15. Computing eigenvalues and eigenvectors

- power iteration
- shift and inverse techniques
- simultaneous (subspace) iteration
- QR iteration

Eigenvalue problem

given $A \in \mathbb{R}^{n\times n}$, find eigenvector x and eigenvalue λ:

$$Ax = \lambda x$$

- for simplicity, we assume that A has only real eigenvalues/eigenvectors
- we discuss methods for finding eigenvalues and eigenvectors

Need for iterative methods

- polynomial $\det(\lambda I - A) = \lambda^n + c_{n-1}\lambda^{n-1} + \cdots + c_1\lambda + a_0$ roots are eig. values of

$$A = \begin{bmatrix} -c_{n-1} & -c_{n-2} & -c_{n-3} & \cdots & -c_1 & -c_0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \in \mathbb{R}^{n\times n}$$

- no closed-form formula exists for roots of a general polynomial of degree $n \geq 5$
- hence, no finite algorithm exists for eigenvalues of general matrix of order $n \geq 5$

The power iteration

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given $A \in \mathbb{R}^{n \times n}$ and nonzero $v^{(0)} \in \mathbb{R}^n$ with $\|v^{(0)}\| = 1$

for $k = 1, 2, \ldots$

1. $\tilde{v} = Av^{(k-1)}$
2. $v^{(k)} = \tilde{v}/\|\tilde{v}\|$ (or $v^{(k)} = \tilde{v}/\|\tilde{v}\|_\infty$)
3. $\lambda^{(k)} = v^{(k)T} A v^{(k)}$ (or $\lambda^{(k)} = \|\tilde{v}\|_\infty$)

- if $v \in \mathbb{C}^n$ and $\lambda \in \mathbb{C}$, we replace v^T by the conjugate transpose v^H
- if λ_1 is the unique largest eigenvalue (*dominant eigenvalue*)
- $\lambda^{(k)}$ (or $\|\tilde{v}\|_\infty$) converges to λ_1
- $v^{(k)}$ converges to multiple of the corresponding eigenvector x_1
- reason for normalization is to keep the iterate magnitude in check (avoid overflow)

Convergence of the power method

- let the eigenvalues and eigenvectors of A be $\{\lambda_j, x_j\}$ for $j = 1, \ldots, n$
- assume $\lambda_1, \lambda_2, \ldots, \lambda_n$ are sorted in decreasing order in terms of their magnitude

$$|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|$$

Dominant eigenvector

- output at the kth step is $v^{(k)} = \gamma_k A^k v^{(0)}$, where γ_k guarantees $\|v^{(k)}\| = 1$
- assume $v^{(0)} \in \text{span}(x_1, \ldots, x_n)$, *i.e.*, $v^{(0)} = \sum_{j=1}^{n} \beta_j x_j$ for some β_j
- multiplying $v^{(0)}$ by A we obtain

$$Av^{(0)} = \sum_{j=1}^{n} \beta_j Ax_j = \sum_{j=1}^{n} \beta_j \lambda_j x_j$$

- continuing, for any positive integer k we have

$$A^k v^{(0)} = \sum_{j=1}^{n} \beta_j \lambda_j^k x_j$$

Convergence of the power method

- suppose that $\beta_1 \neq 0$, then

$$v^{(k)} = \gamma_k \lambda_1^k \sum_{j=1}^{n} \beta_j \left(\lambda_j/\lambda_1\right)^k x_j = \gamma_k \lambda_1^k \left(\beta_1 x_1 + \sum_{j=2}^{n} \beta_j \left(\lambda_j/\lambda_1\right)^k x_j\right)$$

- it follows that for $j \geq 2$ we have $(\lambda_j/\lambda_1)^k \to 0$ as $k \to \infty$
- the power method converges linearly with rate $|\lambda_2/\lambda_1|$:
  in the limit we obtain a normalized vector in the direction of x_1

Dominant eigenvalue

- suppose v is an approximate eigenvector for real A
- the "best" estimate of λ is the minimum of the least squares objective $\|v\lambda - Av\|^2$
- solution is the *Rayleigh quotient* $\mu(v) = v^T Av/v^T v$
- if v were an eigenvector, then $\mu(v)$ gives the associated eigenvalue
- note that by the normalization of $v^{(k)}$, we have $\mu(v^{(k)}) = v^{(k)\,T} A v^{(k)}$

Limitations of the power method

- initialization may have no component in the dominant eigenvector x_1: $\beta_1 = 0$
  - this is extremely unlikely if $v^{(0)}$ is chosen randomly
  - in practice $\beta_1 \neq 0$ due to roundoff errors
- there may be more than one eigenvalue having the same (maximum) modulus
  - iteration may converge to a linear combination of the corresponding eigenvectors
- for real matrix and real initialization, iteration cannot converge to complex vector
- $v^{(0)}$ may not belong to the span of eigenvectors (*e.g.*, A is defective)

  power method for such matrices can still be applied, but convergence can be slow

Example

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$$

with starting vector $v^{(0)} = (0, 1)$, then we obtain the following sequence

using 2-norm

k	$v^{(k)}$	$\lambda^{(k)}$
1	(0.3162, 0.9487)	3.6000
2	(0.5145, 0.8575)	3.8824
3	(0.6139, 0.7894)	3.9692
4	(0.6616, 0.7498)	3.9922
5	(0.6847, 0.7288)	3.9980
6	(0.6960, 0.7181)	3.9995
7	(0.7016, 0.7126)	3.9999
8	(0.7043, 0.7099)	4.0000
9	(0.7057, 0.7085)	4.0000

using ∞-norm

k	$v^{(k)}$	$\|\tilde{v}\|_\infty$
1	(0.333, 1.0)	3.000
2	(0.600, 1.0)	3.333
3	(0.778, 1.0)	3.600
4	(0.882, 1.0)	3.778
5	(0.939, 1.0)	3.882
6	(0.969, 1.0)	3.939
7	(0.984, 1.0)	3.969
8	(0.992, 1.0)	3.984
9	(0.996, 1.0)	3.992

converges to multiple of $x_1 = (1, 1)$ and $\lambda_1 = 4$

Example: PageRank

Problem: rank relevant webpages and determine their importance

- models internet as directed network with n nodes (webpages)
- PageRank computes the importance or *rank* $x_i \geq 0$ of a webpage i by counting the number of pages pointing to i
- set B_i gives indices of pages related to x_i
- if page $j \in B_i$ points to N_j pages including page i, then we set

$$x_i = \sum_{j \in B_i} \frac{1}{N_j} x_j, \quad i = 1, \ldots, n$$

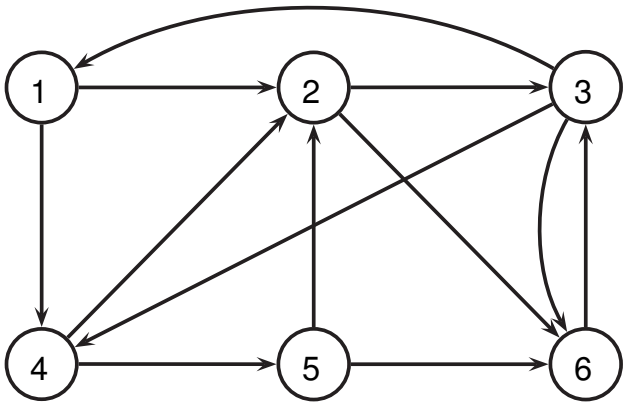
- an eigenvalue problem: $x = Ax$, where $A_{ij} = 1/N_j$ if $j \in B_i$ and zero otherwise
- if $v^{(0)} = \frac{1}{n}\mathbf{1}$, then, for $k = 0, 1, \ldots$, the iteration is defined by

$$v_i^{(k+1)} = \sum_{j \in B_i} \frac{1}{N_j} v_j^{(k)}, \quad i = 1, \ldots, n$$

(without normalization and eigenvalue estimation-operations)

Example: PageRank

webpages are nodes in the graph, numbered 1 through 6



$$A = \begin{bmatrix} 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 1 \\ \frac{1}{2} & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{3} & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

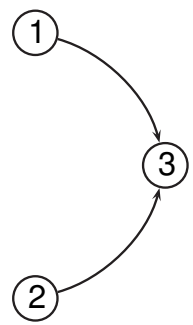
- jth column represents the outlinks from page j; rows indicate the inlinks
- columns sum up to 1; such a matrix is called *column* or *left stochastic*
- matrix A is elementwise nonnegative
- Perron-Frobenius theorem ensures for this matrix that
  - a unique, simple eigenvalue 1 exists
  - all other eigenvalues of A are smaller than one in magnitude
  - the associated eigenvector of the dominant eigenvalue has real entries

Example: PageRank

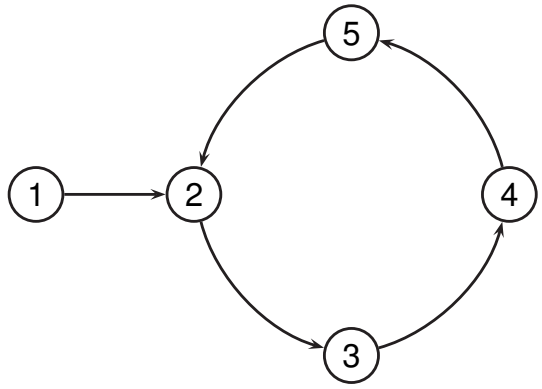
- to compute PageRank, we start with $v^{(0)} = (1/6, 1/6, 1/6, 1/6, 1/6, 1/6)$
- eventually, the method converges to the desired PageRank vector

$$x = (0.0994, 0.1615, 0.2981, 0.1491, 0.0745, 0.2174)$$

- this shows that node 3 is the top-ranked entry
- the ranking according to the values of x is $(3, 6, 2, 4, 1, 5)$
- interpretation: gives probability of a surfer being at a given webpage after a long ("infinite") time, regardless of where they started their journey
- when there are no outlinks from a certain webpage we can replace the whole column from zeros to entries all equal to $1/n$ (in our example, $1/6$)



Example: PageRank



- entering a “dead end,” as shown in diagram can be fixed by forming:

$$\alpha A + (1-\alpha) u \mathbf{1}^T$$

  where α is a damping factor and u is a personalization vector

- interpretation: if $\alpha = 0.85$ and $u = \frac{1}{n}\mathbf{1}$, then with probability 0.85 a surfer follows links and 0.15 probability jump randomly to anywhere

- $\alpha A + (1-\alpha) u \mathbf{1}^T$ has dominant eigenvalue is 1, the rest of its eigenvalues (which are generally complex) are bounded in magnitude by α

Outline

- power iteration
- **shift and inverse techniques**
- simultaneous (subspace) iteration
- QR iteration

Shifted power iteration

- recall that the eigenvalues of $A - \alpha I$ are $\lambda_i - \alpha$ with same eigenvectors of A
- using shifts convergence maybe enhanced to $|\lambda_2 - \alpha|/|\lambda_1 - \alpha| < |\lambda_2/\lambda_n|$

Power iteration with shifts

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given $A \in \mathbb{R}^{n\times n}$ and nonzero $v^{(0)} \in \mathbb{R}^n$

for $k = 1, 2, \ldots$

1. $\tilde{v} = (A - \alpha I)v^{(k-1)}$
2. $v^{(k)} = \tilde{v}/\|\tilde{v}\|$ (or $v^{(k)} = \tilde{v}/\|\tilde{v}\|_\infty$)
3. $\lambda^{(k)} = v^{(k)T} A v^{(k)}$ (or $\lambda^{(k)} = \|\tilde{v}\|_\infty + \alpha$)

Two extreme eigenvalues: shift allows us to find extreme eigenvectors λ_1 or λ_n

- converges to λ_1 if $|\lambda_1 - \alpha| > |\lambda_n - \alpha|$
- converges to λ_n if $|\lambda_n - \alpha| > |\lambda_1 - \alpha|$

The inverse iteration

Inverse iteration: power iteration applied to $(A - \alpha I)^{-1}$

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given $A \in \mathbb{R}^{n \times n}$, nonzero $v^{(0)} \in \mathbb{R}^n$, and shift α

for $k = 1, 2, \ldots$

1. solve $(A - \alpha I)\tilde{v} = v^{(k-1)}$
2. $v^{(k)} = \tilde{v}/\|\tilde{v}\|$ (or $v^{(k)} = \tilde{v}/\|\tilde{v}\|_\infty$)
3. $\lambda^{(k)} = v^{(k)T} A v^{(k)}$ (or $\lambda^{(k)} = 1/(\|\tilde{v}\|_\infty + \alpha)$)

- requires solving a linear equation in each iteration
- eigenvalues of $(A - \alpha I)^{-1}$ are $1/(\lambda_j - \alpha)$ with same eigenvectors as A
- converges to λ_j with largest $1/|\lambda_j - \alpha|$, *i.e.*, λ_j is the eigenvalue closest to α
  - this can allow us to find *any* eigenvalue
  - to converge to λ_1 taking $\alpha = \|A\|_1$ may be a reasonable since $\rho(A) \leq \|A\|$
- useful to find eigenvector corresponding to a known approximate eigenvalue

Example

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$$

- with starting vector $v^{(0)} = (0, 1)$ and $\alpha = 0$, we obtain the following sequence

k	$v^{(k)}$	$\|\tilde{v}\|_\infty$
0	$(0.000,\ 1.0)$	
1	$(-0.333,\ 1.0)$	0.375
2	$(-0.600,\ 1.0)$	0.417
3	$(-0.778,\ 1.0)$	0.450
4	$(-0.882,\ 1.0)$	0.472
5	$(-0.939,\ 1.0)$	0.485
6	$(-0.969,\ 1.0)$	0.492
7	$(-0.984,\ 1.0)$	0.496
8	$(-0.992,\ 1.0)$	0.498
9	$(-0.996,\ 1.0)$	0.499

- converge to eigenvector $(-1\ \ 1)$ with dominant eigenvalue of A^{-1}, which is 0.5
- this vector is an eigenvector corresponding to smallest eigenvalue of A, $\lambda_2 = 2$

Selecting shift dynamically

Rayleigh Quotient iteration

given $A \in \mathbb{R}^{n\times n}$ and nonzero normalized $v^{(0)} \in \mathbb{R}^n$; set $\lambda^{(0)} = v^{(0)T} A v^{(0)}$

for $k = 1, 2, \ldots$

1. solve $(A - \lambda^{(k-1)} I)\tilde{v} = v^{(k-1)}$
2. $v^{(k)} = \tilde{v}/\|\tilde{v}\|$ (or $v^{(k)} = \tilde{v}/\|\tilde{v}\|_\infty$)
3. $\lambda^{(k)} = v^{(k)T} A v^{(k)}$ (or $v^{(k)} = (v^{(k)T} A v^{(k)})/\|\tilde{v}\|^2$)

- selecting shift $\alpha = \lambda^{(k)} = v^{(k)T} A v^{(k)}$ to be the Rayleigh quotient
- improves convergence rate as we get closer to the desired eigenvalue
- requires refactoring $A - \lambda^{(k-1)} I$ each iteration for the solution step 1
- example: using same matrix as before, we get

k	$v^{(k)} = \tilde{v}/\|\tilde{v}\|_\infty$	$\lambda^{(k)}$
0	$(0.807,\ 0.397)$	3.792
1	$(0.924,\ 1.000)$	3.997
2	$(1.000,\ 1.000)$	4.000

Approach to find non-dominant eigenvalues

let u_1 be any vector such that $u_1^T x_1 = \lambda_1$, then the matrix

$$A - x_1 u_1^T$$

has eigenvalues $0,\ \lambda_2,\ \ldots,\ \lambda_n$

- after dominant eigenpair (λ_1, x_1) is found, we form new matrix $A - x_1 u_1^T$
- matrix has same original eigenvalues except λ_1 is replaced by 0

Possible choices of u_1

- $u_1 = \lambda_1 x_1$, if A is symmetric and x_1 is normalized so that $\|x_1\|_2 = 1$
- $u_1 = \lambda_1 y_1$, where y_1 is corresponding left eigenvector normalized $y_1^T x_1 = 1$
- $u_1 = A^T e_k$, if x_1 is normalized $\|x_1\|_\infty = 1$, and the kth component of x_1 is 1

Remarks

- the process becomes increasingly cumbersome
- numerical accuracy may deteriorate
- better alternatives exists

Outline

- power iteration
- shift and inverse techniques
- **simultaneous (subspace) iteration**
- QR iteration

Eigenspace

Invariant subspace: for $A \in \mathbb{R}^{n \times n}$ a subspace $\mathcal{S}$ is an *invariant subspace* if

$$x \in \mathcal{S} \quad \Longrightarrow \quad Ax \in \mathcal{S}$$

Eigenspace: for $A \in \mathbb{R}^{n \times n}$, the *eigenspace* is the set

$$\mathcal{S}_\lambda = \{x \mid Ax = \lambda x\}$$

- an eigenspace is an invariant subspace of $\mathbb{R}^n$ (or $\mathbb{C}^n$)
- if $x_1, \ldots, x_p$ are eigenvectors, then span$(x_1, \ldots, x_p)$ is an invariant subspace

Simultaneous iteration

Simultaneous (subspace) iteration

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given $A \in \mathbb{R}^{n\times n}$ and $V_0 = [v_1^{(0)} \ \cdots \ v_p^{(0)}] \in \mathbb{R}^{n\times p}$ with full column rank

for $k = 1, 2, \ldots$

$V_k = AV_{k-1}$

- power iteration with p starting points
- columns of V_k can be normalized to avoid overflow

Convergence

- let $x_1, \ldots, x_p$ be eigenvectors with eigenvalues $\lambda_1, \ldots, \lambda_p$ and $|\lambda_p| > |\lambda_{p+1}|$
- let $\mathcal{S}_0 = \text{span}(v_1^{(0)}, \ldots, v_p^{(0)})$ and $\mathcal{S} = \text{span}(x_1, \ldots, x_p)$
- assume no nonzero vector in $\mathcal{S}$ is orthogonal to $\mathcal{S}_0$
- then, columns of $V_k = A^k V_0$ converge to a basis for $\text{span}(x_1, \ldots, x_p)$

Convergence discussion

- assume A has $v_i^{(0)} \in \text{span}(x_1, \ldots, x_n)$ such that $v_i^{(0)} = \sum_{j=1}^{n} \beta_{i,j} x_j$ for some $\beta_{i,j}$
- we have for $i = 1, 2, \ldots, p$

$$\begin{aligned} v_i^{(k)} &= \lambda_1^k \beta_{i,1} x_1 + \cdots + \lambda_n^k \beta_{i,n} x_n \\ &= \lambda_p^k \left(\sum_{j=1}^{p} (\lambda_j/\lambda_p)^k \beta_{i,j} x_j + \sum_{j=p+1}^{n} (\lambda_j/\lambda_p)^k \beta_{i,j} x_j \right) \end{aligned}$$

- columns of $V_k = A^k V_0$ converge to basis for $\text{span}(x_1, \ldots, x_p)$ if $|\lambda_p| > |\lambda_{p+1}|$
- columns of V_k become increasingly ill-conditioned basis:
  - each column will be very close to x_1
  - so columns become almost linearly dependent
  - can be addressed by "orthonormalizing" the columns of V_k at each iteration

Outline

- power iteration
- shift and inverse techniques
- simultaneous (subspace) iteration
- **QR iteration**

Orthogonal iteration

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given $A \in \mathbb{R}^{n \times n}$ and an $n \times p$ matrix U_0 with orthonormal columns

for $k = 1, 2, \ldots$

1. compute: $V_k = AU_{k-1}$
2. QR factorization: $V_k = U_k R_k$

- V_k and U_k span the same subspace
- columns of U_k converge to an orthonormal basis for span$(x_1, \ldots, x_p)$
- for $U_0 = I$, $U_k^T A U_k \longrightarrow$ upper triangular matrix with eigenvalues on diagonal if
  - the eigenvalues of A are all real and distinct
  - all the principal submatrices of A are nonsingular
- if the eigenvalues are not all distinct, then $U_k^T A U_k$ will be *block* triangular
  - blocks have size 1×1 or 2×2
  - pair of complex conjugate eigenvalues of a real matrix represented by 2×2 block

Interpretation as QR factorization of powers of A

let $p = n$ and $U_0 = I$, then orthogonal iteration is

$$AU_{k-1} = U_k R_k \quad k = 1, 2, \ldots$$

with U_k orthogonal, R_k upper triangular

- repeated substitution gives:

  $$A = U_1 R_1, \quad A^2 = AU_1 R_1 = U_2 R_2 R_1, \quad A^3 = AU_2 R_2 R_1 = U_3 R_3 R_2 R_1, \quad \ldots$$

- after k steps,

  $$A^k = U_k S_k \quad \text{where} \quad S_k = R_k R_{k-1} \cdots R_1$$

- the product $S_k = R_k R_{k-1} \cdots R_1$ is upper triangular

- so orthogonal iteration produces QR factorizations of successive powers of A

Reorganization of orthogonal iteration

- assume $p = n$ so that U_k is orthogonal and let $U_0 = I$
- from $AU_{k-1} = U_k R_k$, we have

$$U_k^T A U_{k-1} = R_k$$

and

$$A_k = U_{k-1}^T A U_{k-1} = U_{k-1}^T U_k R_k = Q_k R_k$$

last equation is QR factorization with $Q_k = U_{k-1}^T U_k$

- from this it follows that

$$A_{k+1} = U_k^T A U_k = (U_k^T A U_{k-1})(U_{k-1}^T U_k) = R_k Q_k$$

Relation to orthogonal iteration

$$A_0 = A, \quad A_k = Q_k R_k, \quad A_{k+1} = R_k Q_k \quad (\text{for } k \geq 0)$$

- the matrices A_{k+1} and A_k are orthogonaly similar

$$A_{k+1} = R_k Q_k = Q_k^T A_k Q_k$$

- continuing recursively, we see that an orthogonal similarity relates A_k and A:

$$\begin{aligned} A_{k+1} &= (Q_1 Q_2 \cdots Q_k)^T A (Q_1 Q_2 \cdots Q_k) \\ &= U_k^T A U_k \quad \text{where} \quad U_k = Q_1 Q_2 \cdots Q_k \end{aligned}$$

  therefore the matrices A_k all have the same eigenvalues as A

- the orthogonal matrices $U_k = Q_1 Q_2 \cdots Q_k$ and the upper triangular R_k satisfy

$$A U_{k-1} = U_{k-1} A_k = U_{k-1} Q_k R_k = U_k R_k$$

  hence, equivalence to orthogonal iteration is $U_k = Q_1 Q_2 \cdots Q_k$

QR algorithm

most popular method for finding all eigenvalues of a matrix

QR iteration

---

given $A \in \mathbb{R}^{n \times n}$; set $A_0 = A$

for $k = 0, 1, 2, \ldots$

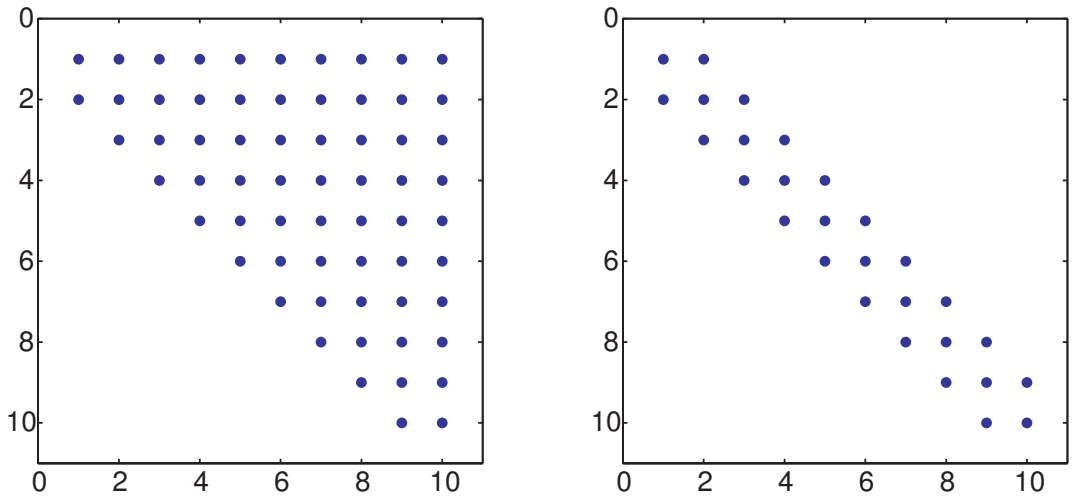
1. QR factorization: $A_k = Q_k R_k$
2. compute: $A_{k+1} = R_k Q_k$

- QR factorization step for rank deficient A_k exists with some zero diagonal on R_k
- A_k converges to upper (block) triangular matrix with eigenvalues in diagonal
- columns of $U_k = Q_1 \cdots Q_k$ converges to orthonormal basis for span$(x_1, \ldots, x_n)$
- for symmetric matrix, U_k converges to matrix of eigenvectors

Two stages

Stage 1: orthogonal similarity transformation

- idea: orthogonally transforming the matrix into simpler form
- general $A \longrightarrow$ upper Hessenberg matrix; symmetric $A \longrightarrow$ tridiagonal matrix



Stage 2

- apply QR iteration
- QR factorization of an upper Hessenberg matrix requires order n^2 operations compared to the order n^3 for a full matrix

Example

$$A = \begin{bmatrix} 0.5 & -0.1 & -0.5 & 0.4 \\ -0.1 & 0.3 & -0.2 & -0.3 \\ -0.3 & -0.2 & 0.6 & 0.3 \\ 0.1 & -0.3 & 0.3 & 1 \end{bmatrix}$$

First stage

- use Householder reflections (page 6.31) to orthogonaly transform matrix into upper Hessenberg $H^T A H$
- we let H_1 denote elementary transformation matrix to zero out element $A_{1,3:4}$:

  find a reflector u_1 such that $(-0.1, -0.3, 0.1)$ turns into $(\alpha, 0, 0)$ (see page 6.33)
- the vector is $u_1 = (-0.8067, -0.5606, 0.1869)$, and we have an orthogonal 3×3 matrix of the form $P^{(1)} = I_3 - 2u_1 u_1^T$; we then define

$$H_1^T = \begin{bmatrix} 1 & \\ & P^{(1)} \end{bmatrix}$$

- $H_1^T A$ now has two zeros in the $(3,1)$ and $(4,1)$ positions

Example

- multiplying by H_1^T on the left does not touch the first row of A
- multiplying by H_1 on the right does not touch the first column of $H_1^T A$
- the first similarity transformation gives

$$H_1^T A H_1 = \begin{bmatrix} 0.5 & 0.6030 & -0.0114 & 0.2371 \\ 0.3317 & 0.3909 & -0.1203 & 0.0300 \\ 0 & -0.1203 & 0.6669 & 0.5255 \\ 0 & 0.03 & 0.5255 & 0.8422 \end{bmatrix}$$

  and by construction the eigenvalues of A are preserved

- we now zero out the last element in the second column
- the reflector is $u_2 = (-0.9925, 0.1221)$, and

$$H_2^T = \begin{bmatrix} I_2 & 0 \\ 0 & P^{(2)} \end{bmatrix}$$

  where $P^{(2)} = I_2 - 2u_2 u_2^T$

Example

- this leads to $H = H_1 H_2$, which transforms A into upper Hessenberg for, given by

$$H_2^T H_1^T A H_1 H_2 = \begin{bmatrix} 0.5 & 0.6030 & 0.0685 & 0.2273 \\ 0.3317 & 0.3909 & 0.1240 & 0 \\ 0 & 0.1240 & 0.4301 & -0.4226 \\ 0 & 0 & -0.4226 & 1.0790 \end{bmatrix}$$

- only $n-1$ nonzeros out of $\frac{(n-1)n}{2}$ are left in the entire strictly lower left triangle

MATLAB code

```
function A = houseeig(A)
%
% reduce A to upper Hessenberg form using Householder reflections
n = size(A,1);
for k = 1:n-2
z=A(k+1:n,k);
e1=[1; zeros(n-k-1,1)];
u=z+sign(z(1))*norm(z)*e1;
u = u/norm(u);
% multiply from left and from right by Q = eye(n-k)-2*u*u';
A(k+1:n,k:n) = A(k+1:n,k:n) - 2*u*(u'*A(k+1:n,k:n));
A(1:n,k+1:n) = A(1:n,k+1:n) - 2*(A(1:n,k+1:n)*u)*u';
end
```

QR algorithm with shifts

in practice, including shift typically leads improved convergence

QR iteration with shifts

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given $A_0 = A$ transformed into upper Hessenberg or tridiagonal form

for $k = 1, 2, \ldots$

1. choose shift α_k
2. QR factorization: $A_k - \alpha_k I = Q_k R_k$
3. compute: $A_{k+1} = R_k Q_k + \alpha_k I$

- it often suffices to take α_k as a value along the diagonal
- common practice: use last diagonal entry of the matrix as a shift
- with properly chosen shifts, the iteration always converges

MATLAB implementation

```
function [lambda,itn] = qreig (A,tol)
% First stage, bring to upper Hessenberg form
A = houseeig(A);
% second stage: deflation loop
n = size(A,1); lambda = []; itn = [];
for j = n:-1:1
% find jth eigenvalue
[lambda(j),itn(j),A] = qrshift(A(1:j,1:j),tol);
end
function [alph,iter,A] = qrshift(A,tol)
m = size(A,1); alph = A(m,m); iter=0; I = eye(m);
if m == 1, return, end
while (iter < 100) % max number of iterations
if (abs(A(m,m-1)) < tol), return, end % check convergence
iter=iter+1;
[Q,R]=qr(A-alph*I); % compute the QR decomposition
A=R*Q+alph*I; % find the next iterate
alph = A(m,m); % next shift
end
```

Example

find eigenvalues λ and corresponding eigenfunctions $u(t)$ such that

$$u''(t) - u'(t) = \lambda u(t), \quad 0 < t < L, \qquad u(0) = u(L) = 0$$

- we regard L as a parameter and seek nontrivial solutions
- eigenvalues for this differential problem are given by

$$\lambda_j^{\text{de}} = -\frac{1}{4} - \left(\frac{j\pi}{L}\right)^2, \quad j = 1, 2, \ldots$$

- discretization: for small value h, we look for λ, $u = (u_1, u_2, \ldots, u_{N-1})$:

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{u_{i+1} - u_{i-1}}{2h} = \lambda u_i, \quad i = 1, 2, \ldots, N-1,$$

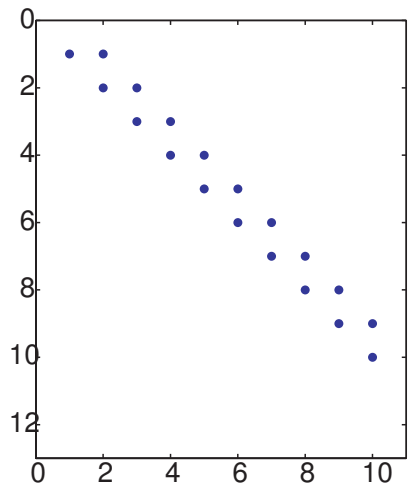
with $u_0 = u_N = 0$ and $N = L/h$

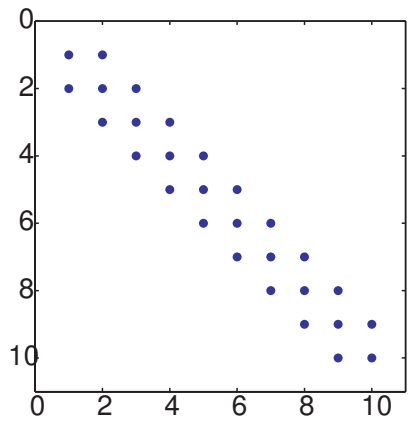
Example

- writing this as $Au = \lambda u$, we have a nonsymmetric, potentially large tridiagonal matrix A of size $n = N - 1$ and hopefully real eigenvalues
- we apply `qreig` $L = 10$ using $h = 0.1$ ($n = 99$) with tolerance 1e-4
- the maximum absolute difference between the first largest six eigenvalues λ_j and their corresponding continuous comrades λ_j^{de} is 0.015; the discrepancy arises because of the discretization error
- applying `qreig` to $L = 80$ with $h = .1$ ($n = 799$) does not converge
- applying MATLAB `eig` for $L = 80$ results in complex eigenvalues even though λ_j^{de} are real
- the reason for the sudden appearance of complex eigenvalues has to do with ill-conditioning of the differential problem and is not our focus here

Computing the SVD

- before, we applied same orthogonal transformation on left and right (transposed)
- for SVD $A = U\Sigma V^T$, there is no need to perform the same operations
- we search for a procedure that would reduce A into bidiagonal form, using different orthogonal transformations on the left and on the right
- note that the eigenvalues of A^TA are the squares of the singular values of A, and for the former we have a technique of reducing the matrix into tridiagonal form





the result of the first stage of the computation of the SVD is a bidiagonal matrix C (left); the corresponding tridiagonal matrix C^TC is given on the right

Example: reduction to bidiagonal

- to illustrate the idea, suppose the nonzero structure of a 5×4 matrix A is given by

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

- applying U_1^T on the left using Householder transformations, we have

$$U_1^T A = \begin{bmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix}$$

Example: reduction to bidiagonal

- we apply a different orthogonal transformation on the right that zeros out the entries to the right of the $(1,2)$ element:

$$U_1^T A V_1 = \begin{bmatrix} \times & \times & 0 & 0 \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix}$$

- another step gives

$$U_2^T U_1^T A V_1 V_2 = \begin{bmatrix} \times & \times & 0 & 0 \\ 0 & \times & \times & 0 \\ 0 & 0 & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & \times & \times \end{bmatrix}$$

- this continues until we get a bidiagonal form
- traditional methods involve an adaptation of the QR to zero out off-diagonal entries

References and further readings

- L. Vandenberghe. *EE133B Lecture Notes*, Univ. of California, Los Angeles.
- M. T. Heath. *Scientific Computing: An Introductory Survey* (revised second edition). Society for Industrial and Applied Mathematics, 2018.
- U. M. Ascher. *A First Course on Numerical Methods*. Society for Industrial and Applied Mathematics, 2011.