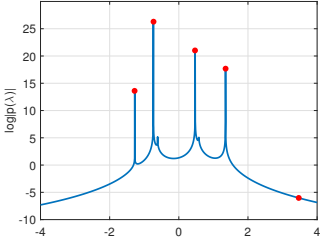


QR with shifts



underlying functions (red dots: eigvals)





QR algorithm: other improvements/simplifications (nonexaminable)

- Double-shift strategy for $A \in \mathbb{R}^{n \times n}$
  - $(A - sI)(A - \bar{s}I) = QR$ using only real arithmetic if A real
- Aggressive early deflation [Braman-Byers-Mathias 2002]
  - Examine lower-right (say 100×100) block instead of $(n, n-1)$ element
  - dramatic speedup ($\approx \times 10$)
- Balancing $A \leftarrow DAD^{-1}$, D: diagonal
  - reduce $\|DAD^{-1}\|$: better-conditioned eigenvalues

- For nonsymmetric A, global convergence is NOT established
  (except [Banks-Garza-Vargas-Srivastava 2021] for possible argument)
  - of course it always converges in practice.. another big open problem in numerical linear algebra

QR algorithm for symmetric A

- Initial reduction to Hessenberg form $\rightarrow$ tridiagonal

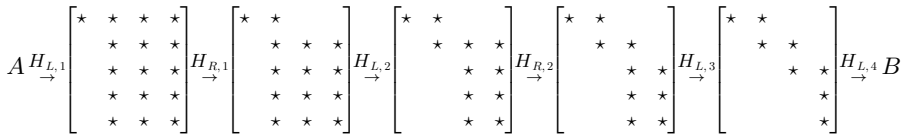
$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{Q_1}{\rightarrow} \begin{bmatrix} * & * & & & \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix} \overset{Q_2}{\rightarrow}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

- QR steps for tridiagonal: $O(n)$ instead of $O(n^2)$ per step
- Powerful alternatives available for tridiagonal eigenproblem (divide-conquer [Gu-Eisenstat 95], HODLR [Kressner-Susnjara 19],...)
- Cost: $\frac{4}{3}n^3$ flops for eigvals, $\approx 10n^3$ for eigvecs (store Givens rotations)

Golub-Kahan for SVD

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

$$A \to B = H_{L,n} \cdots H_{L,1} A H_{R,1} H_{R,2} \cdots H_{R,n-2}$$



- $\sigma_i(A) = \sigma_i(B)$
- Once bidiagonalized,
  - Mathematically, do QR alg on $B^T B$ (symmetric tridiagonal)
  - More elegant: divide-and-conquer [Gu-Eisenstat 1995] or dqds algorithm [Fernando-Parlett 1994]; nonexaminable
- Cost: $\approx 4mn^2$ flops for singvals Σ, $\approx 20mn^2$ flops for singvecs U, V

QZ algorithm for generalised eigenvalue problems

Generalised eigenvalue problem

$$Ax = \lambda Bx, \qquad A, B \in \mathbb{C}^{n \times n}$$

- A, B given, find eigenvalues λ and eigenvector x
- n eigenvalues, roots of $\det(A - \lambda B)$
- Important case: A, B symmetric, B positive definite: λ all real

QZ algorithm: look for unitary Q, Z s.t. QAZ, QBZ both upper triangular

- then $\mathrm{diag}(QAZ)/\mathrm{diag}(QBZ)$ are eigenvalues
- Algorithm: first reduce A, B to Hessenberg-triangular form
- then implicitly do QR to $B^{-1}A$ (without inverting B)
- Cost: $\approx 50n^3$
- See [Golub-Van Loan] for details

Tractable eigenvalue problems

- Standard eigenvalue problems $Ax = \lambda x$
  - symmetric ($4/3n^3$ flops for eigvals, $+9n^3$ for eigvecs)
  - nonsymmetric ($10n^3$ flops for eigvals, $+15n^3$ for eigvecs)
- SVD $A = U\Sigma V^T$ for $A \in \mathbb{C}^{m\times n}$: ($\frac{8}{3}mn^2$ flops for singvals, $+20mn^2$ for singvecs)
- Generalized eigenvalue problems $Ax = \lambda Bx$, $A, B \in \mathbb{C}^{n\times n}$
- Polynomial eigenvalue problems, e.g. (degree $k = 2$)
  $P(\lambda)x = (\lambda^2 A + \lambda B + C)x = 0$, $A, B, C \in \mathbb{C}^{n\times n}$:$\approx 20(nk)^3$
- Nonlinear problems, e.g. $N(\lambda)x = (A\exp(\lambda) + B)x = 0$
  - often solved via approximating by polynomial $N(\lambda) \approx P(\lambda)$
  - more difficult: $A(x)x = \lambda x$: eigenvector nonlinearity

Further speedup when structure present (e.g. sparse, low-rank)

Iterative methods

We've covered direct methods (LU for $Ax = b$, QR for $\min \|Ax - b\|_2$, QRalg for $Ax = \lambda x$). These are

- Incredibly reliable, backward stable
- Works like magic if $n \lesssim 10000$
- But not if n larger!

A 'big' matrix problem is one for which direct methods aren't feasible. Historically,

- 1950: $n \geq 20$
- 1965: $n \geq 200$
- 1980: $n \geq 2000$
- 1995: $n \geq 20000$
- 2010: $n \geq 100000$
- 2020: $n \geq 1000000$ ($n \geq 50000$ on a standard desktop)

was considered 'very large'. For such problems, we need to turn to alternative algorithms: we'll cover **iterative** and **randomised** methods.

Direct vs. iterative methods

Idea of iterative methods:

- gradually refine solution iteratively
- each iteration should be (a lot) cheaper than direct methods, usually $O(n^2)$ or less
- can be (but not always) much faster than direct methods
- tends to be (slightly) less robust, nontrivial/problem-dependent analysis
- often, after $O(n^3)$ work it still gets the exact solution (ignoring roundoff errors)

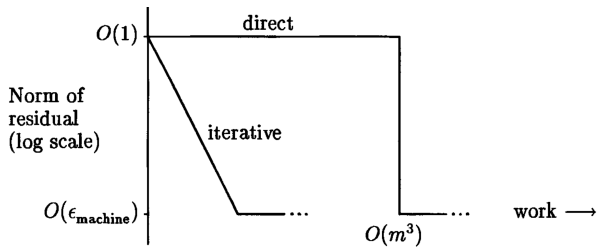


image from [Trefethen-Bau]

We'll focus on **Krylov subspace methods**.

Basic idea of Krylov: polynomial approximation

In Krylov subspace methods, we look for an (approximate) solution $\hat{x}$ (for $Ax = b$ or $Ax = \lambda x$) of the form (after kth iteration)

$$\hat{x} = p_{k-1}(A)v\,,$$

where p_{k-1} is a polynomial of degree $k-1$, and $v \in \mathbb{R}^n$ arbitrary (usually $v = b$ for linsys, for eigenproblems v usually random)

Natural questions:

- Why would this be a good idea?
  - Clearly, 'easy' to compute
  - One example: recall power method $\hat{x} = A^{k-1}v = p_{k-1}(A)v$
    Krylov finds a "better/optimal" polynomial $p_{k-1}(A)$
  - We'll see more cases where Krylov is powerful
- How to turn into an algorithm?
  - Arnoldi (next), Lanczos

Orthonormal basis for $\mathcal{K}_k(A, b)$

Find approximate solution $\hat{x} = p_{k-1}(A)b$, i.e. in Krylov subspace

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

First step: form an orthonormal basis Q, s.t. solution can be written as $x = Qy$

- Naive idea: Form matrix $[b, Ab, A^2b, \ldots, A^{k-1}b]$, then QR
  - $[b, Ab, A^2b, \ldots, A^{k-1}b]$ is usually terribly conditioned! Dominated by leading eigvec
  - Q is therefore extremely ill-conditioned, inaccurately computed

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  - $[b, Ab, A^2b, \ldots, A^{k-1}b]$ is usually terribly conditioned! Dominated by leading eigvec
  - Q is therefore extremely ill-conditioned, inaccurately computed
- Much better solution: Arnoldi process
  - Multiply A once at a time to the latest orthonormal vector q_i
  - Then orthogonalise Aq_i against previous q_j's $(j = 1, \ldots, i-1)$ (as in Gram-Schmidt)
  - Even better news: **Arnoldi decomposition** makes subsequent computation very convenient

Arnoldi iteration and Arnoldi decomposition

Set $q_1 = b/\|b\|_2$
For $k = 1, 2, \ldots,$
  set $v = Aq_k$
    for $j = 1, 2, \ldots, k$
      $h_{jk} = q_j^T v$, $v = v - h_{jk} q_j$ % orthogonalise against q_j via modified G-S
    end for
      $h_{k+1,k} = \|v\|_2$, $q_{k+1} = v/h_{k+1,k}$
End for

Theorem

Suppose that $h_{k+1,k} \neq 0$ *for* $k = 1, \ldots, \ell$. *Then for* $k = 1, \ldots, \ell$,

$$\mathit{Span}(q_1, \ldots, q_k) = \mathcal{K}_k(A, b).$$

Proof: Induction on ℓ. Suppose true for $\ell = \hat{\ell}$ with $q_{\hat{\ell}} = p_{\ell-1}(A)b$. Then $q_{\hat{\ell}+1} = \frac{1}{h_{\hat{\ell}+1,\hat{\ell}}}(Aq_{\hat{\ell}} - \sum_{j=1}^{\hat{\ell}} h_{j,\hat{\ell}} q_j)$, which is of exact degree $\hat{\ell}$.

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For $k = 1, 2, \ldots,$

set $v = Aq_k$

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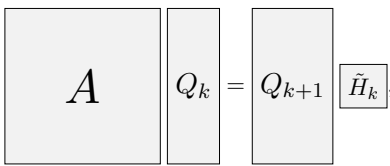
end for

$h_{k+1,k} = \|v\|_2$, $q_{k+1} = v/h_{k+1,k}$

End for

- After k steps, $AQ_k = Q_{k+1}\tilde{H}_k = Q_k H_k + q_{k+1}[0, \ldots, 0, h_{k+1,k}]$, with $Q_k = [q_1, q_2, \ldots, q_k], Q_{k+1} = [Q_k, q_{k+1}]$, span$(Q_k)$ = span$([b, Ab, \ldots, A^{k-1}b])$



$$\tilde{H}_k = \underbrace{\begin{bmatrix} h_{1,1} & h_{1,2} & \ldots & h_{1,k} \\ h_{2,1} & h_{2,2} & \ldots & h_{2,k} \\ & \ddots & & \vdots \\ & & h_{k,k-1} & h_{k,k} \\ & & & h_{k+1,k} \end{bmatrix}}_{\mathbb{R}^{(k+1)\times k} \text{ upper Hessenberg}}, \quad Q_{k+1}^T Q_{k+1} = I_{k+1}$$

- Cost k A-multiplications+$O(k^2)$ inner products ($O(nk^2)$)

GMRES for $Ax = b$

Idea (very simple!): minimise residual in Krylov subspace: [Saad-Schulz 86]

$$x_k = \text{argmin}_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

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$$x_k = \text{argmin}_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

Algorithm: Given $AQ_k = Q_{k+1}\tilde{H}_k$ and writing $x_k = Q_k y$, rewrite as

$$\begin{aligned}
\min_y \|AQ_k y - b\|_2 &= \min_y \|Q_{k+1}\tilde{H}_k y - b\|_2 \\
&= \min_y \left\| \begin{bmatrix} \tilde{H}_k \\ 0 \end{bmatrix} y - \begin{bmatrix} Q_k^T \\ Q_{k,\perp}^T \end{bmatrix} b \right\|_2 \\
&= \min_y \left\| \begin{bmatrix} \tilde{H}_k \\ 0 \end{bmatrix} y - \|b\|_2 e_1 \right\|_2, \quad e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n
\end{aligned}$$

(where $[Q_k, Q_{k,\perp}]$ orthogonal; same trick as in least-squares)

- Minimised when $\|\tilde{H}_k y - \tilde{Q}_k^T b\| \to \min$; Hessenberg least-squares problem
- Solve via QR (k Givens rotations)+triangular solve, $O(k^2)$ in addition to Arnoldi

GMRES convergence: polynomial approximation

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

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

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

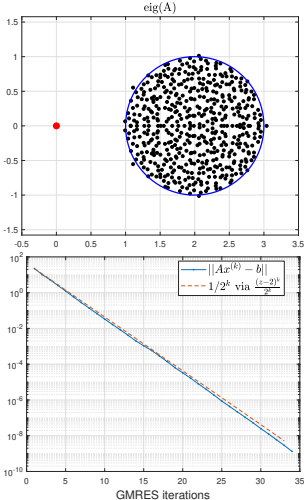
$$\begin{aligned}\|p(A)\|_2 &= \|Xp(\Lambda)X^{-1}\|_2 \leq \|X\|_2 \|X^{-1}\|_2 \|p(\Lambda)\|_2 \\ &= \kappa_2(X) \max_{z \in \lambda(A)} |p(z)|\end{aligned}$$

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

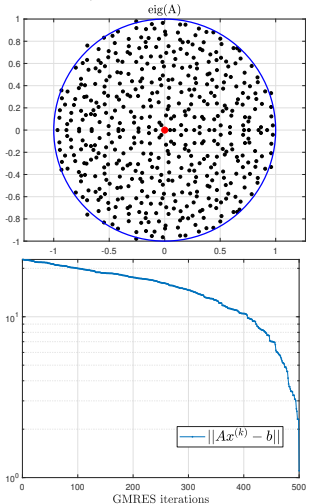
GMRES example

G: Gaussian random matrix ($G_{ij} \sim N(0,1)$, i.i.d.) $G/\sqrt{n}$: eigvals in unit disk

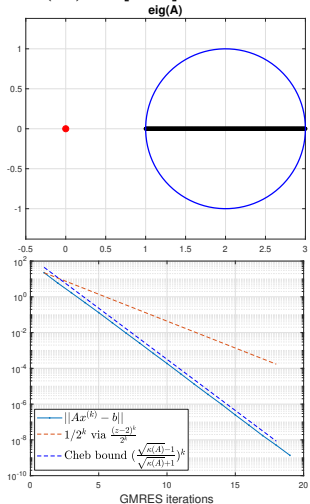
$A = 2I + G/\sqrt{n}$,
$p(z) = 2^{-k}(z-2)^k$



$A = G/\sqrt{n}$



$\mathrm{eig}(A) \in [1, 3]$



When does GMRES converge fast?

Recall GMRES solution satisfies (assuming A diagonalisable+nonsingular)

$$\min_{x_k \in \mathcal{K}_k(A,b)} \|Ax_k - b\|_2 = \min_{p \in \mathcal{P}_k, p(0)=1} \|p(A)b\|_2 \leq \kappa_2(X) \max_{z \in \lambda(A)} |p(z)| \|b\|_2.$$

$\max_{z \in \lambda(A)} |p(z)|$ is small when

- $\lambda(A)$ are clustered away from 0
  - a good p can be found quite easily
  - e.g. example 2 slides ago

- When $\lambda(A)$ takes $k (\ll n)$ distinct values
  - Then convergence in k GMRES iterations (why?)

Preconditioning for GMRES

We've seen that GMRES is great if spectrum clustered away from 0. If not true with

$$Ax = b,$$

then precondition: find $M \in \mathbb{R}^{n \times n}$ and solve

$$MAx = Mb$$

Desiderata of M:

- M simple enough s.t. applying M to vector is easy (note that each GMRES iteration requires MA-multiplication), and one of
  1. MA has clustered eigenvalues away from 0
  2. MA has a small number of distinct eigenvalues
  3. MA is well-conditioned $\kappa_2(MA) = O(1)$; then solve normal equation $(MA)^T MAx = (MA)^T Mb$

Preconditioners: examples

- ILU (Incomplete LU) preconditioner: $A \approx LU, M = (LU)^{-1} = U^{-1}L^{-1}$, L, U 'as sparse as A' $\Rightarrow MA \approx I$ (hopefully; 'cluster away from 0')
- For $\tilde{A} = \begin{bmatrix} A & B \\ C & 0 \end{bmatrix}$, set $M = \begin{bmatrix} A^{-1} & \\ & (CA^{-1}B)^{-1} \end{bmatrix}$. Then if M nonsingular, $M\tilde{A}$ has eigvals$\in \{1, \frac{1}{2}(1 \pm \sqrt{5})\} \Rightarrow$ 3-step convergence [Murphy-Golub-Wathen 2000]
- Multigrid-based, operator preconditioning, ...

Finding effective preconditioners is never-ending research topic

Prof. Andy Wathen is our Oxford expert!

Restarted GMRES

For k iterations, GMRES costs k matrix multiplications$+O(nk^2)$ for orthogonalization $\rightarrow$ Arnoldi eventually becomes expensive.

Practical solution: restart by solving 'iterative refinement':

1. Stop GMRES after $k_{\max}$ (prescribed) steps to get approx. solution $\hat{x}_1$
2. Solve $A\tilde{x} = b - A\hat{x}_1$ via GMRES
3. Obtain solution $\hat{x}_1 + \tilde{x}$

Sometimes multiple restarts needed

Lanczos iteration

Recall Arnoldi decomposition $AQ_k = Q_{k+1}\tilde{H}_k = Q_k H_k + q_{k+1}[0, \ldots, 0, h_{k+1,k}]$.
When A symmetric, Arnoldi decomposition simplifies to

$$AQ_k = Q_k T_k + q_{k+1}[0, \ldots, 0, t_{k+1,k}],$$

where T_k is symmetric tridiagonal (proof: just note $H_k = Q_k^T A Q_k$ in Arnoldi)

$$A \; Q_k = Q_{k+1} \; \boxed{\tilde{T}_k}, \quad \tilde{T}_k = \underbrace{\begin{bmatrix} t_{1,1} & t_{1,2} & & & \\ t_{2,1} & t_{2,2} & \ddots & & \\ & \ddots & & & t_{k-1,k} \\ & & & t_{k,k-1} & t_{k,k} \\ & & & & t_{k+1,k} \end{bmatrix}}_{\mathbb{R}^{(k+1)\times k} \text{ symmetric tridiagonal}}, \; Q_{k+1}^T Q_{k+1} = I_{k+1}$$

- 3-term recurrence $t_{k+1,k} q_{k+1} = (A - t_{k,k}) q_k - t_{k-1,k} q_{k-1}$; orthogonalisation necessary only against last two vecs q_k, q_{k-1}
- Significant speedup over Arnoldi; cost k A-mult.$+O(k)$ inner products ($O(nk)$)

CG: Conjugate Gradient method for $Ax = b$, $A \succ 0$

When A symmetric, Lanczos gives $AQ_k = Q_k T_k + q_{k+1}[0, \ldots, 0, 1]$, T_k: tridiagonal

CG: when $A \succ 0$ PD, solve $Q_k^T(AQ_k y - b) = T_k y - Q_k^T b = 0$, and $x = Q_k y$
$\rightarrow$"Galerkin orthogonality": residual $Ax - b$ orthogonal to Q_k

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- $T_k y = Q_k^T b$ is tridiagonal linear system, $O(k)$ operations to solve
- three-term recurrence reduces cost to $O(k)$ A-multiplications
- minimises A-norm of error $x_k = \text{argmin}_{x \in Q_k} \|x - x_*\|_A$ ($Ax_* = b$):

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

minimiser is $y = (Q_k^T A Q_k)^{-1} Q_k^T b$, so $Q_k^T(AQ_k y - b) = 0$

- Note $\|x\|_A = \sqrt{x^T A x}$ defines a norm (exercise)
- More generally, for inner-product norm $\|z\|_M = \sqrt{< z, z >_M}$, $\min_{x=Qy} \|x_* - x\|_M$ attained when $< q_i, x_* - x >_M = 0$, $\forall q_i$ (cf. Part A NA)

CG algorithm for $Ax = b$, $A \succ 0$

Set $x_0 = 0$, $r_0 = -b$, $p_0 = r_0$ and do for $k = 1, 2, 3, \ldots$

$$\begin{aligned}
\alpha_k &= \langle r_k, r_k \rangle / \langle p_k, Ap_k \rangle \\
x_{k+1} &= x_k + \alpha_k p_k \\
r_{k+1} &= r_k - \alpha_k A p_k \\
\beta_k &= \langle r_{k+1}, r_{k+1} \rangle / \langle r_k, r_k \rangle \\
p_{k+1} &= r_{k+1} + \beta_k p_k
\end{aligned}$$

where $r_k = Ax_k - b$ (residual) and p_k (search direction).

One can show among others (exercise/sheet)

- $\mathcal{K}_k(A, b) = \mathsf{span}(r_0, r_1, \ldots, r_{k-1}) = \mathsf{span}(x_1, x_2, \ldots, x_k)$ (also equal to $\mathsf{span}(p_0, p_1, \ldots, p_{k-1})$)
- $r_j^T r_k = 0$, $j = 0, 1, 2, \ldots, k-1$

Thus x_k is kth CG solution, satisfying orthogonality $Q_k^T(Ax_k - b) = 0$

CG convergence

Let $e_k := x_* - x_k$. We have $e_0 = x_*$ ($x_0 = 0$), and

$$\begin{aligned}
\frac{\|e_k\|_A}{\|e_0\|_A} &= \min_{x \in \mathcal{K}_k(A,b)} \|x_k - x_*\|_A / \|x_*\|_A \\
&= \min_{p_{k-1} \in \mathcal{P}_{k-1}} \|p_{k-1}(A)b - A^{-1}b\|_A / \|e_0\|_A \\
&= \min_{p_{k-1} \in \mathcal{P}_{k-1}} \|(p_{k-1}(A)A - I)e_0\|_A / \|e_0\|_A \\
&= \min_{p \in \mathcal{P}_k, p(0)=1} \|p(A)e_0\|_A / \|e_0\|_A \\
&= \min_{p \in \mathcal{P}_k, p(0)=1} \left\| V \begin{bmatrix} p(\lambda_1) & & \\ & \ddots & \\ & & p(\lambda_n) \end{bmatrix} V^T e_0 \right\|_A / \|e_0\|_A
\end{aligned}$$

Now (blue)$^2 = \sum_i \lambda_i p(\lambda_i)^2 (V^T e_0)_i^2 \le \max_j p(\lambda_j)^2 \sum_i \lambda_i (V^T e_0)_i^2 = \max_j p(\lambda_j)^2 \|e_0\|_A^2$

CG convergence cont'd

We've shown

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{p\in\mathcal{P}_k, p(0)=1} \max_j |p(\lambda_j)| \leq \min_{p\in\mathcal{P}_k, p(0)=1} \max_{x\in[\lambda_{\min}(A),\lambda_{\max}(A)]} |p(x)|$$

Now

$$\min_{p\in\mathcal{P}_k, p(0)=1} \max_{x\in[\lambda_{\min}(A),\lambda_{\max}(A)]} |p(x)| \leq 2\left(\frac{\sqrt{\kappa_2(A)}-1}{\sqrt{\kappa_2(A)}+1}\right)^k$$

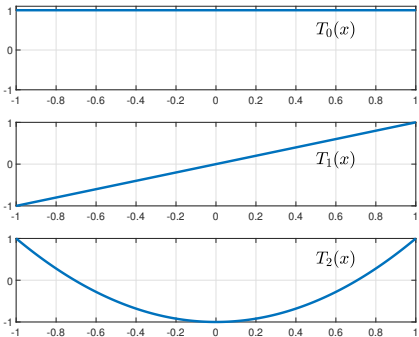
- note $\kappa_2(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)} = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} (=: \frac{b}{a})$
- above bound obtained by Chebyshev polynomials on $[\lambda_{\min}(A), \lambda_{\max}(A)]$

Chebyshev polynomials

For $z = \exp(i\theta)$, $x = \frac{1}{2}(z + z^{-1}) = \cos\theta \in [-1, 1]$, $\theta = \text{acos}(x)$,
$T_k(x) = \frac{1}{2}(z^k + z^{-k}) = \cos(k\theta)$. $T_k(x)$ is a polynomial in x:

$$\frac{1}{2}(z+z^{-1})(z^k+z^{-k}) = \frac{1}{2}(z^{k+1}+z^{-(k+1)})+\frac{1}{2}(z^{k-1}+z^{-(k-1)}) \Leftrightarrow \underbrace{2xT_k(x) = T_{k+1}(x) + T_{k-1}(x)}_{\text{3-term recurrence;}}$$

$2\cos\theta\cos(k\theta)=\cos((k+1)\theta)+\cos((k-1)\theta)$



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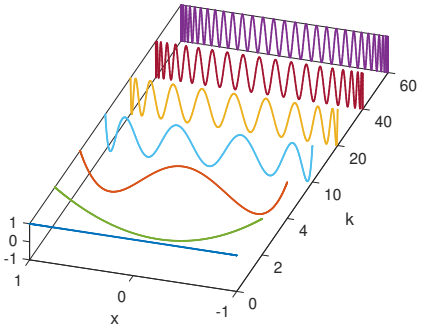
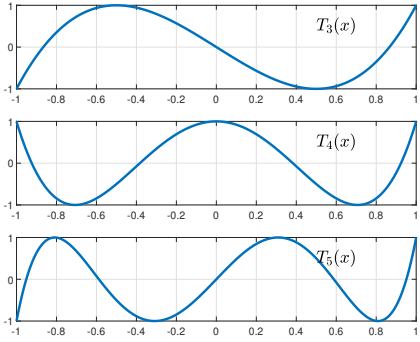
$2\cos\theta\cos(k\theta)=\cos((k+1)\theta)+\cos((k-1)\theta)$





Chebyshev polynomials

For $z = \exp(i\theta)$, $x = \frac{1}{2}(z + z^{-1}) = \cos\theta \in [-1, 1]$, $\theta = \text{acos}(x)$,
$T_k(x) = \frac{1}{2}(z^k + z^{-k}) = \cos(k\theta)$. $T_k(x)$ is a polynomial in x:

$$\frac{1}{2}(z+z^{-1})(z^k+z^{-k}) = \frac{1}{2}(z^{k+1}+z^{-(k+1)})+\frac{1}{2}(z^{k-1}+z^{-(k-1)}) \Leftrightarrow \underbrace{2xT_k(x) = T_{k+1}(x) + T_{k-1}(x)}_{\text{3-term recurrence;}}$$

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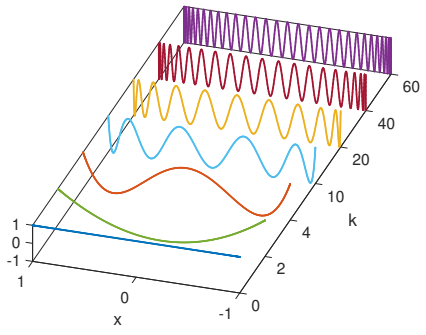

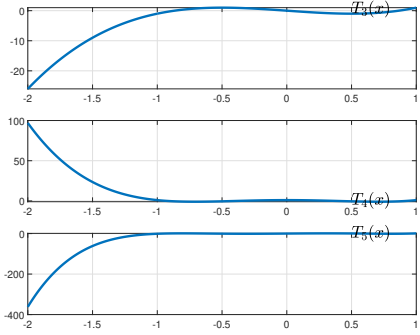

Chebyshev polynomials cont'd

For $z = \exp(i\theta)$, $x = \frac{1}{2}(z + z^{-1}) = \cos\theta \in [-1, 1]$, $\theta = \operatorname{acos}(x)$,
$T_k(x) = \frac{1}{2}(z^k + z^{-k}) = \cos(k\theta)$.

- Inside $[-1, 1]$, $|T_k(x)| \leq 1$
- Outside $[-1, 1]$, $|T_k(x)| \gg 1$ grows rapidly with $|x|, k$(fastest growth among $\mathcal{P}_k$)

Shift+scale s.t. $p(x) = c_k T_k(\frac{2x-b-a}{b-a})$ where $c_k = 1/T_k(\frac{-(b+a)}{b-a})$ so $p(0) = 1$. Then

- $|p(x)| \leq 1/|T_k(\frac{-(b+a)}{b-a})| = 1/|T_k(\frac{b+a}{b-a})|$ on $x \in [a, b]$
- $T_k(z) = \frac{1}{2}(z^k + z^{-k})$ with $\frac{1}{2}(z + z^{-1}) = \frac{b+a}{b-a} \Rightarrow z = \frac{\sqrt{b/a}+1}{\sqrt{b/a}-1} = \frac{\sqrt{\kappa_2(A)}+1}{\sqrt{\kappa_2(A)}-1}$, so

$$|p(x)| \leq 1/T_k(\frac{b+a}{b-a}) \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k$$

For much more about T_k, see C6.3 Approximation of Functions

MINRES: symmetric (indefinite) version of GMRES (nonexaminable)

Recall GMRES

$$x = \text{argmin}_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

Algorithm: Given $AQ_k = Q_{k+1}\tilde{H}_k$ and writing $x = Q_k y$, rewrite as

$$\begin{aligned}
\min_y \|AQ_k y - b\|_2 &= \min_y \|Q_{k+1}\tilde{H}_k y - b\|_2 \\
&= \min_y \left\| \begin{bmatrix} \tilde{H}_k \\ 0 \end{bmatrix} y - \begin{bmatrix} Q_k^T \\ Q_{k,\perp}^T \end{bmatrix} b \right\|_2 \\
&= \min_y \left\| \begin{bmatrix} \tilde{H}_k \\ 0 \end{bmatrix} y - \|b\|_2 e_1 \right\|_2, \quad e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n
\end{aligned}$$

(where $[Q_k, Q_{k,\perp}]$ orthogonal; same trick as in least-squares)

- Minimised when $\|\tilde{T}_k y - \tilde{Q}_k^T b\| \to \min$; Hessenberg least-squares problem
- Solve via QR (k Givens rotations)+triangular solve, $O(k^2)$ in addition to Arnoldi

MINRES: symmetric (indefinite) version of GMRES (nonexaminable)

MINRES (minimum-residual method) for $A = A^T$ (but not necessarily $A \succ 0$)

$$x = \text{argmin}_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

Algorithm: Given $AQ_k = Q_{k+1}\tilde{T}_k$ and writing $x = Q_k y$, rewrite as

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\end{aligned}$$

(where $[Q_k, Q_{k,\perp}]$ orthogonal; same trick as in least-squares)

- Minimised when $\|\tilde{T}_k y - \tilde{Q}_k^T b\| \to \min$; tridiagonal least-squares problem
- Solve via QR (k Givens rotations)+tridiagonal solve, $O(k)$ in addition to Lanczos

MINRES convergence (nonexaminable)

As in GMRES,

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

Since $A=A^T$, A is diagonalisable $A=Q\Lambda Q^T$ with Q orthogonal, so

$$\|p(A)\|_2 = \|Qp(\Lambda)Q^T\|_2 \le \|Q\|_2\|Q^T\|_2\|p(\Lambda)\|_2$$
$$= \max_{z\in\lambda(A)} |p(z)|$$

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

MINRES convergence cont'd (nonexaminable)

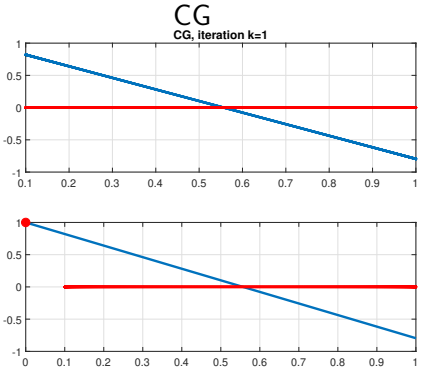
$$\frac{\|Ax-b\|_2}{\|b\|_2} \leq \min_{p\in\mathcal{P}_k, p(0)=1} \max |p(\lambda_i)|$$

One can prove (nonexaminable)

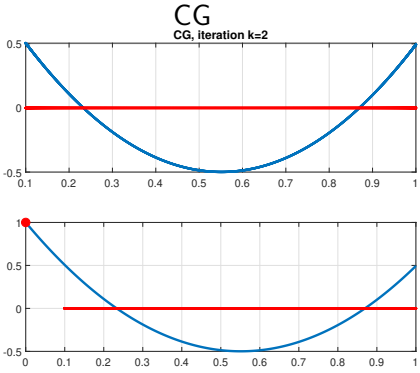
$$\min_{p\in\mathcal{P}_k, p(0)=1} \max |p(\lambda_i)| \leq 2\left(\frac{\kappa_2(A)-1}{\kappa_2(A)+1}\right)^{k/2}$$

- obtained by Chebyshev+Möbius change of variables [Greenbaum's book 97]
- minimisation needed on positive **and** negative sides, hence slower convergence when A indefinite

CG and MINRES, optimal polynomials



CG and MINRES, optimal polynomials



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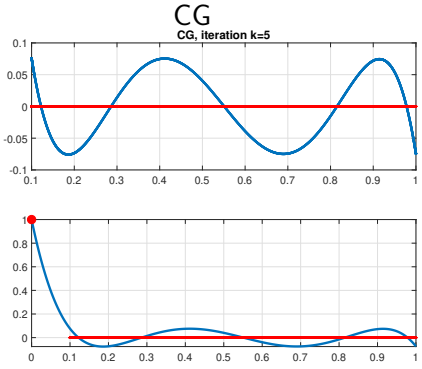

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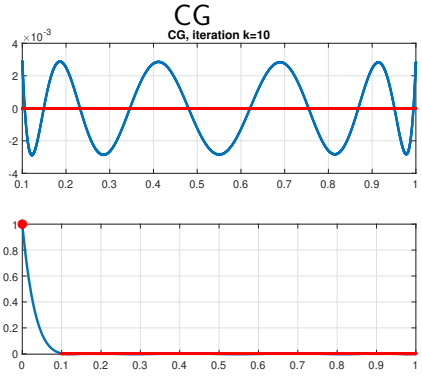

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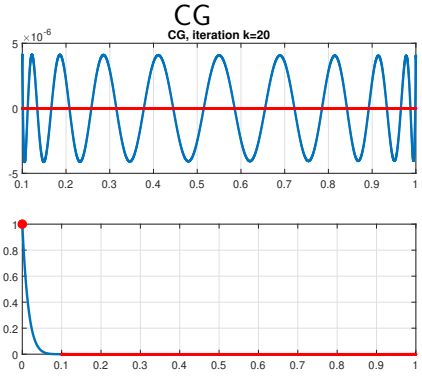

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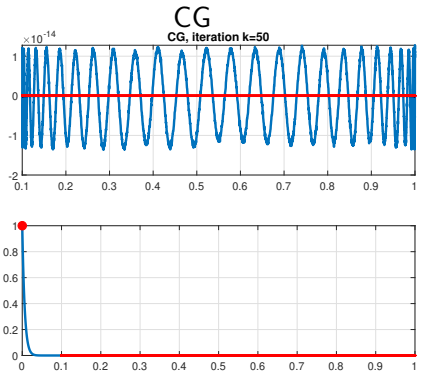

CG and MINRES, optimal polynomials

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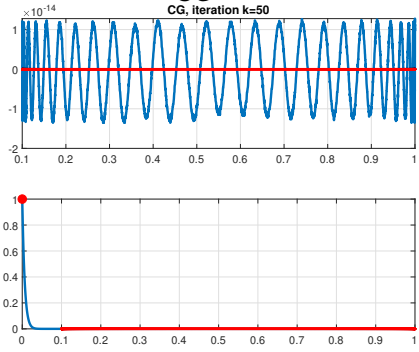
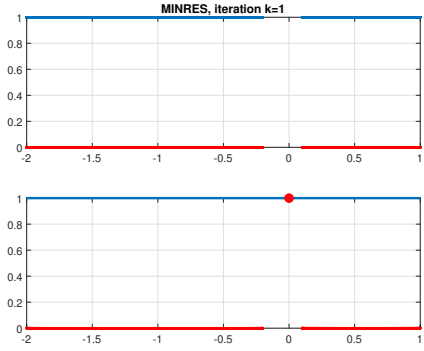


MINRES



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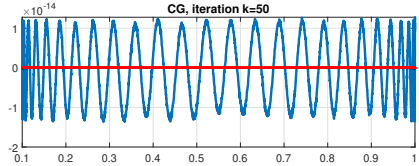

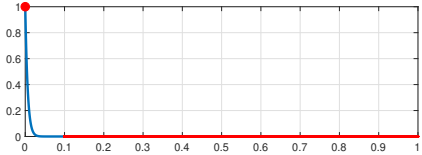

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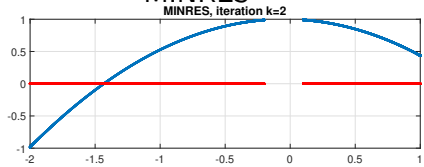

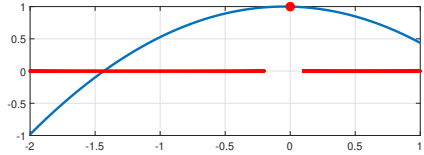

CG and MINRES, optimal polynomials

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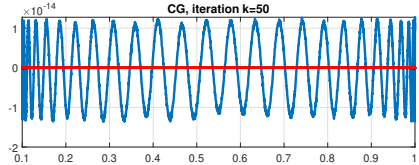

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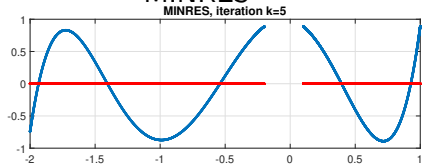

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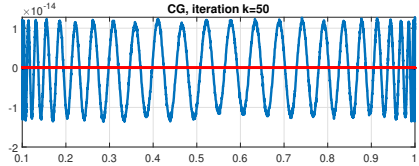

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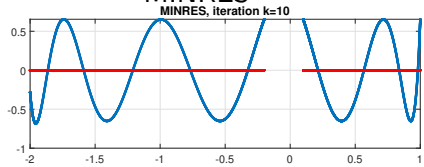

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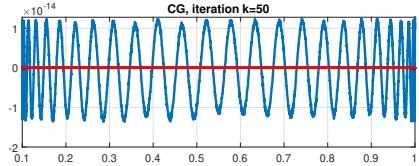

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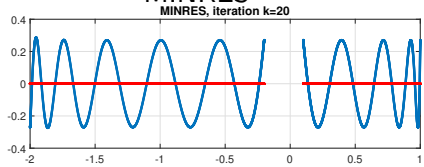

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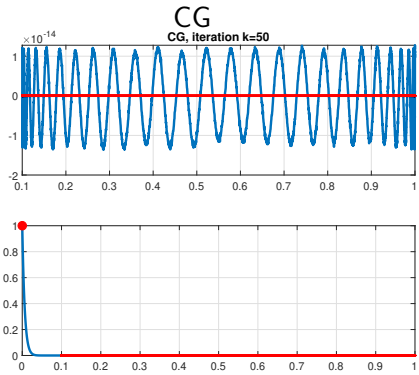
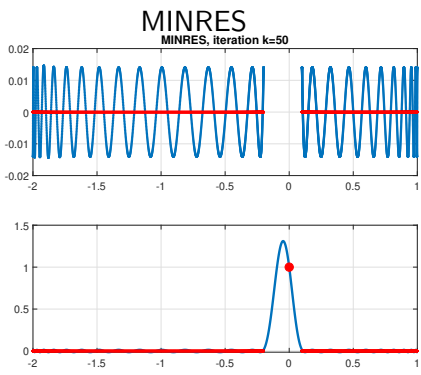




- CG employs Chebyshev polynomials
- MINRES is more complicated+slower convergence

Preconditioned CG/MINRES

$$Ax = b, \quad A \succ 0$$

Find preconditioner M s.t. "$M^T M \approx A^{-1}$" and solve

$$M^T A M y = M^T b, \quad My = x$$

As before, desiderata of M:

- $M^T A M$ simple to apply
- $M^T A M$ has clustered eigenvalues

Note that reducing $\kappa_2(M^T A M)$ directly implies rapid convergence

- Possible to implement with just $M^T M$ (no need to find M)

The Lanczos algorithm for symmetric eigenproblem (nonexaminable)

Rayleigh-Ritz: given symmetric A and orthonormal Q, find approximate eigenpairs

1. Compute $Q^T AQ$
2. Eigenvalue decomposition $Q^T AQ = V\hat{\Lambda}V^T$
3. Approximate eigenvalues $\mathrm{diag}(\hat{\Lambda})$ (Ritz values) and eigenvectors QV (Ritz vectors)

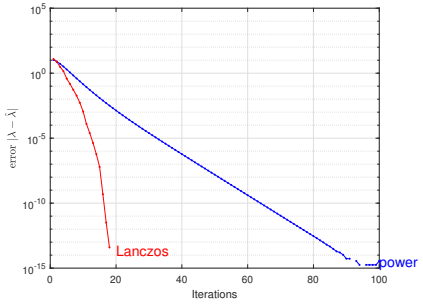
This is a **projection** method (similar alg. available for SVD)

Lanczos algorithm=Lanczos iteration+Rayleigh-Ritz

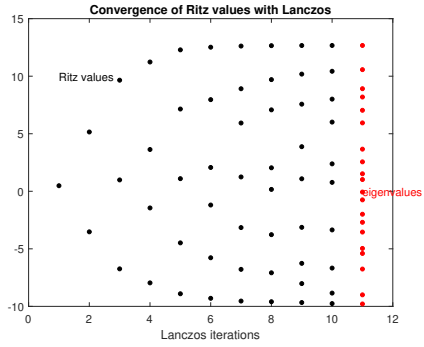
- In this case $Q = Q_k$, so simply $Q_k^T AQ_k = T_k$ (tridiagonal eigenproblem)
- Very good convergence to extremal eigenpairs
  - Recall from Courant-Fisher $\lambda_{\max}(A) = \max_x \frac{x^T Ax}{x^T x}$
  - Hence $\lambda_{\max}(A) \geq \underbrace{\max_{x \in \mathcal{K}_k(A,b)} \frac{x^T Ax}{x^T x}}_{\text{Lanczos output}} \geq \underbrace{\frac{v^T Av}{v^T v}, \quad v = A^{k-1}b}_{k-1 \text{ power method}}$, as $v \in \mathcal{K}_k(A, b)$
  - Same for $\lambda_{\min}$, similar for e.g. λ_2

Experiments with Lanczos (nonexaminable)

Symmetric $A \in \mathbb{R}^{n \times n}, n = 100$, Lanczos/power method with random initial vector b



Convergence to dominant eigenvalue



Convergence of all eigenvalues

Arnoldi for nonsymmetric eigenvalue problems (nonexaminable)

Arnoldi for eigenvalue problems: Arnoldi iteration+Rayleigh-Ritz (just like Lanczos alg)

1. Compute $Q^T A Q$
2. Eigenvalue decomposition $Q^T A Q = X \hat{\Lambda} X^{-1}$
3. Approximate eigenvalues $\text{diag}(\hat{\Lambda})$ (Ritz values) and eigenvectors QX (Ritz vectors)

As in Lanczos, $Q = Q_k = \mathcal{K}_k(A, b)$, so simply $Q_k^T A Q_k = H_k$ (Hessenberg eigenproblem, ideal for QRalg)

Which eigenvalues are found by Arnoldi?

- Krylov subspace is invariant under shift: $\mathcal{K}_k(A, b) = \mathcal{K}_k(A - sI, b)$
- Thus any eigenvector that power method applied to $A - sI$ converges to should be contained in $\mathcal{K}_k(A, b)$
- To find other (e.g. interior) eigvals, shift-invert Arnoldi: $Q = \mathcal{K}_k((A - sI)^{-1}, b)$

Randomised algorithms in NLA

So far, all algorithms have been deterministic (always same output)

- Direct methods (LU for $Ax = b$, QRalg for $Ax = \lambda x$ or $A = U\Sigma V^T$):
  - Incredibly reliable, backward stable
  - Works like magic if $n \lesssim 10000$
  - But not beyond; cubic complexity $O(n^3)$ or $O(mn^2)$
- Iterative methods (GMRES, CG, Arnoldi, Lanczos)
  - Very fast when it works (nice spectrum etc)
  - Otherwise, not so much; need for preconditioning

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  - Otherwise, not so much; need for preconditioning
- Randomised algorithms
  - Output differs at every run
  - Ideally succeed with enormous probability, e.g. $1 - \exp(-cn)$
  - Often by far the fastest&only feasible approach
  - Not for all problems—active field of research

We'll cover two NLA topics where randomisation very successful: **low-rank approximation (randomised SVD)**, and overdetermined **least-squares problems**

Gaussian random matrices

Gaussian $G \in \mathbb{R}^{m \times n}$: Takes iid (independent identically distributed) entries drawn from the standard normal (Gaussian) distribution $G_{ij} \sim N(0, 1)$.

Key properties of Gaussian matrices:

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  1. Linear combination of Gaussian random variables is Gaussian.
  2. The distribution of a Gaussian r.v. is determined by its mean and variance.
  3. $\mathbb{E}[(Qg_i)] = Q\mathbb{E}[g_i] = 0$ (g_i: ith column of G), and $\mathbb{E}[(Qg_i)^T(Qg_i)] = Q\mathbb{E}[g_i^T g_i]Q^T = I$, so each Qg_i is multivariate Gaussian with the same distribution as g_i. Independence of Qg_i, Qg_j is immediate.

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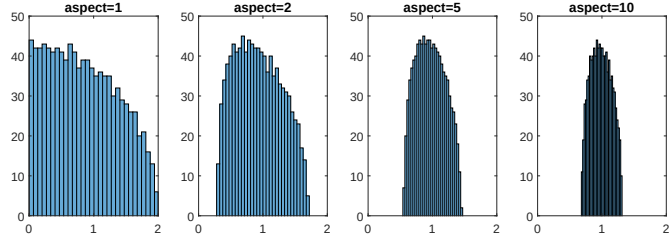
  Alternatively: joint pdf of $g_i = [g_{11}, \ldots, g_{n1}]^T$ is $\frac{1}{(2\pi)^{n/2}} \exp(-\frac{1}{2}(g_{11}^2 + \cdots + g_{n1}^2))$, and that of $Qg_i = [\tilde{g}_{11}, \ldots, \tilde{g}_{n1}]^T$ is (change of variables, note $\det Q = 1$) is $\frac{1}{(2\pi)^{n/2}} \exp(-\frac{1}{2}(\tilde{g}_{11}^2 + \cdots + \tilde{g}_{n1}^2))$
- Marchenko-Pastur rule: "Rectangular random matrices are well conditioned"

Tool from RMT: Rectangular random matrices are well conditioned

Singvals of random matrix $X \in \mathbb{R}^{m\times n}$ ($m \geq n$) with iid X_{ij} (mean 0, variance 1) follow Marchenko-Pastur (M-P) distribution (proof nonexaminable)



density $\sim \frac{1}{x}\sqrt{((1+\sqrt{\frac{m}{n}})-x)(x-(1-\sqrt{\frac{m}{n}}))}$, support $[\sqrt{m}-\sqrt{n}, \sqrt{m}+\sqrt{n}]$

$\sigma_{\max}(X) \approx \sqrt{m}+\sqrt{n}$, $\sigma_{\min}(X) \approx \sqrt{m}-\sqrt{n}$, hence $\kappa_2(X) \approx \frac{1+\sqrt{m/n}}{1-\sqrt{m/n}} = O(1)$,

Key fact in many breakthroughs in computational maths!

- Randomised SVD, Blendenpik (randomised least-squares)
- (nonexaminable:) Compressed sensing (RIP) [Donoho 06, Candes-Tao 06], Matrix concentration inequalities [Tropp 11], Function approx. by least-squares [Cohen-Davenport-Leviatan 13]

'Fast' (but fragile) alg for $\min_x \|Ax - b\|_2$

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

Consider 'row-subselection' algorithm: select $s(> n)$ rows A_1, b_1, and solve $\hat{x} := \operatorname{argmin}_x \|A_1 x - b_1\|_2$

- $\hat{x}$ exact solution if $Ax_* = b$ (consistent LS) and A_1 full rank
- If $Ax_* \neq b$, $\hat{x}$ can be terrible: e.g. $A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_k \end{bmatrix}$, $b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix}$ where $A_1 = \epsilon I_n (\epsilon \ll 1)$, and $A_i = I_n$ for $i \geq 2$, and $b_i = b_j$ if $i, j \geq 2$. Then $x_* \approx b_2$, but $\hat{x} = \operatorname{argmin}_x \|A_1 x - b_1\|_2$ has $\hat{x} = \frac{1}{\epsilon} b_1$.

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  How to avoid such choices? **Randomisation**

Sketch and solve for $\min_x \|Ax - b\|_2$

A simple randomised algorithm for $\min_x \|Ax - b\|_2$,: *sketch and solve*; draw Gaussian $G \in \mathbb{R}^{s \times m}$ $(s > n)$ and

$$\underset{x}{\text{minimize}} \|G(Ax - b)\|_2.$$

Suppose $G \in \mathbb{C}^{\tilde{r} \times n} (n < \tilde{r} \ll m)$ Gaussian and let $[A\ b] = QR \in \mathbb{C}^{m \times (n+1)}$.

- Note $\boxed{GQ}$ is $s \times n$ Gaussian (by orth. invariance); so $\sigma_i(GQ) \in [\sqrt{s} - \sqrt{n+1}, \sqrt{s} + \sqrt{n+1}]$
- $\|G(Av - b)\|_2 = \|G[A, b] \begin{bmatrix} v \\ -1 \end{bmatrix} \|_2 \leq (\sqrt{s} + \sqrt{n+1}) \|R \begin{bmatrix} v \\ -1 \end{bmatrix} \|_2 =$ $(\sqrt{s} + \sqrt{n+1}) \|Av - b\|_2$, $\forall v$, and similarly $\|G(Av - b)\|_2 \geq (\sqrt{s} - \sqrt{n+1}) \|Av - b\|_2$.
- Since by definition $\|G(A\hat{x} - b)\|_2 \leq \|G(Ax - b)\|_2$, it follows that

$$\|A\hat{x} - b\|_2 \leq \frac{1}{\sqrt{s} - \sqrt{n+1}} \|G(Ax - b)\|_2 \leq \frac{\sqrt{s} + \sqrt{n+1}}{\sqrt{s} - \sqrt{n+1}} \|Ax - b\|_2.$$

If $s = 4(n+1)$, we have $\frac{\sqrt{s}+\sqrt{n+1}}{\sqrt{s}-\sqrt{n+1}} = 3$, so
$\|Ax_* - b\|_2 = 10^{-10} \Rightarrow \|A\hat{x} - b\|_2 \leq 3 \cdot 10^{-10}$

Randomised least-squares: Blendenpik

[Avron-Maymounkov-Toledo 2010]

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

- Traditional method: normal eqn $x = (A^TA)^{-1}A^Tb$ or $A = QR, x = R^{-1}(Q^Tb)$, both $O(mn^2)$ cost
- Randomised: generate random $G \in \mathbb{R}^{4n\times m}$, and $GA = \hat{Q}\hat{R}$ (QR factorisation), then solve $\min_y \|(A\hat{R}^{-1})y - b\|_2$'s normal eqn via Krylov
  - $O(mn\log m + n^3)$ cost using fast FFT-type transforms for G
  - Successful because $A\hat{R}^{-1}$ is well-conditioned

Explaining Blendenpik via Marchenko-Pastur

Claim: $A\hat{R}^{-1}$ is well-conditioned with $G\,A = \hat{Q}\,\hat{R}$ (QR)

Show this for $G \in \mathbb{R}^{4n \times m}$ Gaussian:

Proof: Let $A = QR$. Then $GA = (GQ)R =: \tilde{G}R$

- $\tilde{G}$ is $4n \times n$ rectangular Gaussian, hence well-cond
- So by M-P, $\kappa_2(\tilde{R}^{-1}) = O(1)$ where $\tilde{G} = \tilde{Q}\tilde{R}$ is QR
- Thus $\tilde{G}R = (\tilde{Q}\tilde{R})R = \tilde{Q}(\tilde{R}R) = \tilde{Q}\hat{R}$, so $\hat{R}^{-1} = R^{-1}\tilde{R}^{-1}$
- Hence $A\hat{R}^{-1} = Q\tilde{R}^{-1}$, $\kappa_2(A\hat{R}^{-1}) = \kappa_2(\tilde{R}^{-1}) = O(1)$

Blendenpik: solving $\min_x \|Ax - b\|_2$ using $\hat{R}$

We have $\kappa_2(A\hat{R}^{-1}) =: \kappa_2(B) = O(1)$;
defining $\hat{R}x = y$, $\min_x \|Ax - b\|_2 = \min_y \|(A\hat{R}^{-1})y - b\|_2 = \min_y \|By - b\|_2$

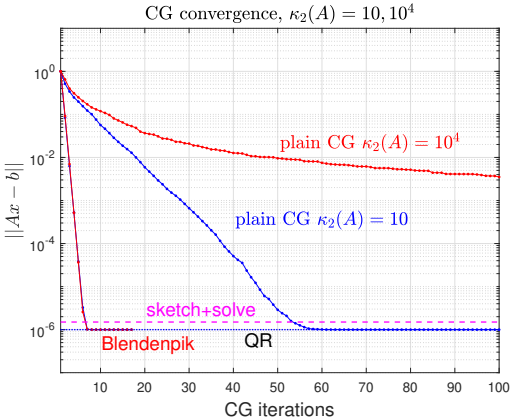
- B well-conditioned⇒in normal equation

$$B^T B y = B^T b \tag{1}$$

  B well-conditioned $\kappa_2(B) = O(1)$;

- solve (1) via CG (or a tailor-made method LSQR; nonexaminable)
  - exponential convergence, $O(1)$ iterations! (or $O(\log \frac{1}{\epsilon})$ iterations for ϵ accuracy)
  - each iteration requires $w \leftarrow Bw$, consisting of $w \leftarrow \hat{R}^{-1}w$ ($n \times n$ triangular solve) and $w \leftarrow Aw$ ($m \times n$mat-vec multiplication); $O(mn)$ cost overall

Blendenpik experiments



Solving $\min_x \|Ax - b\|_2$ via CG for $A^T Ax = A^T b$ vs. Blendenpik $(AR^{-1})^T (AR^{-1})x = (AR^{-1})^T b$, $m = 10000, n = 100$

In practice, Blendenpik gets $\approx \times 5$ speedup over classical (Householder-QR based) method when $m \gg n$

SVD: the most important matrix decomposition

- **Symmetric eigenvalue decomposition**: $A = V\Lambda V^T$
  for symmetric $A \in \mathbb{R}^{n\times n}$, where $V^TV = I_n$, $\Lambda = \mathsf{diag}(\lambda_1, \ldots, \lambda_n)$.
- **Singular Value Decomposition (SVD)**: $A = U\Sigma V^T$
  for any $A \in \mathbb{R}^{m\times n}$, $m \geq n$. Here $U^TU = V^TV = I_n$, $\Sigma = \mathsf{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

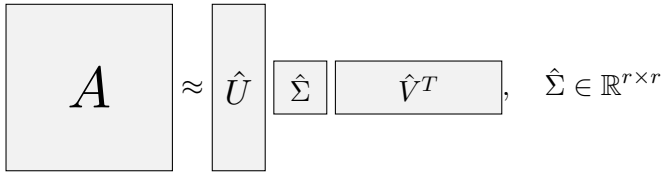
SVD proof: Take Gram matrix A^TA and its eigendecomposition $A^TA = V\Lambda V^T$. Λ is nonnegative, and $(AV)^T(AV)$ is diagonal, so $AV = U\Sigma$ for some orthonormal U. Right-multiply V^T.

SVD useful for

- Finding column space, row space, null space, rank, ...
- Matrix analysis, polar decomposition, ...
- **Low-rank approximation**

(Most) important result in Numerical Linear Algebra

Given $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$, find low-rank (rank r) approximation



- Optimal solution $A_r = U_r \Sigma_r V_r^T$ via truncated SVD
  $U_r = U(:, 1:r), \Sigma_r = \Sigma(1:r, 1:r), V_r = V(:, 1:r)$, giving

$$\|A - A_r\| = \|\mathsf{diag}(\sigma_{r+1}, \ldots, \sigma_n)\|$$

  in any unitarily invariant norm [Horn-Johnson 1985]
- But that costs $O(mn^2)$ (bidiagonalisation+QR); look for cheaper approximation

Randomised SVD by HMT

[Halko-Martinsson-Tropp, SIAM Review 2011]

1. Form a random (Gaussian) matrix $X \in \mathbb{R}^{n \times r}$, usually $r \ll n$.
2. Compute AX.
3. QR factorisation $AX = QR$.
4. $A \approx Q \boxed{Q^T A}$ $(= (QU_0)\Sigma_0 V_0^T)$ is rank-r approximation.

- $O(mnr)$ cost for dense A
- Near-optimal approximation guarantee: for any $\hat{r} < r$,

$$\mathbb{E}\|A - \hat{A}\|_F \leq \left(1 + \frac{r}{r - \hat{r} - 1}\right) \|A - A_{\hat{r}}\|_F$$

where $A_{\hat{r}}$ is the rank $\hat{r}$-truncated SVD (expectation w.r.t. random matrix X)

Goal: understand this, or at least why $\mathbb{E}\|A - \hat{A}\| = O(1)\|A - A_{\hat{r}}\|$

Pseudoinverse and projectors

Given $M \in \mathbb{R}^{m\times n}$ with economical SVD $M = U_r \Sigma_r V_r^T$
($U_r \in \mathbb{R}^{m\times r}, \Sigma_r \in \mathbb{R}^{r\times r}, V_r \in \mathbb{R}^{n\times r}$ where $r = \text{rank}(M)$ so that $\Sigma_r \succ 0$), the **pseudoinverse** $M^\dagger$ is

$$M^\dagger = V_r \Sigma_r^{-1} U_r^T \in \mathbb{R}^{n\times m}$$

- satisfies $MM^\dagger M = M$, $M^\dagger M M^\dagger = M^\dagger$, $MM^\dagger = (MM^\dagger)^T$, $M^\dagger M = (M^\dagger M)^T$ (which are often taken to be the definition—above is much simpler IMO)
- $M^\dagger = M^{-1}$ if M nonsingular, $M^\dagger M = I_n (MM^\dagger = I_m)$ if $m \geq n (m \geq n)$ and M full rank

A square matrix $P \in \mathbb{R}^{n\times n}$ is called a **projector** if $P^2 = P$

- P diagonalisable and all eigenvalues 1 or 0
- $\|P\|_2 \geq 1$ and $\|P\|_2 = 1$ iff $P = P^T$; in this case P is called orthogonal projector
- $I - P$ is another projector, and unless $P = 0$ or $P = I$, $\|I - P\|_2 = \|P\|_2$: Schur form $QPQ^* = \left[\begin{smallmatrix} I & B \\ 0 & 0 \end{smallmatrix}\right]$, $Q(I-P)Q^* = \left[\begin{smallmatrix} 0 & -B \\ 0 & I \end{smallmatrix}\right]$; see [Szyld 2006]

HMT approximant: analysis (down from 70 pages!)

$\hat{A} = QQ^T A$, where $AX = QR$. Goal: $\|A - \hat{A}\| = \|(I_m - QQ^T)A\| = O(\|A - A_{\hat{r}}\|)$.

1. $QQ^T AX = AX$ (QQ^T is orthogonal projector onto span(AX)). Hence $(I_m - QQ^T)AX = 0$, so $A - \hat{A} = (I_m - QQ^T)A(I_n - XM^T)$ for any $M \in \mathbb{R}^{n \times r}$.

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2. Set $M^T = (V^T X)^\dagger V^T$ where $V = [v_1, \ldots, v_{\hat{r}}] \in \mathbb{R}^{n \times \hat{r}}$ top sing vecs of A ($\hat{r} \leq r$).

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4. Taking norms, $\|A - \hat{A}\|_2 = \|(I_m - QQ^T)A(I - VV^T)(I_n - XM^T)\|_2 = \|(I_m - QQ^T)U_2\Sigma_2 V_2^T(I_n - XM^T)\|_2$ where $[V, V_2]$ is orthogonal, so

$$\|A - \hat{A}\|_2 \le \|\Sigma_2\|_2 \|(I_n - XM^T)\|_2 = \underbrace{\|\Sigma_2\|_2}_{\text{optimal rank-}\hat{r}} \quad \|XM^T\|_2$$

To see why $\|XM^T\|_2 = O(1)$ (with high probability), we need random matrix theory

$\|XM^T\|_2 = O(1)$

Recall we've shown for $M^T = (V^T X)^\dagger V^T \ X \in \mathbb{R}^{n\times r}$

$$\|A - \hat{A}\|_2 \leq \|\Sigma_2\|_2 \|(I_n - XM^T)\|_2 = \underbrace{\|\Sigma_2\|_2}_{\text{optimal rank-}\hat{r}} \quad \|XM^T\|_2$$

Now $\|XM^T\|_2 = \|X(V^T X)^\dagger V^T\|_2 = \|X(V^T X)^\dagger\|_2 \leq \|X\|_2 \|(V^T X)^\dagger\|_2$.
Assume X is random Gaussian $X_{ij} \sim \mathcal{N}(0,1)$. Then

- $V^T X$ is a Gaussian matrix (orthogonal$\times$Gaussian=Gaussian (in distribution); exercise), hence $\|(V^T X)^\dagger\| = 1/\sigma_{\min}(V^T X) \lesssim 1/(\sqrt{r} - \sqrt{\hat{r}})$ by M-P
- $\|X\|_2 \lesssim \sqrt{m} + \sqrt{r}$ by M-P

Together we get $\|XM^T\|_2 \lesssim \frac{\sqrt{m}+\sqrt{r}}{\sqrt{r}-\sqrt{\hat{r}}} = "O(1)"$

- When X non-Gaussian random matrix, perform similarly, harder to analyze

Precise analysis for HMT (nonexaminable)

Theorem (Reproduces HMT 2011 Thm.10.5)

If X Gaussian, for any $\hat{r} < r$, $\mathbb{E}\|E_{\mathrm{HMT}}\|_F \le \sqrt{\mathbb{E}\|E_{\mathrm{HMT}}\|_F^2} = \sqrt{1 + \frac{r}{r-\hat{r}-1}}\,\|A - A_{\hat{r}}\|_F.$

PROOF. First ineq: Cauchy-Schwarz. $\|E_{\mathrm{HMT}}\|_F^2$ is

$$\begin{aligned}&\|A(I - VV^T)(I - \mathcal{P}_{X,V})\|_F^2 = \|A(I - VV^T)\|_F^2 + \|A(I - VV^T)\mathcal{P}_{X,V}\|_F^2 \\ &= \|\Sigma_2\|_F^2 + \|\Sigma_2 \mathcal{P}_{X,V}\|_F^2 = \|\Sigma_2\|_F^2 + \|\Sigma_2 (V_\perp^T X)(V^T X)^\dagger V^T\|_F^2.\end{aligned}$$

Now if X is Gaussian then $V_\perp^T X \in \mathbb{R}^{(n-\hat{r})\times r}$ and $V^T X \in \mathbb{R}^{\hat{r}\times r}$ are independent Gaussian. Hence by [HMT Prop. 10.1] $\mathbb{E}\|\Sigma_2 (V_\perp^T X)(V^T X)^\dagger\|_F^2 = \frac{r}{r-\hat{r}-1}\|\Sigma_2\|_F^2$, so

$$\mathbb{E}\|E_{\mathrm{HMT}}\|_F^2 = \left(1 + \frac{r}{r-\hat{r}-1}\right)\|\Sigma_2\|_F^2.$$

Generalized Nyström (nonexaminable)

$X \in \mathbb{R}^{n\times r}$ as before; set $Y \in \mathbb{R}^{n\times(r+\ell)}$, and [N. 2020]

$$\hat{A} = (AX(Y^TAX)^\dagger Y^T)A = \mathcal{P}_{AX,Y}A$$

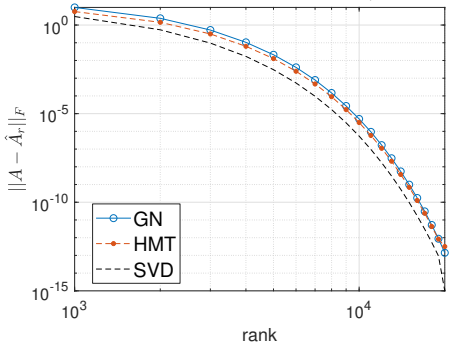
Then $A - \hat{A} = (I - \mathcal{P}_{AX,Y})A = (I - \mathcal{P}_{AX,Y})A(I - XM^T)$; choose M s.t. $XM^T = X(V^TX)^\dagger V^T = \mathcal{P}_{X,V}$. Then $\mathcal{P}_{AX,Y}, \mathcal{P}_{X,V}$ projections, and

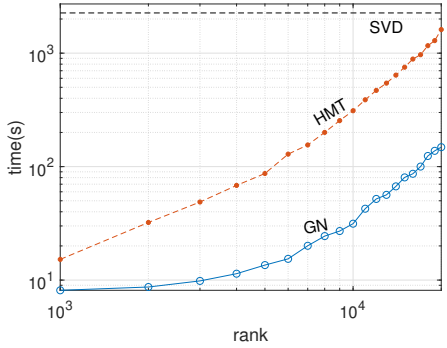
$$\begin{aligned}\|A - \hat{A}\| &= \|(I - \mathcal{P}_{AX,Y})A(I - \mathcal{P}_{X,V})\| \\ &\le \|(I - \mathcal{P}_{AX,Y})A(I - VV^T)(I - \mathcal{P}_{X,V})\| \\ &\le \|A(I - VV^T)(I - \mathcal{P}_{X,V})\| + \|\mathcal{P}_{AX,Y}A(I - VV^T)(I - \mathcal{P}_{X,V})\|.\end{aligned}$$

- Note $\|A(I - VV^T)(I - \mathcal{P}_{X,V})\|$ exact same as HMT error
- Extra term $\|\mathcal{P}_{AX,Y}\|_2 = O(1)$ as before if $c > 1$ in $Y \in \mathbb{R}^{m\times cr}$
- Overall, about $(1 + \|\mathcal{P}_{AX,Y}\|_2) \approx (1 + \frac{\sqrt{n}+\sqrt{r+\ell}}{\sqrt{r+\ell}-\sqrt{r}})$ times bigger expected error than HMT, **still near-optimal** and **much faster** $O(mn\log n + r^3)$

Experiments: dense matrix

Dense $30,000 \times 30,000$ matrix w/ geometrically decaying σ_i





HMT: Halko-Martinsson-Tropp 11, GN: generalized Nyström , SVD: full svd

- Randomised algorithms are very competitive until $r \approx n$
- error $\|A - \hat{A}_r\| = O(\|A - A_{\hat{r}}\|)$, as theory predicts

MATLAB codes

Setup:

```
n = 1000; % size
A = gallery('randsvd',n,1e100); % geometrically decaying singvals
r = 200;  % rank
```

Then

HMT:

```
X = randn(n,r);
AX = A*X;
[Q,R] = qr(AX,0); % QR fact.
At = Q*(Q'*A);

norm(At-A,'fro')/norm(A,'fro')
ans = 1.2832e-15
```

Generalized Nyström :

```
X = randn(n,r); Y = randn(n,1.5*r);
AX = A*X;  YA = Y'*A;  YAX = YA*X;
[Q,R] = qr(YAX,0);  % stable p-inv
At = (AX/R)*(Q'*YA);

norm(At-A,'fro')/norm(A,'fro')
ans = 2.8138e-15
```

Important (N)LA topics not treated

- tensors [Kolda-Bader 2009]
- FFT (values$\leftrightarrow$coefficients map for polynomials) [e.g. Golub and Van Loan 2012]
- sparse direct solvers [Duff, Erisman, Reid 2017]
- multigrid [e.g. Elman-Silvester-Wathen 2014]
- functions of matrices [Higham 2008]
- generalised, polynomial eigenvalue problems [Guttel-Tisseur 2017]
- perturbation theory (Davis-Kahan etc) [Stewart-Sun 1990]
- compressed sensing [Foucart-Rauhut 2013]
- model order reduction [Benner-Gugercin-Willcox 2015]
- communication-avoiding algorithms [e.g. Ballard-Demmel-Holtz-Schwartz 2011]

C6.1 Numerical Linear Algebra, summary

1st half

- SVD and its properties (Courant-Fisher etc), applications (low-rank)
- Direct methods (LU) for linear systems and least-squares problems (QR)
- Stability of algorithms

2nd half

- Direct method (QR algorithm) for eigenvalue problems, SVD
- Krylov subspace methods for linear systems (GMRES, CG) and eigenvalue problems (Arnoldi, Lanczos)
- Randomised algorithms for SVD and least-squares

Where does this course lead to?

Courses with significant intersection

- C6.3 Approximation of Functions (Prof. Nick Trefethen, MT): Chebyshev polynomials/approximation theory
- C7.7 Random Matrix Theory (Prof. Jon Keating): for theoretical underpinnings of Randomised NLA
- C6.4 Finite Element Method for PDEs (Prof. Patrick Farrell): NLA arising in solutions of PDEs
- C6.2 Continuous Optimisation (Prof. Cora Cartis): NLA in optimisation problems

and many more: differential equations, data science, optimisation, machine learning,...
NLA is everywhere in computational maths

Thank you for your interest in NLA!