Chapter 11 Approximating Eigenvalues

Baodong LIU
baodong@sdu.edu.cn

December 12, 2018

- **Standard eigenvalue problem** : Given $n \times n$ matrix $\mathbf{A}$, find scalar λ and **nonzero vector** $\mathbf{x}$ such that

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

  - λ is eigenvalue;
  - $\mathbf{x}$ is **corresponding eigenvector**.

Notes about Eigenvalues and Eigenvectors

- λ may be complex even if $\mathbf{A}$ is real.
- An $n \times n$ matrix $\mathbf{A}$ has precisely n (not necessarily distinct)eigenvalues that are the roots of the polynomial
$$p(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I}).$$
- $\mathbf{x}$ can be viewed as **right eigenvector**, thus we can also define **left eigenvector**
$$\mathbf{y}^T\mathbf{A} = \lambda\mathbf{y}^T$$
- If $\mathbf{y}$ is left eigenvector of $\mathbf{A}$, then it is right eigenvector of $\mathbf{A}^T$, since
$$\mathbf{A}^T\mathbf{y} = \lambda\mathbf{y}.$$
- **Spectrum** (谱) of $\mathbf{A}$ $=$ set of eigenvalues of $\mathbf{A}$, denoted by $\lambda(\mathbf{A})$.
- **Spectral radius**(谱半径) of $\mathbf{A}$
$$\rho(A) = \max\{|\lambda| : \lambda \in \lambda(\mathbf{A})\}.$$

Geometric Interpretation

- Matrix expands or shrinks any vector lying in direction of eigenvector by scalar factor.
- Expansion or contraction factor is given by corresponding eigenvalue λ
- Eigenvalues and eigenvectors decompose complicated behavior of general linear transformation into simpler actions.

Existence and Uniqueness

- Equation $\mathbf{Ax} = \lambda\mathbf{x}$ is equivalent to

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}$$

  which has nonzero solution $\mathbf{x}$, if and only if, its matrix $(\mathbf{A} - \lambda\mathbf{I})$ is singular.
- Eigenvalues of $\mathbf{A}$ are roots λ_i of **characteristic polynomial**

$$p(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I}) = \mathbf{0}$$

  in λ of degree n.
- Fundamental Theorem of Algebra implies that $n \times n$ matrix $\mathbf{A}$ always has n eigenvalues, but they may not be real nor distinct
- Complex eigenvalues of **real matrix** occur in complex conjugate pairs: if $\alpha + i\beta$ is eigenvalue of real matrix, then so is $\alpha - i\beta$, where $i = \sqrt{-1}$.

Steps on Finding eigenvalues and eigenvectors of $\mathbf{A}$

- Solving $p(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I}) = 0.$
- Get its solution $\lambda_j, j = 1, 2, \cdots, n.$
- Finding corresponding eigenvector $\mathbf{v}_j$ for λ_j:

$$\mathbf{A}\mathbf{v}_j = \lambda_j\mathbf{v}_j, j = 1, 2, \cdots, n$$

- **Note:**
  1. In practices, it is difficult to determine the root of an nth-degree polynomial.
  2. Approximation techniques are needed for finding eigenvalues and eigenvectors.

Multiplicity (重根) and Diagonalizability

- Multiplicity is number of times root appears when polynomial is written as product of linear factors
- Eigenvalue of multiplicity 1 is simple(简根)
- **Defective matrix**(亏损矩阵) has eigenvalue of multiplicity $k > 1$ with fewer than k linearly independent corresponding eigenvectors
- **Nondefective matrix** $\mathbf{A}$ has n linearly independent eigenvectors, so it is diagonalizable

$$\mathbf{X}^{-1}\mathbf{A}\mathbf{X} = \mathbf{D}$$

where $\mathbf{X}$ is nonsingular matrix of eigenvectors.

- Eigenvectors can be scaled arbitrarily: if $\mathbf{Ax} = \lambda \mathbf{x}$, then
$$\mathbf{A}(\gamma \mathbf{x}) = \lambda(\gamma \mathbf{x})$$
for any scalar γ, so $\gamma \mathbf{x}$ is also eigenvector corresponding to λ.
- Eigenvectors are usually normalized by requiring some norm of eigenvector to be 1.
- **Eigenspace:** $\mathcal{S}_\lambda = \{\mathbf{x} : \mathbf{Ax} = \lambda \mathbf{x}\}$
- A subspace $\mathcal{S}$ of $\mathbb{R}^n$ (or $\mathcal{C}^n$) is said to be **invariant subspace** if $\mathbf{A}\mathcal{S} \subseteq \mathcal{S}$
- For eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n$, $span(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n)$ is invariant subspace

Relevant Properties of Matrices

Property	Definition
diagonal	$a_{ij} = 0$ for $i \neq j$
tridiagonal	$a_{ij} = 0$ for $\lvert i-j \rvert > 1$
triangular	$a_{ij} = 0$ for $i > j$ (upper)
	$a_{ij} = 0$ for $i < j$ (lower)
Hessenberg	$a_{ij} = 0$ for $i > j+1$ (upper)
	$a_{ij} = 0$ for $i < j-1$ (lower)
orthogonal	$\mathbf{A}^T\mathbf{A} = \mathbf{A}\mathbf{A}^T = \mathbf{I}$
unitary(酉矩阵)	$\mathbf{A}^H\mathbf{A} = \mathbf{A}\mathbf{A}^H = \mathbf{I}$
symmetric	$\mathbf{A} = \mathbf{A}^T$
Hermitian(厄密特矩阵)	$\mathbf{A} = \mathbf{A}^H$
normal(正规矩阵)	$\mathbf{A}^H\mathbf{A} = \mathbf{A}\mathbf{A}^H$

Examples

- Transpose(转置): $\begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix}^T = \begin{bmatrix}1 & 3\\ 2 & 4\end{bmatrix}$
- Conjugate transpose(共轭转置):
  $\begin{bmatrix}1+i & 1+2i\\ 2-i & 2-2i\end{bmatrix}^H = \begin{bmatrix}1-i & 2+i\\ 1-2i & 2+2i\end{bmatrix}$
- Hermitian(厄密特矩阵): $\begin{bmatrix}1 & 1+i\\ 1-i & 2\end{bmatrix}$,
- nonHermitian: $\begin{bmatrix}1 & 1+i\\ 1+i & 2\end{bmatrix}$
- Orthogonal: $\begin{bmatrix}\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2}\\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2}\end{bmatrix}$, $\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$, $\begin{bmatrix}-1 & 0\\ 0 & -1\end{bmatrix}$

- unitary(酉矩阵): $\begin{bmatrix} \frac{\sqrt{2}}{2}i & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2}i \end{bmatrix}$
- Normal(正规或正则矩阵): $\begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 2 \\ 2 & 0 & 1 \end{bmatrix}$
- Nonnormal: $\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$

Theorem 11.1

If $\mathbf{A}$ is a matrix and $\lambda_1, \cdots, \lambda_k$ are distinct eigenvalues of $\mathbf{A}$ with associated eigenvectors

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \cdots, \mathbf{x}^{(k)},$$

then

$$\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \cdots, \mathbf{x}^{(k)}\}$$

is linearly independent.

Definition 11.2

A set of vectors

$$\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}, \cdots, \mathbf{v}^{(n)}$$

is called **orthogonal** if

$$(\mathbf{v}^{(i)})^T \mathbf{v}^{(j)} = 0, \quad \texttt{for all} \quad i \neq j.$$

If, in addition ,

$$(\mathbf{v}^{(i)})^T \mathbf{v}^{(i)} = 1, \quad \texttt{for all} \quad i = 1, 2, \cdots, n,$$

then the set is **orthonormal**.

Theorem 11.3

An orthogonal set of vectors that does not contain the zero vector is linearly independent.

Definition 11.4

A matrix $\mathbf{P}$ is said to be an orthogonal matrix if $\mathbf{P}^{-1} = \mathbf{P}^T$.

Definition 11.5

Two matrices $\mathbf{A}$ and $\mathbf{B}$ are said to be **similar** if a nonsingular matrix $\mathbf{S}$ exists with

$$\mathbf{A} = \mathbf{S}^{-1}\mathbf{B}\mathbf{S}.$$

Theorem 11.6

- Suppose $\mathbf{A}$ and $\mathbf{B}$ are similar matrices and λ is an eigenvalue of $\mathbf{A}$ with associated eigenvector $\mathbf{x}$.
- Then λ is also an eigenvalue of $\mathbf{B}$, and if $\mathbf{A} = \mathbf{S}^{-1}\mathbf{B}\mathbf{S}$, then $\mathbf{S}\mathbf{x}$ is an eigenvector associated with λ for the matrix $\mathbf{B}$.

Theorem 11.7 (Schur)

Let $\mathbf{A}$ be an arbitrary matrix. A nonsingular matrix $\mathbf{U}$ exists with the property that

$$\mathbf{T} = \mathbf{U}^{-1}\mathbf{A}\mathbf{U}$$

where $\mathbf{T}$ is an upper-triangular matrix whose diagonal entries consist of the eigenvalues of $\mathbf{A}$.

Theorem 11.8

If $\mathbf{A}$ is a **symmetric matrix** and $\mathbf{D}$ is a **diagonal matrix** whose diagonal entries are the eigenvalues of $\mathbf{A}$,then there exists an orthogonal matrix $\mathbf{P}$ such that

$$\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{P}^{T}\mathbf{A}\mathbf{P}$$

Corollary 11.9

If $\mathbf{A}$ is a real symmetric $n \times n$ matrix , then the eigenvalues of $\mathbf{A}$ are real numbers , and there exist n eigenvectors of $\mathbf{A}$ that form an orthonormal set.

推论11.9证明

记$\mathbf{v}=(\mathbf{v}_1,\mathbf{v}_2,\cdots,\mathbf{v}_n)$ 为$\mathbf{A}$ 的n 个特征向量构成的矩阵；$\mathbf{D}=(d_{ii})$ 为$\mathbf{A}$ 的n 个特征值构成的对角矩阵；则

$$\mathbf{D}=\mathbf{v}^{-1}\mathbf{A}\mathbf{v}\text{或}\quad \mathbf{A}\mathbf{v}=\mathbf{D}\mathbf{v}.$$

对任一$1\le i\le n$ 有

$$\mathbf{A}\mathbf{v}_i=d_{ii}\mathbf{v}_i,$$

其中d_{ii} 是$\mathbf{A}$ 的特征值，$\mathbf{v}_i$ 是其对应的特征向量.
等式两端同乘 $\mathbf{v}_i^T$，得

$$\mathbf{v}_i^T A\mathbf{v}_i=d_{ii}\mathbf{v}_i^T\mathbf{v}_i.$$

由矩阵$\mathbf{A}$ 是对称的，则$\mathbf{v}_i^T A\mathbf{v}_i$ 和$\mathbf{v}_i^T\mathbf{v}_i$ 都是实数，且$\mathbf{v}_i^T\mathbf{v}_i=1$, 从而特征值$d_{ii}=\mathbf{v}_i^T A\mathbf{v}_i$ 也是实数.■

Theorem 11.10

A symmetric matrix $\mathbf{A}$ is positive definite if and only if all the eigenvalues of $\mathbf{A}$ are positive.

Theorem 4.11 (Gerschgorin Circle Theorem–圆盘定理)

- Let $\mathbf{A}$ be an $n \times n$ matrix
- $\mathbb{R}_i$ denote the circle in the complex plane with center a_{ii} and radius $\sum_{j=1, j\neq i}^{n} |a_{ij}|$;
- that is

$$\mathbb{R}_i = \left\{ z \in \mathcal{C} \middle| |z - a_{ii}| \leq \sum_{j=1, j\neq i}^{n} |a_{ij}| \right\}$$

  where $\mathcal{C}$ denotes the complex plane.
- The eigenvalues of $\mathbf{A}$ are contained with $\mathbb{R} = \cup_{i=1}^{n} \mathbb{R}_i$
- Moreover , the union (并集) of any k of these circles that do not intersect the remaining $(n-k)$ contains precisely k (counting multiplicities) of the eigenvalues.

圆盘定理的证明

- Suppose that λ is an eigenvalue of $\mathbf{A}$ with associated eigenvector $\mathbf{x}$, where $\|\mathbf{x}\|_\infty = 1$.
- Since $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, the equivalent component representation is

$$\sum_{j=1}^{n} a_{ij}x_j = \lambda x_i, \text{for each} \quad i = 1, 2, \cdots, n.$$

- If k is an integer with $|x_k| = \|\mathbf{x}\|_\infty = 1$, this equation, with $i = k$, implies that

$$\sum_{j=1}^{n} a_{kj}x_j = \lambda x_k.$$

- Thus

$$\sum_{j=1, j\neq k} a_{kj}x_j = \lambda x_k - a_{kk}x_k = (\lambda - a_{kk})x_k,$$

- So

$$|\lambda - a_{kk}| \cdot |x_k| = \left| \sum_{j=1, j\neq k}^{n} a_{kj} x_j \right| \leq \sum_{j=1, j\neq k}^{n} |a_{kj}||x_j|.$$

- Since $|x_j| \leq |x_k| = 1$, for all $j = 1, 2, \cdots, n$,

$$|\lambda - a_{kk}| \leq \sum_{j=1, j\neq k}^{n} |a_{kj}|$$

- Thus , $\lambda \in R_k$, which proves the first assertion in the theorem.
- 定理的第二部分证明需要连通性理论，不再证明.

Problem Transformations

- **Shift** : If $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ and σ is any scalar, then

$$(\mathbf{A} - \sigma\mathbf{I})\mathbf{x} = (\lambda - \sigma)\mathbf{x},$$

  so eigenvalues of **shifted matrix** (转移矩阵) are shifted eigenvalues of original matrix
- **Inversion** : If $\mathbf{A}$ is nonsingular and $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ with $\mathbf{x} \neq 0$, then $\lambda \neq 0$ and $\mathbf{A}^{-1}\mathbf{x} = \frac{1}{\lambda}\mathbf{x}$, so eigenvalues of inverse are reciprocals of eigenvalues of original matrix
- **Powers** : If $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, then $\mathbf{A}^k\mathbf{x} = \lambda^k\mathbf{x}$, so eigenvalues of power of matrix are same power of eigenvalues of original matrix
- **Polynomial** : If $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ and $p(t)$ is polynomial, then

$$p(\mathbf{A})\mathbf{x} = p(\lambda)\mathbf{x},$$

  so eigenvalues of polynomial in matrix are values of polynomial evaluated at eigenvalues of original matrix

Similarity Transformation

- $\mathbf{B}$ is similar to $\mathbf{A}$ if there is nonsingular matrix $\mathbf{P}$ such that

$$\mathbf{B} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}.$$

- Then

$$\mathbf{B}\mathbf{y} = \lambda\mathbf{y}, \Rightarrow \mathbf{P}^{-1}\mathbf{A}\mathbf{P}\mathbf{y} = \lambda\mathbf{y}, \Rightarrow \mathbf{A}(\mathbf{P}\mathbf{y}) = \lambda(\mathbf{P}\mathbf{y})$$

  so $\mathbf{A}$ and $\mathbf{B}$ have same eigenvalues, and if $\mathbf{y}$ is eigenvector of $\mathbf{B}$, then $\mathbf{x} = \mathbf{P}\mathbf{y}$ is eigenvector of $\mathbf{A}$.
- Similarity transformations preserve eigenvalues and eigenvectors are easily recovered

11.2 Computing Eigenvalues and Eigenvectors: power method

Iterative Power method

- assume that the $n \times n$ matrix $\mathbf{A}$ has n eigenvalues

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

  with an associated collection of linearly independent eigenvectors

$$\{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}, \cdots, \mathbf{v}^{(n)}\}.$$

- If $\mathbf{x}$ is any vector in $\mathbb{R}^n$, then constants $\beta_1, \beta_2, \cdots, \beta_n$ exist with

$$\mathbf{x} = \beta_1 \mathbf{v}^1 + \cdots + \beta_n \mathbf{v}^n = \sum_{j=1}^{n} \beta_j \mathbf{v}^{(j)}$$

- Multiplying both sides of this equation by $\mathbf{A}, \mathbf{A}^2, \cdots, \mathbf{A}^k$,we obtain:

$$
\begin{aligned}
\mathbf{A}\mathbf{x} &= \sum_{j=1}^{n} \beta_j A \mathbf{v}^{(j)} = \sum_{j=1}^{n} \beta_j \lambda_j \mathbf{v}^{(j)} \\
\mathbf{A}^2\mathbf{x} &= \sum_{j=1}^{n} \beta_j \lambda_j A \mathbf{v}^{(j)} = \sum_{j=1}^{n} \beta_j \lambda_j^2 \mathbf{v}^{(j)} \\
&\vdots \\
\mathbf{A}^k\mathbf{x} &= \sum_{j=1}^{n} \beta_j \lambda_j^k \mathbf{v}^{(j)} = \lambda_1^k \sum_{j=1}^{n} \beta_j \left(\frac{\lambda_j}{\lambda_1}\right)^k \mathbf{v}^{(j)} \\
&= \lambda_1^k \left(\beta_1 \mathbf{v}^{(1)} + \sum_{j=2}^{n} \beta_j \left(\frac{\lambda_j}{\lambda_1}\right)^k \mathbf{v}^{(j)} \right)
\end{aligned}
$$

- Since $|\lambda_1| > |\lambda_j|$ for all $j = 2, 3, \cdots, n$, we have

$$\lim_{k\to\infty} (\lambda_j/\lambda_1)^k = 0,$$

$$\lim_{k\to\infty} \mathbf{A}^k\mathbf{x} = \lim_{k\to\infty} \lambda_1^k \beta_1 \mathbf{v}^{(1)} \tag{1}$$

- This gives us the way to proceed to find λ_1 and an associated eigenvector.
- but we can not use the sequence in (1) directly since it converges to zero if $\lambda_1 < 1$ and diverges if $\lambda_1 > 1$, provided , of course , that $\beta_1 \neq 0$.
- Advantage can be made of the relationship expressed in Eq.(1) by scaling the powers of $A^k\mathbf{x}$ in an appropriate manner to ensure that the limit in Eq.(1) is finite and nonzero

Scaling Method(比例方法):

Step 1

- Choose an arbitrary unit vector $\mathbf{x}^{(0)}$ relative to $\|\cdot\|_\infty$.
- Suppose a component $x_{p_0}^{(0)}$ of $\mathbf{x}^{(0)}$ with

$$x_{p_0}^{(0)} = 1 = \|\mathbf{x}^{(0)}\|_\infty$$

- Let $\mathbf{y}^{(1)} = \mathbf{A}\mathbf{x}^{(0)}$, and define: $\mu^{(1)} = y_{p_0}^{(1)}$.
- With this notation ,

$$\begin{aligned}
\mu^{(1)} &= y_{p_0}^{(1)} = \frac{y_{p_0}^{(1)}}{x_{p_0}^{(0)}} = \frac{\beta_1 \lambda_1 v_{p_0}^{(1)} + \sum_{j=2}^{n} \beta_j \lambda_j v_{p_0}^{(j)}}{\beta_1 v_{p_0}^{(1)} + \sum_{j=2}^{n} \beta_j v_{p_0}^{(j)}} \\
&= \lambda_1 \left[\frac{\beta_1 v_{p_0}^{(1)} + \sum_{j=2}^{n} \beta_j (\lambda_j/\lambda_1) v_{p_0}^{(j)}}{\beta_1 v_{p_0}^{(1)} + \sum_{j=2}^{n} \beta_j v_{p_0}^{(j)}} \right]
\end{aligned}$$

- Then let p_1 be the least integer such that

$$y_{p_1}^{(1)} = \| \mathbf{y}^{(1)} \|_\infty$$

- Define $\mathbf{x}^{(1)}$ by

$$\mathbf{x}^{(1)} = \frac{1}{y_{p_1}^{(1)}}\mathbf{y}^{(1)} = \frac{1}{y_{p_1}^{(1)}}A\mathbf{x}^{(0)}$$

- Then

$$x_{p_1}^{(1)} = 1 = \|\mathbf{x}^{(1)}\|_\infty$$

Step 2

- Define

$$\mathbf{y}^{(2)} = \mathbf{A}\mathbf{x}^{(1)} = \frac{1}{y_{p_1}^{(1)}}\mathbf{A}^2\mathbf{x}^{(0)}$$

- Let

$$\begin{aligned}\mu^{(2)} = y_{p_1}^{(2)} &= \frac{y_{p_1}^{(2)}}{x_{p_1}^{(1)}} = \frac{\left[\beta_1\lambda_1^2 v_{p_1}^{(1)} + \sum_{j=2}^{n}\beta_j\lambda_j^2 v_{p_1}^{(j)}\right] \Big/ y_{p_1}^{(1)}}{\left[\beta_1\lambda_1 v_{p_1}^{(1)} + \sum_{j=2}^{n}\beta_j\lambda_j v_{p_1}^{(j)}\right] \Big/ y_{p_1}^{(1)}} \\ &= \lambda_1\left[\frac{\beta_1 v_{p_1}^{(1)} + \sum_{j=2}^{n}\beta_j(\lambda_j/\lambda_1)^2 v_{p_1}^{(j)}}{\beta_1 v_{p_1}^{(1)} + \sum_{j=2}^{n}\beta_j(\lambda_j/\lambda_1) v_{p_1}^{(j)}}\right].\end{aligned}$$

- Let p_2 be the smallest integer with

$$|y_{p_2}^{(2)}| = \|\mathbf{y}^{(2)}\|_\infty$$

- Define: $\mathbf{x}^{(2)} = \frac{1}{y_{p_2}^{(2)}}\mathbf{y}^{(2)} = \frac{1}{y_{p_2}^{(2)}}\mathbf{A}\mathbf{x}^{(1)} = \frac{1}{y_{p_2}^{(2)}y_{p_1}^{(1)}}\mathbf{A}^2\mathbf{x}^{(0)}.$

Step m

- In a similar manner , define sequences of vectors $\{\mathbf{x}^{(m)}\}_{m=1}^{\infty}$ and $\{\mathbf{y}^{(m)}\}_{m=1}^{\infty}$, and a sequence of scalars $\{\mu^{(m)}\}_{m=1}^{\infty}$.
- $\mathbf{y}^{(m)} = \mathbf{A}\mathbf{x}^{(m-1)}$
- $\mu^{(m)} = y_{p_{m-1}}^{(m)} = \lambda_1 \left[\dfrac{\beta_1 v_{p_{m-1}}^{(1)} + \sum_{j=2}^{n} \beta_j (\lambda_j/\lambda_1)^m v_{p_{m-1}}^{(j)}}{\beta_1 v_{p_{m-1}}^{(1)} + \sum_{j=2}^{n} \beta_j (\lambda_j/\lambda_1)^{m-1} v_{p_{m-1}}^{(j)}} \right]$
- Let p_m be the smallest integer with

$$|y_{p_m}^{(m)}| = \|\mathbf{y}^{(m)}\|_{\infty}$$

- Let $\mathbf{x}^{(m)} = \dfrac{\mathbf{y}^{(m)}}{y_{p_m}^{(m)}} = \dfrac{\mathbf{A}^m \mathbf{x}^{(0)}}{\prod_{k=1}^{m} y_{p_k}^{(k)}}$

- At each step, p_m is used to represent the smallest integer for which

$$|y_{p_m}^{(m)}| = \| \mathbf{y}^{(m)} \|_\infty$$

- Since $|\lambda_j/\lambda_1| < 1$ for each $j = 2, 3, \cdots, n$, then

$$\lim_{m\to\infty} \mu^{(m)} = \lambda_1,$$

ALGORITHM 1: the Power method

- To approximate the dominant eigenvalue and an associated eigenvector of the $n \times n$ matrix $\mathbf{A}$ given a nonzero vector **x**
- **INPUT** dimension n; matrix $\mathbf{A}$; vector $\mathbf{x}$; tolerance TOL; maximum number of iterations N.
- **OUTPUT** approximate eigenvalue μ; approximate eigenvector $\mathbf{x}$ (with $\|\|\mathbf{x}\|_\infty\| = 1$) or a message that the maximum number of iterations was exceeded.
- **Step 1** Set $k = 1$.
- **Step 2** Find the smallest integer p with $1 \leq p \leq n$ and $|x_p| = \|\mathbf{x}\|_\infty$.
- **Step 3** Set $\mathbf{x} = \mathbf{x}/x_p$.

- **Step 4** While $(k \leq N)$ do Steps 5-11.
  - **Step 5** Set $\mathbf{y} = A\mathbf{x}$.
  - **Step 6** Set $\mu = y_p$.
  - **Step 7** Find the smallest integer p with $1 \leq p \leq n$ and $|y_p| = \|\mathbf{y}\|_\infty$.
  - **Step 8** If $y_p = 0$ then
    - OUTPUT ('Eigenvector', $\mathbf{x}$);
    - OUTPUT ('A has the eigenvalue 0, select a new vector $\mathbf{x}$ and restart');
    - STOP.
  - **Step 9** Set $ERR = \|\mathbf{x} - (\mathbf{y}/y_p)\|_\infty; \mathbf{x} = \mathbf{y}/y_p$.
  - **Step 10** If $ERR < TOL$ then OUTPUT $(\mu, \mathbf{x})$;(Procedure completed successfully.).STOP.
  - **Step 11** Set $k = k + 1$.
- **Step 12** OUTPUT ('Maximum number of iterations exceeded');(Procedure completed unsuccessfully.)
- STOP.

Remarks:

- **Choosing the smallest integer of** $\|\cdot\|_\infty$: Choosing, in Step 7, the smallest integer p_m for which $|p_m| = \|\mathbf{y}^{(m)}\|_\infty$ will generally ensure that this index eventually becomes invariant.
- **Rate of Convergence:** The rate at which $\{\mu^{(m)}\}_{m=1}^{\infty}$ converges to λ_1 is determined by the ratios $|\lambda_j/\lambda_1|^m$, for $j = 2, 3, \cdots, n$, and in particular by $|\lambda_2/\lambda_1|^m$,.
- The rate of convergence is $O(|\lambda_2/\lambda_1|^m)$, so there is a constant k such that for large m,

$$|\mu^{(m)} - \lambda_1| \approx k\left|\frac{\lambda_2}{\lambda_1}\right|^m,$$

which implies that

$$\lim_{m\to\infty} \frac{|\mu^{(m+1)} - \lambda_1|}{|\mu^{(m)} - \lambda_1|} \approx \left|\frac{\lambda_2}{\lambda_1}\right| < 1.$$

- The **Inverse Power method** is a modification of the Power method that gives faster convergence.
- It is used to determine the eigenvalue of $\mathbf{A}$ that is closest to a specified number q.
- Assume that the matrix $\mathbf{A}$ has eigenvalues

$$\lambda_1, \cdots, \lambda_n$$

with linearly independent eigenvectors

$$\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \cdots, \mathbf{v}^{(n)}.$$

- Suppose that $q \neq \lambda_i$ for $i = 1, 2, 3, \cdots, n$
- We can easily get that the eigenvalues of the matrix $(\mathbf{A} - q\mathbf{I})^{-1}$ are

$$\frac{1}{\lambda_1 - q}, \frac{1}{\lambda_2 - q}, \cdots, \frac{1}{\lambda_n - q}$$

with eigenvectors

$$\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \cdots, \mathbf{v}^{(n)}$$

- Applying the Power method to $(A - qI)^{-1}$ gives

$$\mathbf{y}^{(m)} = (\mathbf{A} - q\mathbf{I})^{-1}\mathbf{x}^{(m-1)}$$

- Let

$$\mu^{(m)} = y^{(m)}_{p_{m-1}} = \frac{y^{(m)}_{p_{m-1}}}{x^{(m-1)}_{p_{m-1}}} = \frac{\sum_{j=1}^{n} \beta_j \frac{1}{(\lambda_j - q)^m} v^{(j)}_{p_{m-1}}}{\sum_{j=1}^{n} \beta_j \frac{1}{(\lambda_j - q)^{m-1}} v^{(j)}_{p_{m-1}}} \qquad (2)$$

- Let p_m represents the smallest integer for which

$$|y^{(m)}_{p_m}| = \| \mathbf{y}^{(m)} \|_\infty$$

- Define

$$\mathbf{x}^{(m)} = \frac{\mathbf{y}^{(m)}}{y^{(m)}_{p_m}}$$

- The sequence $\{\mu^{(m)}\}$ in Eq . (2) converges to

$$\frac{1}{|\lambda_k - q|} = \max_{1 \le j \le n} \frac{1}{\lambda_i - q}$$

- With k known , Eq.(2) can be written as

$$\mu^{(m)} = \frac{1}{\lambda_k - q}\left[\frac{\beta_k v_{p_{m-1}}^{(k)} + \sum_{j=1, j\neq k}^{n} \beta_j \left[\frac{\lambda_k - q}{\lambda_j - q}\right]^m v_{p_{m-1}}^{(j)}}{\beta_k v_{p_{m-1}}^{(k)} + \sum_{j=1, j\neq k}^{n} \beta_j \left[\frac{\lambda_k - q}{\lambda_j - q}\right]^{m-1} v_{p_{m-1}}^{(j)}}\right] \tag{3}$$

- Thus the choice of q determines the convergence.
- $\frac{1}{\lambda_k - q}$ is a unique dominant eigenvalue of $(\mathbf{A} - q\mathbf{I})^{-1}$.
- The closer q is to an eigenvalue λ_k of $\mathbf{A}$, the faster the convergence since the convergence is of order

$$O\left(\left|\frac{(\lambda - q)^{-1}}{(\lambda_k - q)^{-1}}\right|^m\right) = O\left(\left|\frac{(\lambda_k - q)}{(\lambda - q)}\right|^m\right)$$

where λ represents the eigenvalue of A that is second closest to q .

- The determination of $\mathbf{y}^{(m)}$ in iteration

$$\mathbf{y}^{(m)} = (\mathbf{A} - q\mathbf{I})^{-1}\mathbf{x}^{(m-1)}$$

can be obtained from the equation

$$(\mathbf{A} - q\mathbf{I})\mathbf{y}^{(m)} = \mathbf{x}^{(m)}$$

- In general , Gaussian elimination with pivoting is used to solve this system.
- Although the Inverse Power method requires the solution of an $n \times n$ system at each step , the multipliers can be saved to reduce the computation .
- The selection of q can be based on the Gerschgorin Circle Theorem or on any other means of localizing an eigenvalue.

ALGORITHM 2: the Inverse Power method

To approximate an eigenvalue and an associated eigenvector of the $n \times n$ matrix $\mathbf{A}$ given a nonzero vector **x**:

- **INPUT:** Dimension n; matrix $\mathbf{A}$; vector $\mathbf{x}$; tolerance TOL; maximum number of iterations N.
- **OUTPUT:** Approximate eigenvalue μ; approximate eigenvector $\mathbf{x}$ (with $\|\|\mathbf{x}\|_\infty\| = 1$) or a message that the maximum number of iterations was exceeded.
- **Step 1:** Set $q = \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$.
- **Step 2:** Set $k = 1$.
- **Step 3:** Find the smallest integer p with $1 \leq p \leq n$ and $|x_p| = \|\mathbf{x}\|_\infty$.
- **Step 4** Set $\mathbf{x} = \mathbf{x}/x_p$.

- **Step 5:** While $(k \leq N)$ do Steps 6-12.
  - **Step 6:** Set the linear system $(\mathbf{A} - q\mathbf{I}))\mathbf{y} = \mathbf{x}$.
  - **Step 7:** If the system doesn't have a unique solution, then OUTPUT ('q is an eigenvalue',q);
  - **Step 8:** Set $\mu = y_p$.
  - **Step 9:** Find the smallest integer p with $1 \leq p \leq n$ and $|y_p| = \|\mathbf{y}\|_\infty$.
  - **Step 10:** Set $ERR = \|\mathbf{x} - (\mathbf{y}/y_p)\|_\infty; \mathbf{x} = \mathbf{y}/y_p$.
  - **Step 11:** If $ERR < TOL$ then set $\mu = (1/\mu) + q$;
    - OUTPUT $(\mu, \mathbf{x})$;
    - (Procedure was successfully.)
    - STOP.
  - **Step 12:** Set $k = k + 1$.
- **Step 13:** OUTPUT ('Maximum number of iterations exceeded');(Procedure completed unsuccessfully.)
- STOP.

Rayleigh Quotient Iteration–Rayleigh 商迭代方法

- If $\mathbf{x}$ is an eigenvector of $\mathbf{A}$ with respect to the eigenvalue λ , then $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$. So , $\mathbf{x}^T\mathbf{A}\mathbf{x} = \lambda\mathbf{x}^T\mathbf{x}$ and

$$\lambda = \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\|\mathbf{x}\|_2^2}.$$

- The quantity $\frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$, known as Rayleigh Quotient, has many useful properties.
- It can be use to accelerate the convergence of a method, such as power iteration or inverse power iteration method, since at the kth iteration, the Rayleigh quotient $\frac{\mathbf{x}_k^T\mathbf{A}\mathbf{x}_k}{\mathbf{x}_k^T\mathbf{x}_k}$ gives a better approximation than the basic method alone.

Symmetric Power Method(对称幂法)

- Suppose that the $n \times n$ matrix $\mathbf{A}$ is **symmetric**, thus $\mathbf{A}$ has n eigenvalues

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

with real number, and a collection of eigenvectors

$$\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \cdots, \mathbf{v}^{(n)}$$

which are orthonormal.

- For any vector $\mathbf{x}_0$ in $\mathbb{R}^n$, there exists a set of constants $\beta_1, \beta_2, \cdots, \beta_n$, such that:

$$x_0 = \beta_1 \mathbf{v}^{(1)} + \beta_2 \mathbf{v}^{(2)} + \cdots + \beta_n \mathbf{v}^{(n)}$$

- Then for the power of $\mathbf{x}_k = \mathbf{A}^k \mathbf{x}_0$, it can be rewritten as

$$\mathbf{x}_k = \mathbf{A}^k \mathbf{x} = \beta_1 \lambda_1^k \mathbf{v}^{(1)} + \beta_2 \lambda_2^k \mathbf{v}^{(2)} + \cdots + \beta_n \lambda_n^k \mathbf{v}^{(n)}$$

- Since the set of eigenvectors $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \cdots, \mathbf{v}^{(n)}$ are orthonormal, it can be seen that

$$\mathbf{x}_k^T \mathbf{x}_k = \sum_{j=1}^{n} \beta_j^2 \lambda_j^{2k} = \beta_1^2 \lambda_1^{2k} \left\{ 1 + \sum_{j=2}^{n} \left(\frac{\beta_j}{\beta_1} \right)^2 \left(\frac{\lambda_j}{\lambda_1} \right)^{2k} \right\},$$

and

$$\begin{aligned} \mathbf{x}_k^T \mathbf{A} \mathbf{x}_k &= \sum_{j=1}^{n} \beta_j^2 \lambda_j^{2k+1} \\ &= \beta_1^2 \lambda_1^{2k+1} \left\{ 1 + \sum_{j=2}^{n} \left(\frac{\beta_j}{\beta_1} \right)^2 \left(\frac{\lambda_j}{\lambda_1} \right)^{2k+1} \right\}. \end{aligned}$$

- Thus

$$\lim_{k\to\infty} \frac{\mathbf{x}_k^T \mathbf{A}\mathbf{x}_k}{\mathbf{x}_k^T \mathbf{x}_k} = \lambda_1$$

$$\lim_{k\to\infty} \frac{\mathbf{x}_k}{\|\mathbf{x}_k\|_2} = \frac{\mathbf{v}^{(1)}}{\|\mathbf{v}^{(1)}\|_2}.$$

- The rate of convergence of the modified procedure given in Rayleigh Method for symmetric matrix is $O(|\lambda_2/\lambda_1|^{2m})$.
- The sequence $\{\mu^{(m)}\}_{m=1}^{\infty}$ is still linearly convergent.

ALGORITHM 3 Symmetric Power Method

- To approximate the dominant eigenvalue and an associated eigenvector of the $n \times n$ symmetric matrix $\mathbf{A}$, given a nonzero vector $\mathbf{x}$:
- **INPUT** dimension n; matrix $\mathbf{A}$; vector $\mathbf{x}$; tolerance TOL; maximum number of iterations N.
- **OUTPUT** approximate eigenvalue μ; approximate eigenvector $\mathbf{x}$ (with $\|\mathbf{x}\|_2 = 1$) or a message that the maximum number of iterations was exceeded.
- **Step 1** Set $k = 1$;

$$\mathbf{x} = \mathbf{x}/\|\mathbf{x}\|_2.$$

- **Step 2** While $(k \leq N)$ do Steps 3-8.
  - **Step 3** Set $\mathbf{y} = A\mathbf{x}$.
  - **Step 4** Set $\mu = \mathbf{x}^T\mathbf{y}$.
  - **Step 5** If $\|\mathbf{y}\|_2 = 0$, then OUTPUT ('Eigenvector', $\mathbf{x}$); OUTPUT ('A has eigenvalue 0, select new vector $\mathbf{x}$ and restart'); STOP.
  - **Step 6** Set

$$
\begin{aligned}
ERR &= \left\| \mathbf{x} - \frac{\mathbf{y}}{\|\mathbf{y}\|_2} \right\|_2 \\
\mathbf{x} &= \mathbf{y}/\|\mathbf{y}\|_2.
\end{aligned}
$$

  - **Step 7** If $ERR < TOL$ then OUTPUT $(\mu, \mathbf{x})$; (Procedure completed successfully.) STOP.
  - **Step 8** Set $k = k + 1$.
- **Step 9** OUTPUT ('Maximum number of iterations exceeded'); (Procedure completed unsuccessfully.) STOP.

Remarks

- If $\mathbf{A}$ is symmetric, then for any real number q, $(\mathbf{A} - q\mathbf{I})^{-1}$ is also symmetric.
- the Symmetric Power method, Algorithm can be applied to $(\mathbf{A} - q\mathbf{I})^{-1}$ to speed the convergence to
$$O\left(\left|\frac{\lambda_k - q}{\lambda - q}\right|^{2m}\right)$$
- Numerous techniques are available for obtaining approximations to other eigenvalues are the same as those of $\mathbf{A}$, except that the dominant eigenvalue of $\mathbf{A}$ is replaced by the eigenvalue 0.

Deflation–求全部特征值的收缩算法

Theorem 4.12

- Suppose $\lambda_1, \lambda_2, \cdots, \lambda_n$ are eigenvalues of $\mathbf{A}$ with associated eigenvectors $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \cdots, \mathbf{v}^{(n)}$ and λ_1 has multiplicity 1.
- Let $\mathbf{x}$ be a vector with $\mathbf{x}^T\mathbf{v}^{(1)} = 1$.
- Then the matrix

$$\mathbf{B} = \mathbf{A} - \lambda_1 \mathbf{v}^{(1)} \mathbf{x}^T$$

has eigenvalues 0 , $\lambda_2, \lambda_3, \cdots, \lambda_n$ with associated eigenvectors $\mathbf{v}^{(1)}, \mathbf{w}^{(2)}, \mathbf{w}^{(3)}, \cdots, \mathbf{w}^{(n)}$, where $\mathbf{v}^{(i)}$ and $\mathbf{w}^{(i)}$ are related by the equation

$$\mathbf{v}^{(i)} = (\lambda_i - \lambda_1)\mathbf{w}^{(i)} + \lambda_1(\mathbf{x}^T\mathbf{w}^{(i)})\mathbf{v}^{(1)} \tag{4}$$

for each $i = 2, 3, \cdots, n$.■

- After eigenvalue λ_1 and corresponding eigenvector $\mathbf{x}_1$ have been computed, then additional eigenvalues $\lambda_2, \lambda_3, \cdots, \lambda_n$ of $\mathbf{A}$ can be computed by deflation, which effectively removes known eigenvalue.
- Let $\mathbf{H}$ be any nonsingular matrix such that $\mathbf{H}\mathbf{x}_1 = \alpha\mathbf{e}_1$ scalar multiple of first column of identity matrix (Householder transformation is good choice for $\mathbf{H}$)
- Then similarity transformation determined by H transforms $\mathbf{A}$ into form

$$\mathbf{H}\mathbf{A}\mathbf{H}^{-1} = \begin{bmatrix} \lambda_1 & \mathbf{b}^T \\ 0 & \mathbf{B} \end{bmatrix}$$

where $\mathbf{B}$ is matrix of order $n-1$ having eigenvalues $\lambda_2, \lambda_3, \cdots, \lambda_n$.

- Thus, we can work with $\mathbf{B}$ to compute next eigenvalue λ_2.
- Moreover, if $\mathbf{y}_2$ is eigenvector of $\mathbf{B}$ corresponding to λ_2, then

$$\mathbf{x}_2 = \mathbf{H}^{-1} \begin{bmatrix} \gamma \\ \mathbf{y}_2 \end{bmatrix}, \texttt{where} \quad \gamma = \frac{\mathbf{b}^T \mathbf{y}_2}{\lambda_2 - \lambda_1}$$

  is eigenvector corresponding to λ_2 for original matrix $\mathbf{A}$, provided $\lambda_1 = \lambda_2$.
- Process can be repeated to find additional eigenvalues and eigenvectors

- Alternative approach to deflation is to let $\mathbf{u}_1$ be any vector such that

$$\mathbf{u}_1^T \mathbf{x}_1 = \lambda_1$$

- Then the matrix $\mathbf{A} - \mathbf{x}_1 \mathbf{u}_1^T$ has eigenvalues

$$0, \lambda_2, \cdots, \lambda_n.$$

- Possible choices for $\mathbf{u}_1$ include
  - $\mathbf{u}_1 = \lambda_1 \mathbf{x}_1$, if $\mathbf{A}$ is symmetric and $\mathbf{x}_1$ is normalized so that $\|\mathbf{x}_1\|_2 = 1$.
  - $\mathbf{u}_1 = \lambda_1 \mathbf{y}_1$, where $\mathbf{y}_1$ is corresponding left eigenvector (i.e., $\mathbf{A}^T \mathbf{y}_1 = \lambda_1 \mathbf{y}_1$) normalized so that $\mathbf{y}_1^T \mathbf{x}_1 = 1$.
  - $\mathbf{u}_1 = \mathbf{A}^T \mathbf{e}_k$, if $\mathbf{x}_1$ is normalized so that $\|\mathbf{x}_1\|_\infty = 1$ and kth component of $\mathbf{x}_1$ is 1.

Wielandt deflation

- **Wielandt deflation** proceeds from defining

$$\mathbf{x} = \frac{1}{\lambda_1 v_i^{(1)}} \begin{bmatrix} a_{i1} \\ a_{i2} \\ \vdots \\ a_{in} \end{bmatrix} \tag{5}$$

where $v_i^{(1)}$ is a coordinate of $\mathbf{v}^{(1)}$ that is nonzero , and the values $a_{i1}, a_{i2}, \cdots , a_{in}$ are the entries in the ith row of $\mathbf{A}$.

- With this definition ,

$$\begin{aligned}
\mathbf{x}^T\mathbf{v}^{(1)} &= \frac{1}{\lambda_1 v_i^{(1)}}[a_{i1}, a_{i2}, \cdots, a_{in}]\left(v_1^{(1)}, v_2^{(1)}, \cdots, v_n^{(1)}\right)^T \\
&= \frac{1}{\lambda_1 v_i^{(1)}}\sum_{j=1}^{n} a_{ij}v_j^{(1)}
\end{aligned}$$

where the sum is the ith coordinate of the product $A\mathbf{v}^{(1)}$.

- Since $\mathbf{A}\mathbf{v}^{(1)} = \lambda_1\mathbf{v}^{(1)}$, we have

$$\sum_{j=1}^{n} a_{ij}v_j^{(1)} = \lambda_1 v_i^{(1)}$$

which implies that

$$\mathbf{x}^T\mathbf{v}^{(1)} = \frac{1}{\lambda_1 v_i^{(1)}}\left(\lambda_1 v_i^{(1)}\right) = 1.$$

- So $\mathbf{x}$ satisfies the hypotheses of Theorem 4.12

- Moreover , the ith row of $\mathbf{B} = \mathbf{A} - \lambda_1 \mathbf{v}^{(1)} \mathbf{x}^T$ consists entirely of zero entries.
- If $\lambda \neq 0$ is an eigenvalue with associated eigenvector $\mathbf{w}$, the relation $B\mathbf{w} = \lambda \mathbf{w}$ implies that the ith coordinate of $\mathbf{w}$ must also be zero .
- Consequently the ith column of the matrix $\mathbf{B}$ makes no contribution to the product $\mathbf{B}\mathbf{w} = \lambda \mathbf{w}$.
- Thus , the matrix B can be replaced by an $(n-1) \times (n-1)$ matrix $\mathbf{B}'$ has eigenvalues $\lambda_2, \lambda_3, \cdots, \lambda_n$.

- If $|\lambda_2| > |\lambda_3|$, the Power method is reapplied to the matrix B' to determine this new dominant eigenvalue and an eigenvector , $\mathbf{w}^{(2)'}$, associated with λ_2 , with respect to the matrix B' .
- To find the associated eigenvector $\mathbf{w}^{(2)}$ for the matrix B , insert a zero coordinate between the coordinates $w_{i-1}^{(2)'}$ and $w_i^{(2)'}$ of the $(n-1)$-dimensional vector $\mathbf{w}^{(2)'}$ and then calculate $\mathbf{v}^{(2)}$ by the use of Eq.(4).

ALGORITHM 4 Wielandt Deflation Technique

- To approximate the second most dominant eigenvalue and an associated eigenvector of the $n \times n$ matrix $\mathbf{A}$ given an approximation λ to the dominant eigenvalue, an approximation $\mathbf{v}$ to a corresponding eigenvector, and a vector $\mathbf{x} \in \mathbb{R}^{n-1}$:
- **INPUT** dimension n; matrix A; approximate eigenvalue λ with eigenvector $\mathbf{v} \in \Re R^n$; vector $\mathbf{x} \in \Re R^{n-1}$, tolerance TOL, maximum number of iterations N.
- **OUTPUT** approximate eigenvalue μ; approximate eigenvector $\mathbf{u}$ or a message that the method fails.
- **Step 1** Let i be the smallest integer with $1 \leq i \leq n$ and $|v_i| = \max\limits_{1 \leq j \leq n} |v_j|$.

- **Step 2** If $i \neq 1$ then
    - for $k = 1, \cdots, i-1$
        - for $j = 1, \cdots, i-1$
        - set
$$b_{kj} = a_{kj} - \frac{v_k}{v_i} a_{ij};$$
- **Step 3** If $i \neq 1$ and $i \neq n$ then
    - for $k = i, \cdots, n-1$
        - for $j = 1, \cdots, i-1$
        - set
$$\begin{aligned} b_{kj} &= a_{k+1,j} - \frac{v_{k+1}}{v_i} a_{i,j}; \\ b_{jk} &= a_{j,k+1} - \frac{v_j}{v_i} a_{i,k+1}; \end{aligned}$$
- **Step 4** If $i \neq n$ then
    - for $k = i, \cdots, n-1$
        - for $j = i, \cdots, n-1$
        - set $b_{kj} = a_{k+1,j+1} - \frac{v_{k+1}}{v_i} a_{i,j+1};$
- **Step 5** Perform the power method on the $(n-1) \times (n-1)$ matrix $B' = (b_{kj})$ with $\mathbf{x}$ as initial approximation.

- **Step 6** If the method fails, then OUTPUT ('Method fails'); STOP.
  Else let μ be the approximate eigenvalue and $\mathbf{w}' = (w_1', w_2', \cdots, w_{n-1}')$ the approximate eigenvector.
- **Step 7** If $i \neq 1$ then for $k = 1, \cdots, i-1$ set $w_k = w_k'$.
- **Step 8** Set $w_i = 0$.
- **Step 9** If $i \neq n$ then for $k = i+1, \cdots, n$ set $w_k = w_{k-1}'$.
- **Step 10** For $k = 1, \cdots, n$ set

$$u_k = (\mu - \lambda) w_k + \left(\sum_{j=1}^{n} a_{ij} w_j \right) \frac{v_k}{v_i}.$$

  (Compute the eigenvector using Eq. (4).)
- **Step 11** OUTPUT $(\mu, \mathbf{u})$;
  (Procedure completed successfully.)
  STOP.

- Possible methods include:
  - Householder transformations
  - Givens rotations
  - Gram-Schmidt orthogonalization

11.3.1 Householder transformation

- **Householder transformation** has form

$$\mathbf{H} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}$$

for nonzero vector $\mathbf{v}$

- $\mathbf{H}$ is orthogonal and symmetric:

$$\mathbf{H} = \mathbf{H}^T = \mathbf{H}^{-1}$$

- **Notes:**

$$\begin{aligned}\mathbf{H}\mathbf{H} &= (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}) \\ &= \mathbf{I} - 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} + 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \\ &= \mathbf{I}\end{aligned}$$

- **Householder transformation** has form

$$\mathbf{H} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}$$

for nonzero vector $\mathbf{v}$

- $\mathbf{H}$ is orthogonal and symmetric:

$$\mathbf{H} = \mathbf{H}^T = \mathbf{H}^{-1}$$

- **Notes:**

$$\begin{aligned} \mathbf{H}\mathbf{H} &= (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}) \\ &= \mathbf{I} - 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} + 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \\ &= \mathbf{I} \end{aligned}$$

11.3.1 Householder transformation

- **Householder transformation** has form

$$\mathbf{H} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}$$

for nonzero vector $\mathbf{v}$

- $\mathbf{H}$ is orthogonal and symmetric:

$$\mathbf{H} = \mathbf{H}^T = \mathbf{H}^{-1}$$

- **Notes:**

$$\begin{aligned}
\mathbf{H}\mathbf{H} &= (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}) \\
&= \mathbf{I} - 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} + 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \\
&= \mathbf{I}
\end{aligned}$$

- Given vector $\mathbf{a}$, we want to choose $\mathbf{v}$, so that

$$\mathbf{Ha} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \mathbf{e}_1$$

- Substituting into formula for $\mathbf{H}$, we have

$$\alpha \mathbf{e}_1 = \mathbf{Ha} = \left(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \right) \mathbf{a} = \mathbf{a} - 2\mathbf{v}\frac{\mathbf{v}^T\mathbf{a}}{\mathbf{v}^T\mathbf{v}}$$

- then

$$\mathbf{v} = (\mathbf{a} - \alpha \mathbf{e}_1)\frac{\mathbf{v}^T\mathbf{v}}{2\mathbf{v}^T\mathbf{a}}$$

- Given vector $\mathbf{a}$, we want to choose $\mathbf{v}$, so that

$$\mathbf{Ha} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \mathbf{e}_1$$

- Substituting into formula for $\mathbf{H}$, we have

$$\alpha \mathbf{e}_1 = \mathbf{Ha} = \left(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \right) \mathbf{a} = \mathbf{a} - 2\mathbf{v}\frac{\mathbf{v}^T\mathbf{a}}{\mathbf{v}^T\mathbf{v}}$$

- then

$$\mathbf{v} = (\mathbf{a} - \alpha \mathbf{e}_1)\frac{\mathbf{v}^T\mathbf{v}}{2\mathbf{v}^T\mathbf{a}}$$

- Given vector $\mathbf{a}$, we want to choose $\mathbf{v}$, so that

$$\mathbf{Ha} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \mathbf{e}_1$$

- Substituting into formula for $\mathbf{H}$, we have

$$\alpha \mathbf{e}_1 = \mathbf{Ha} = \left(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \right) \mathbf{a} = \mathbf{a} - 2\mathbf{v}\frac{\mathbf{v}^T\mathbf{a}}{\mathbf{v}^T\mathbf{v}}$$

- then

$$\mathbf{v} = (\mathbf{a} - \alpha \mathbf{e}_1)\frac{\mathbf{v}^T\mathbf{v}}{2\mathbf{v}^T\mathbf{a}}$$

- Let $\mathbf{v} = \mathbf{a} - \alpha \mathbf{e}_1$
- To preserve the norm, we let

$$\alpha = \pm \|\mathbf{a}\|_2$$

i.e.,

$$\alpha = -\mathbf{sign}(a_1)\|\mathbf{a}\|_2$$

with sign chosen to avoid cancellation.

- If $\mathbf{a} = [2 \quad 1 \quad 2]^T$, then we take

$$\mathbf{v} = \mathbf{a} - \alpha \mathbf{e}_1 = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \alpha \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} \alpha \\ 0 \\ 0 \end{bmatrix}$$

  where $\alpha = \pm \|\mathbf{a}\|_2 = \pm 3$.
- Since $a_1 > 0$, we choose $\alpha = -\|\mathbf{a}\|_2 = -3$, so

$$\mathbf{v} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

- To confirm that transformation works,

$$\mathbf{H}\mathbf{a} = \mathbf{a} - 2\frac{\mathbf{v}^T\mathbf{a}}{\mathbf{v}^T\mathbf{v}}\mathbf{v} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - 2\frac{15}{30} \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}$$

Householder QR Factorization

- To compute $\mathbf{QR}$ factorization of $\mathbf{A}$, use Householder transformations to annihilate subdiagonal entries of each successive column
- Each Householder transformation is applied to entire matrix, but does not affect prior columns, so zeros are preserved
- In applying Householder transformation $\mathbf{H}$ to arbitrary vector $\mathbf{u}$,

$$\mathbf{Hu} = (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})\mathbf{u} = \mathbf{u} - 2\frac{\mathbf{v}^T\mathbf{u}}{\mathbf{v}^T\mathbf{v}}\mathbf{v}$$

  which is much cheaper than general matrix-vector multiplication and requires only vector $\mathbf{v}$, not full matrix $\mathbf{H}$.

Householder $\mathbf{QR}$ Factorization

- To compute $\mathbf{QR}$ factorization of $\mathbf{A}$, use Householder transformations to annihilate subdiagonal entries of each successive column
- Each Householder transformation is applied to entire matrix, but does not affect prior columns, so zeros are preserved
- In applying Householder transformation $\mathbf{H}$ to arbitrary vector $\mathbf{u}$,

$$\mathbf{H}\mathbf{u} = (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})\mathbf{u} = \mathbf{u} - 2\frac{\mathbf{v}^T\mathbf{u}}{\mathbf{v}^T\mathbf{v}}\mathbf{v}$$

which is much cheaper than general matrix-vector multiplication and requires only vector $\mathbf{v}$, not full matrix $\mathbf{H}$.

Householder $\mathbf{QR}$ Factorization

- To compute $\mathbf{QR}$ factorization of $\mathbf{A}$, use Householder transformations to annihilate subdiagonal entries of each successive column
- Each Householder transformation is applied to entire matrix, but does not affect prior columns, so zeros are preserved
- In applying Householder transformation $\mathbf{H}$ to arbitrary vector $\mathbf{u}$,

$$\mathbf{H}\mathbf{u} = (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})\mathbf{u} = \mathbf{u} - 2\frac{\mathbf{v}^T\mathbf{u}}{\mathbf{v}^T\mathbf{v}}\mathbf{v}$$

which is much cheaper than general matrix-vector multiplication and requires only vector $\mathbf{v}$, not full matrix $\mathbf{H}$.

- Process just described produces factorization

$$\mathbf{H}_n \cdots \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$$

where $\mathbf{R}$ is $n \times n$ and upper triangular.

- If $\mathbf{Q} = \mathbf{H}_1 \cdots \mathbf{H}_n$, then $\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$.
- To preserve solution of linear least squares problem, right-hand side b is transformed by same sequence of Householder transformations.
- Then solve triangular least squares problem

$$\begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix} \mathbf{x} \cong \mathbf{Q}^T \mathbf{b}$$

- Process just described produces factorization

$$\mathbf{H}_n \cdots \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$$

  where $\mathbf{R}$ is $n \times n$ and upper triangular.

- If $\mathbf{Q} = \mathbf{H}_1 \cdots \mathbf{H}_n$, then $\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$.

- To preserve solution of linear least squares problem, right-hand side $\mathbf{b}$ is transformed by same sequence of Householder transformations.

- Then solve triangular least squares problem

$$\begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix} \mathbf{x} \cong \mathbf{Q}^T \mathbf{b}$$

- Process just described produces factorization

$$\mathbf{H}_n \cdots \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$$

  where $\mathbf{R}$ is $n \times n$ and upper triangular.
- If $\mathbf{Q} = \mathbf{H}_1 \cdots \mathbf{H}_n$, then $\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$.
- To preserve solution of linear least squares problem, right-hand side $\mathbf{b}$ is transformed by same sequence of Householder transformations.
- Then solve triangular least squares problem

$$\begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix} \mathbf{x} \cong \mathbf{Q}^T \mathbf{b}$$

- Process just described produces factorization

$$\mathbf{H}_n \cdots \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$$

where $\mathbf{R}$ is $n \times n$ and upper triangular.

- If $\mathbf{Q} = \mathbf{H}_1 \cdots \mathbf{H}_n$, then $\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$.
- To preserve solution of linear least squares problem, right-hand side $\mathbf{b}$ is transformed by same sequence of Householder transformations.
- Then solve triangular least squares problem

$$\begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix} \mathbf{x} \cong \mathbf{Q}^T \mathbf{b}$$

- For solving linear least squares problem, product $\mathbf{Q}$ of Householder transformations need not be formed explicitly.
- $\mathbf{R}$ can be stored in upper triangle of array initially containing $\mathbf{A}$.
- Householder vectors $\mathbf{v}$ can be stored in (now zero) lower triangular portion of $\mathbf{A}$ (almost)
- Householder transformations most easily applied in this form anyway

Example: Householder QR Factorization

- For polynomial data-fitting example given previously, with

$$\mathbf{A} = \begin{bmatrix} 1 & -1 & 1.0 \\ 1 & -0.5 & 0.25 \\ 1 & 0.0 & 0.0 \\ 1 & 0.5 & 0.25 \\ 1 & 1.0 & 1.0 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 0.5 \\ 2.0 \end{bmatrix}$$

- Householder vector $\mathbf{v}_1$ for annihilating subdiagonal entries of first column of $\mathbf{A}$ is

$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} -2.236 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 3.236 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

- Applying resulting Householder transformation $\mathbf{H}_1$ yields transformed matrix and right-hand side:

$$\mathbf{H}_1\mathbf{A} = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & -0.191 & -0.405 \\ 0 & 0.309 & -0.655 \\ 0 & 0.809 & -0.405 \\ 0 & 1.309 & 0.345 \end{bmatrix}, \quad \mathbf{H}_1\mathbf{b} = \begin{bmatrix} -1.789 \\ -0.362 \\ -0.862 \\ -0.362 \\ 1.138 \end{bmatrix}$$

- Householder vector $\mathbf{v}_2$ for annihilating subdiagonal entries of second column of $\mathbf{H}_1\mathbf{A}$ is

$$\mathbf{v}_2 = \begin{bmatrix} 0 \\ -0.191 \\ 0.309 \\ 0.809 \\ 1.309 \end{bmatrix} - \begin{bmatrix} 0 \\ 1.581 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -1.772 \\ 0.309 \\ 0.809 \\ 1.309 \end{bmatrix}$$

- Applying resulting Householder transformation $\mathbf{H}_2$ yields

$$\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & -0.725 \\ 0 & 0 & -0.589 \\ 0 & 0 & 0.047 \end{bmatrix}, \quad \mathbf{H}_2\mathbf{H}_1\mathbf{b} = \begin{bmatrix} -1.789 \\ 0.632 \\ -1.035 \\ -0.816 \\ 0.404 \end{bmatrix}$$

- Householder vector $\mathbf{v}_3$ for annihilating subdiagonal entries of third column of $\mathbf{H}_2\mathbf{H}_1\mathbf{A}$ is

$$\mathbf{v}_3 = \begin{bmatrix} 0 \\ 0 \\ -0.725 \\ -0.589 \\ 0.047 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0.935 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -1.660 \\ -0.589 \\ 0.047 \end{bmatrix}$$

- Applying resulting Householder transformation $\mathbf{H}_3$ yields

$$\mathbf{H}_3\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & 0.935 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{H}_3\mathbf{H}_2\mathbf{H}_1\mathbf{b} = \begin{bmatrix} -1.789 \\ 0.632 \\ 1.336 \\ 0.026 \\ 0.337 \end{bmatrix}$$

- Now solve upper triangular system $\mathbf{R}\mathbf{x} = \mathbf{c}_1$ by back-substitution to obtain $\mathbf{x} = [0.086 \quad 0.400 \quad 1.429]^T$.

Givens Rotations

- Givens rotations introduce zeros one at a time
- Given vector $[a_1 \quad a_2]^T$, choose scalars c and s so that
$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$$
with $c^2 + s^2 = 1$, or equivalently, $\alpha = \sqrt{a_1^2 + a_2^2}$.
- Previous equation can be rewritten
$$\begin{bmatrix} a_1 & a_2 \\ a_2 & -a_1 \end{bmatrix} \begin{bmatrix} c \\ s \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$$

- Gaussian elimination yields triangular system

$$\begin{bmatrix} a_1 & a_2 \\ 0 & -a_1 - a_2^2/a_1 \end{bmatrix} \begin{bmatrix} c \\ s \end{bmatrix} = \begin{bmatrix} \alpha \\ -\alpha\, a_2/a_1 \end{bmatrix}$$

- Back-substitution then gives

$$s = \frac{\alpha\, a_2}{a_1^2 + a_2^2} \quad \text{and} \quad c = \frac{\alpha\, a_1}{a_1^2 + a_2^2}$$

- Finally, $c^2 + s^2 = 1$, or $\alpha = \sqrt{a_1^2 + a_2^2}$, implies

$$s = \frac{a_2}{\sqrt{a_1^2 + a_2^2}} \quad \text{and} \quad c = \frac{a_1}{\sqrt{a_1^2 + a_2^2}}$$

- More generally, to annihilate any desired component of vector in n dimensions, rotate target component with another component say (i, j).
- For example, let $n = 5, i = 4, j = 2$

$$
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & c & 0 & s & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & -s & 0 & c & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\
a_{21} & {\color{blue}a_{22}} & a_{23} & a_{24} & a_{25} \\
a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\
a_{41} & {\color{blue}a_{42}} & a_{43} & a_{44} & a_{45} \\
a_{51} & a_{52} & a_{53} & a_{54} & a_{55}
\end{bmatrix}
$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots \\ ca_{21} + sa_{41} & ca_{22} + sa_{42} & ca_{23} + sa_{43} & ca_{24} + sa_{44} & ca_{25} \cdots \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdots \\ -sa_{21} + ca_{41} & -sa_{22} + ca_{42} & -sa_{23} + ca_{43} & -sa_{24} + ca_{44} & -sa_{\cdots} \\ a_{51} & a_{52} & a_{53} & a_{54} & \cdots \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ \hat{a}_{21} & \hat{a}_{22} & \hat{a}_{23} & \hat{a}_{24} & \hat{a}_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ \hat{a}_{41} & 0 & \hat{a}_{43} & \hat{a}_{44} & \hat{a}_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix}$$

Note that: Let

$$c = \frac{a_{22}}{\sqrt{a_{22}^2 + a_{42}^2}}, s = \frac{a_{42}}{\sqrt{a_{22}^2 + a_{42}^2}}$$

- By systematically annihilating successive entries, we can reduce matrix to upper triangular form using sequence of Givens rotations.
- **Each rotation is orthogonal,** so **their product is orthogonal**, producing $\mathbf{QR}$ factorization.
- Straightforward implementation of Givens method requires about 50% more work than Householder method, and also requires more storage, since each rotation requires two numbers, c and s, to define it.
- These disadvantages can be overcome, but requires more complicated implementation.
- Givens can be advantageous for computing $\mathbf{QR}$ factorization when many entries of matrix are already zero, since those annihilations can then be skipped.

To solve least square problem

$$\mathbf{Ax} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cong \begin{bmatrix} 1237 \\ 1941 \\ 2417 \\ 711 \\ 1177 \\ 475 \end{bmatrix} = \mathbf{b}$$

- First, to eliminate the entry in the position (4,1) of $\mathbf{G_1A}$, since $\sqrt{1^2+(-1)^2}=\sqrt{2}$, so $c=1/\sqrt{2}$, $s=-1/\sqrt{2}$, and the first Givens matrix is

$$\mathbf{G}_1=\begin{bmatrix}0.7071 & 0 & 0 & 0 & -0.7071 & 0\\ 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0\\ 0.7071 & 0 & 0 & 0 & 0.7071 & 0\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}$$

- Applying this rotation to $\mathbf{A}$ and $\mathbf{b}$, yields

$$\mathbf{G}_1\mathbf{A}=\begin{bmatrix}1.4142 & 0 & -0.7071\\ 0 & 1 & 0\\ 0 & 0 & 1\\ -1 & 1 & 0\\ 0 & 0 & 0.7071\\ 0 & -1 & 1\end{bmatrix}, \quad \mathbf{G}_1\mathbf{b}=\begin{bmatrix}42\\ 1941\\ 2417\\ 711\\ 1707\\ 475\end{bmatrix}$$

- Second, to eliminate the entry in the position (4,1), since $\sqrt{1.4142^2 + (-1)^2} = \sqrt{3}$, so $c = \sqrt{2}/\sqrt{3}$, $s = -1/\sqrt{3}$, and the second Givens matrix is

$$\mathbf{G}_2 = \begin{bmatrix} 0.8165 & 0 & 0 & -5774 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0.5774 & 0 & 0 & 0.8165 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

- Applying this rotation to $\mathbf{G_1 A}$ and $\mathbf{G_1 b}$, yields

$$\mathbf{G}_2\mathbf{G}_1\mathbf{A} = \begin{bmatrix} 1.7321 & -0.5774 & -0.5774 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0.8165 & -0.4082 \\ 0 & 0 & 0.7071 \\ 0 & -1 & 1 \end{bmatrix}, \mathbf{G}_2\mathbf{G}_1\mathbf{b} = \begin{bmatrix} -376 \\ 1941 \\ 2417 \\ 605 \\ 1707 \\ 475 \end{bmatrix}$$

- Third working for the bottom of the other column of $\mathbf{G_2 G_1 A}$, to eliminate the entry in the position (6,2),(4,2) and (6,3),(5,3),(4,3) with Givens rotation matrix.
- Finally yields

$$\mathbf{Q}^T\mathbf{A} = \begin{bmatrix} 1.7321 & -0.5774 & -0.5774 \\ 0 & 1.6330 & -0.8165 \\ 0 & 0 & 1.4142 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{Q}^T\mathbf{b} = \begin{bmatrix} -376 \\ 1200 \\ 2417 \\ 5.66 \\ -1.63 \\ -0.56 \end{bmatrix}$$

- We can now solve the upper triangular system by backward-substitution to obtain $\mathbf{x} = [1236 \quad 1943 \quad 2416]^T$

Gram-Schmidt Orthogonalization

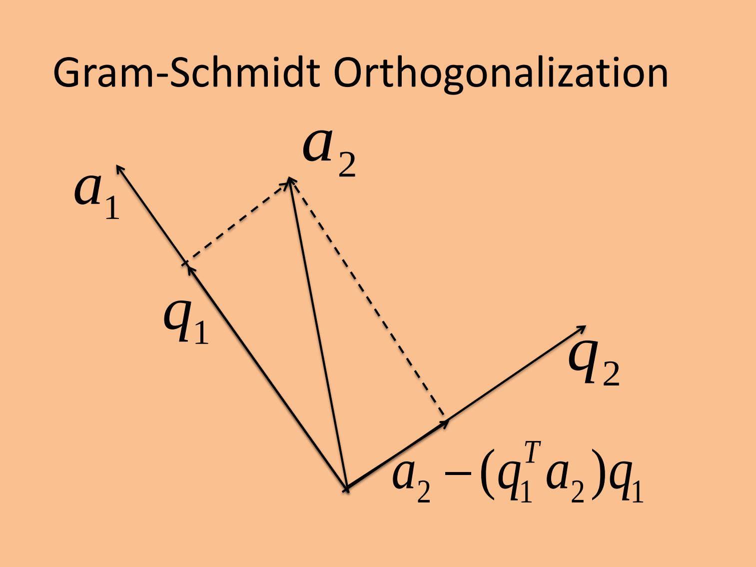
- Given vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, we seek orthonormal vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ having same span.
- We first normalize $\mathbf{a}_1$ to obtain

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{\|\mathbf{a}_1\|_2}.$$

- Next we want to subtract from $\mathbf{a}_2$ its component in $\mathbf{q}_1$, as shown in diagram.

$$\mathbf{q}_2 = \mathbf{a}_2 - (\mathbf{q}_1^T \mathbf{a}_2)\mathbf{q}_1$$

$$\mathbf{q}_2 = \frac{\mathbf{q}_2}{\|\mathbf{q}_2\|}.$$


Gram-Schmidt Orthogonalization
a_2
a_1
q_1
q_2
$a_2-(q_1^T a_2)q_1$

THEOREM: The Orthogonal Decomposition Theorem — 正交分解定理

Let W be a subspace of $\mathbb{R}^n$. Then each $\mathbf{y}$ in $\mathbb{R}^n$ can be written uniquely in the form

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \tag{6}$$

where $\hat{\mathbf{y}}$ is in W and $\mathbf{z}$ is in $W^{\perp}$.

如何求$\hat{\mathbf{y}}$ 和$\mathbf{z}$?

事实上, 若 $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ 是子空间 W 的正交基, 则

$$\hat{\mathbf{y}} = \frac{\mathbf{y}\cdot\mathbf{u}_1}{\mathbf{u}_1\cdot\mathbf{u}_1}\mathbf{u}_1 + \frac{\mathbf{y}\cdot\mathbf{u}_2}{\mathbf{u}_2\cdot\mathbf{u}_2}\mathbf{u}_2 + \cdots + \frac{\mathbf{y}\cdot\mathbf{u}_p}{\mathbf{u}_p\cdot\mathbf{u}_p}\mathbf{u}_p \quad (7)$$

进而，可以很容易地得出:

$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}.$$

定理证明:

- 若 $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ 是$\mathbb{R}^n$ 空间的子空间 W 的一个正交基, 由于 $\hat{\mathbf{y}} \in W$, 则 $\hat{\mathbf{y}} \in W$ 可以写成如下关于正交基 $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ 的线性组合:

$$\hat{\mathbf{y}} = \frac{\mathbf{y}\cdot\mathbf{u}_1}{\mathbf{u}_1\cdot\mathbf{u}_1}\mathbf{u}_1 + \frac{\mathbf{y}\cdot\mathbf{u}_2}{\mathbf{u}_2\cdot\mathbf{u}_2}\mathbf{u}_2 + \cdots + \frac{\mathbf{y}\cdot\mathbf{u}_p}{\mathbf{u}_p\cdot\mathbf{u}_p}\mathbf{u}_p$$

- 令: $\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$.
- 则可以证明: $\mathbf{z} \in W^{\perp}$.

$$\begin{aligned}
\mathbf{z}\cdot\mathbf{u}_1 &= (\mathbf{y}-\hat{\mathbf{y}})\cdot\mathbf{u}_1 \\
&= \mathbf{y}\cdot\mathbf{u}_1 - \frac{\mathbf{y}\cdot\mathbf{u}_1}{\mathbf{u}_1\cdot\mathbf{u}_1}\mathbf{u}_1\cdot\mathbf{u}_1 - 0 - \cdots - 0 \\
&= \mathbf{y}\cdot\mathbf{u}_1 - \mathbf{y}\cdot\mathbf{u}_1 = 0
\end{aligned}$$

- 类似地，可以证明 $\mathbf{z}$ 与 W 中每一个基向量 $\mathbf{u}_i, i = 1, 2, \cdots, p$ 都正交, 而

$$W = \mathrm{Span}\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$$

所以, $\mathbf{z}$ 与 W 中任意向量都正交, 即 $\mathbf{z} \in W^{\perp}$.

- 再证正交分解的唯一性: 设 $\mathbf{y} = \hat{\mathbf{y}}_1 + \mathbf{z}_1$ $(\mathbf{y}_1 \in W, \mathbf{z}_1 \in W^{\perp})$ 是另一个正交分解. 则

$$\hat{\mathbf{y}} + \mathbf{z} = \hat{\mathbf{y}}_1 + \mathbf{z}_1$$

或写成

$$\hat{\mathbf{y}} - \hat{\mathbf{y}}_1 = \mathbf{z}_1 - \mathbf{z}.$$

- 注意到上式左端向量 $(\hat{\mathbf{y}} - \hat{\mathbf{y}}_1) \in W$, 而右端向量 $(\mathbf{z}_1 - \mathbf{z}) \in W^{\perp}$.
此类情况当且仅当两端同时为零向量时方可成立.
于是$\hat{\mathbf{y}} = \hat{\mathbf{y}}_1, \mathbf{z}_1 = \mathbf{z}$, 即正交分解是唯一的.■■

- If $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ is any orthogonal basis of W, and $\mathbf{y} \in W$, then

$$\hat{\mathbf{y}} = \mathrm{Proj}_W \mathbf{y} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1}\mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2}\mathbf{u}_2 + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p}\mathbf{u}_p$$

- **THEOREM—The Best Approximation Theorem(最优逼近定理)**
  Let W be a subspace of $\mathbb{R}^n$, $\mathbf{y}$ any vector in $\mathbb{R}^n$, and $\hat{\mathbf{y}}$ the any orthogonal projection of $\mathbf{y}$ onto W. Then $\hat{\mathbf{y}}$ is the closest point in W to $\mathbf{y}$. In the sense that

$$\|\mathbf{y} - \hat{\mathbf{y}}\| \leq \|\mathbf{y} - \mathbf{v}\|$$

  for all $\mathbf{v} \in W$ distinct from $\hat{\mathbf{y}}$.

Proof of Theorem:

- Suppose $\mathbf{v} \in W$, then $\hat{\mathbf{y}} - \mathbf{v}$ also in W, by the orthogonal decomposition theorem, $\mathbf{y} - \hat{\mathbf{y}}$ is orthogonal to W, that is $\mathbf{y} - \hat{\mathbf{y}}$ is orthogonal to $\hat{\mathbf{y}} - \mathbf{v}$.
- Since $\mathbf{y} - \mathbf{v} = (\mathbf{y} - \hat{\mathbf{y}}) + (\hat{\mathbf{y}} - \mathbf{v})$
- By the Pythagorean Theorem, gives

$$\|\mathbf{y} - \mathbf{v}\|^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2 + \|\hat{\mathbf{y}} - \mathbf{v}\|^2.$$

- If $\hat{\mathbf{y}} \neq \mathbf{v}$, then we have $\|\hat{\mathbf{y}} - \mathbf{v}\|^2 > 0$, so the inequality

$$\|\mathbf{y} - \hat{\mathbf{y}}\| \leq \|\mathbf{y} - \mathbf{v}\|$$

holds immediately.

THEOREM:

If $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ is an orthonormal basis for a subspace W of $\mathbb{R}^n$, then

$$\text{proj}_W \mathbf{y} = (\mathbf{y} \cdot \mathbf{u}_1)\mathbf{u}_1 + (\mathbf{y} \cdot \mathbf{u}_2)\mathbf{u}_2 + \cdots + (\mathbf{y} \cdot \mathbf{u}_p)\mathbf{u}_p$$

If $\mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_p]$, then

$$\text{proj}_W \mathbf{y} = \mathbf{U}^T\mathbf{U}\mathbf{y}, \quad \forall \mathbf{y} \in \mathbb{R}^n$$

证明: 首先由正交投影定理, 可得

$$\text{proj}_W \mathbf{y} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1}\mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2}\mathbf{u}_2 + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p}\mathbf{u}_p$$

进一步地, 由于$\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$为子空间$W$ 的标准正交基, 故有

$$\mathbf{u}_1 \cdot \mathbf{u}_1 = \mathbf{u}_2 \cdot \mathbf{u}_2 = \cdots = \mathbf{u}_p \cdot \mathbf{u}_p = 1.$$

从而有

$$\mathrm{proj}_W \mathbf{y} = (\mathbf{y} \cdot \mathbf{u}_1)\mathbf{u}_1 + (\mathbf{y} \cdot \mathbf{u}_2)\mathbf{u}_2 + \cdots + (\mathbf{y} \cdot \mathbf{u}_p)\mathbf{u}_p$$

成立.又由

$$\mathbf{y} \cdot \mathbf{u}_1 = \mathbf{u}_1^T \mathbf{y}, \mathbf{y} \cdot \mathbf{u}_2 = \mathbf{u}_2^T \mathbf{y}, \cdots, \mathbf{y} \cdot \mathbf{u}_y = \mathbf{u}_p^T \mathbf{y}$$

所以

$$\mathrm{proj}_W \mathbf{y} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \mathbf{u}_p] \begin{bmatrix} \mathbf{u}_1^T \mathbf{y} \\ \mathbf{u}_2^T \mathbf{y} \\ \vdots \\ \mathbf{u}_p^T \mathbf{y} \end{bmatrix} = \mathbf{U}(\mathbf{U}^T \mathbf{y}). \blacksquare\blacksquare$$

若 W 是 $\mathbb{R}^n$ 的子空间, $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_p\}$ 是 W 的基，记

$$\begin{aligned}
\mathbf{v}_1 &= \mathbf{x}_1 \\
\mathbf{v}_2 &= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v_1}}\mathbf{v}_1 \\
\mathbf{v}_3 &= \mathbf{x}_3 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v_1}}\mathbf{v}_1 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v_2}}\mathbf{v}_2 \\
&\vdots \\
\mathbf{v}_p &= \mathbf{x}_p - \frac{\mathbf{x}_p \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v_1}}\mathbf{v}_1 - \frac{\mathbf{x}_p \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v_2}}\mathbf{v}_2 - \cdots - \frac{\mathbf{x}_p \cdot \mathbf{v}_{p-1}}{\mathbf{v}_{p-1} \cdot \mathbf{v}_{p-1}}\mathbf{v}_{p-1}.
\end{aligned}$$

则$\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\}$ 是 W 的正交基.，且

$$\mathrm{Span}\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\} = \mathrm{Span}\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_p\}.$$

证明: 易证按Gram-Schmidt正交化过程产生的p 个向量

$$\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p$$

两两正交. 先证

$$\mathbf{v}_2 \cdot \mathbf{v}_1 = (\mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1) \cdot \mathbf{v}_1 = 0.$$

类似地, 可证对$i = 1, 2, \cdots, p-1$, 有

$$\mathbf{v}_i \cdot \mathbf{v}_j = 0, j = i+1, \cdots, p.$$

即$\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\}$ 两两正交, 故该向量组为线性无关组。由于其无关向量的个数为 p 个, 故该向量组为子空间W 的一个正交基.

由Gram-Schmidt 向量的正交化过程可知:

$$\mathrm{Span}\{\mathbf{x}_1, \cdots, \mathbf{x}_k\} = \mathrm{Span}\{\mathbf{v}_1, \cdots, \mathbf{v}_k\}, k = 1, 2, \cdots, p.$$

即向量组$\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_k\}$ 中任一向量都可以由向量组$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_k\}$线性表出, 反之亦然. 因此

$$\mathrm{Span}\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\} = \mathrm{Span}\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_p\}.$$

Examples

- Let $\mathbf{x}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$, $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$, construct an orthognal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ for W
- Let $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$. Then $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ is a subspace of $\mathbb{R}^4$. Construct an orthogonal basis for W.

- If $\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\}$ is an orthogonal basis for W, then let
$$\mathbf{u}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|}, \mathbf{u}_1 = \frac{\mathbf{v}_2}{\|\mathbf{v}_2\|}, \cdots, \mathbf{u}_p = \frac{\mathbf{v}_p}{\|\mathbf{v}_p\|}$$
Then $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ is an orthonormal basis for W.
- If an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\}$ and $\text{Span}\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\} = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_p\}$. Then is orthonormal sets $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$ also forms an basis for W, and
$$\text{Span}\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\} = \text{Span}\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p\}$$
$$= \text{Span}\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_p\}.$$

THEOREM 11.12: The QR Factorization

If $\mathbf{A}$ is an $m \times n$ matrix with **linearly independent columns**, then $\mathbf{A}$ can be factored as $\mathbf{A} = \mathbf{QR}$, where $\mathbf{Q}$ is an $m \times n$ matrix whose columns form an **orthonormal basis** for $\mathrm{Col}\mathbf{A}$ and $\mathbf{R}$ is an $n \times n$ **upper triangular invertible matrix** with **positive entries on its diagonal**.

证明: 记 $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n$ 为A 的 n 个线性无关列向量, $\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n\}$. 为其按照Gram-Schmidt 方法构造的正交向量组, 而$\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_n\}$ 为由线性无关的正交向量组 $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_n\}$ 标准化后形成的标准正交基.

则有

$$\mathrm{Span}\{\mathbf{x}_1, \cdots, \mathbf{x}_k\} = \mathrm{Span}\{\mathbf{u}_1, \cdots, \mathbf{u}_k\}, k = 1, 2, \cdots, p.$$

即

$$\begin{aligned}
\mathbf{x}_1 &= r_{11}\mathbf{u}_1 + 0 \cdot \mathbf{u}_2 + \cdots + 0 \cdot \mathbf{u}_n \\
\mathbf{x}_2 &= r_{12}\mathbf{u}_1 + r_{22}\mathbf{u}_2 + \cdots + 0 \cdot \mathbf{u}_n \\
&\cdots \\
\mathbf{x}_n &= r_{1n}\mathbf{u}_1 + r_{2n}\mathbf{u}_2 + \cdots + r_{nn}\mathbf{u}_n.
\end{aligned}$$

其中, $r_{i,j}, i,j = 1,2,\cdots,n$ 为组合系数, 且易证$r_{kk}, k = 1,2,\cdots,n$ 均为非负常数.

$$[\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n] = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_n] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}$$

记

$$Q = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_n], \mathbf{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}$$

则$m \times n$ 矩阵$\mathbf{A}$ 可以分解为一个$m \times n$ 阶标准正交矩阵$\mathbf{Q}$和一个$n \times n$ 阶上三角矩阵$\mathbf{R}$ 的乘积的形式. 即

$$\mathbf{A} = \mathbf{QR}.$$

Steps or Algorithm for computing QR factorization for an $m \times n$ matrix $\mathbf{A}$

- Using Gram-Schimdt process, find its corresponding orthogonal set.
- Normalize the orthogonal set, and form $\mathbf{Q}$
- Find $\mathbf{R} = \mathbf{Q}^T\mathbf{A}$.

Example: Find a $\mathbf{QR}$ factorization of $\mathbf{A}$

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

Classical Gram-Schmidt procedure:

For any number of vectors $\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n$, orthogonalizing each successive vector against all preceding ones, giving

Gram-Schmidt procedure

for $k = 1$ to n

$\quad \mathbf{q}_k = \mathbf{a}_k$

$\quad$ for $j = 1$ to $k-1$

$\quad \quad r_{jk} = \mathbf{q}_j^T \mathbf{a}_k, \;\; \mathbf{q}_k = \mathbf{q}_k - r_{jk}\mathbf{q}_j$

$\quad$ end

$\quad r_{kk} = \|\mathbf{q}_k\|_2, \;\; \mathbf{q}_k = \mathbf{q}_k / r_{kk}$

end

Resulting $\mathbf{q}_k$ and r_{jk} form reduced $\mathbf{QR}$ factorization of $\mathbf{A}$.

Modified Gram-Schmidt

- Classical Gram-Schmidt procedure often suffers loss of orthogonality in finite-precision.
- Also, separate storage is required for $\mathbf{A}, \mathbf{Q}$, and $\mathbf{R}$, since original $\mathbf{a}_k$ are needed in inner loop, so $\mathbf{q}_k$ cannot overwrite columns of $\mathbf{A}$.
- Both deficiencies are improved by modified Gram-Schmidt procedure, with each vector orthogonalized in turn against all subsequent vectors, so $\mathbf{q}_k$ can overwrite $\mathbf{a}_k$.

Modified Gram-Schmidt QR Factorization Algorithm

Modified Gram-Schmidt QR Factorization Algorithm

for $k = 1$ to n

$$r_{kk} = \|\mathbf{a}_k\|_2, \quad \mathbf{q}_k = \mathbf{a}_k / r_{kk}$$

for $j = k + 1$ to n

$$r_{kj} = \mathbf{q}_k^T \mathbf{a}_j, \quad \mathbf{a}_j = \mathbf{a}_j - r_{kj}\mathbf{q}_k$$

end

end

Rank Deficiency

- If $\mathrm{rank}(\mathbf{A}) < n$, then $\mathbf{QR}$ factorization still exists, but yields singular upper triangular factor $\mathbf{R}$, and multiple vectors $\mathbf{x}$ give minimum residual norm.
- Common practice selects minimum residual solution $\mathbf{x}$ having smallest norm.
- Can be computed by $\mathbf{QR}$ factorization with column pivoting or by **singular value decomposition (SVD)**?
- Rank of matrix is often not clear cut in practice, so relative tolerance is used to determine rank

Example: Near Rank Deficiency

- Consider 3×2 matrix

$$\mathbf{A} = \begin{bmatrix} 0.641 & 0.242 \\ 0.321 & 0.121 \\ 0.962 & 0.363 \end{bmatrix}$$

- Computing $\mathbf{QR}$ factorization,

$$R = \begin{bmatrix} 1.1997 & 0.4527 \\ 0 & 0.0002 \end{bmatrix}$$

$\mathbf{R}$ is extremely close to singular (exactly singular to 3-digit accuracy of problem statement).

Example: Near Rank Deficiency

- Consider 3×2 matrix

$$\mathbf{A} = \begin{bmatrix} 0.641 & 0.242 \\ 0.321 & 0.121 \\ 0.962 & 0.363 \end{bmatrix}$$

- Computing $\mathbf{QR}$ factorization,

$$R = \begin{bmatrix} 1.1997 & 0.4527 \\ 0 & 0.0002 \end{bmatrix}$$

$\mathbf{R}$ is extremely close to singular (exactly singular to 3-digit accuracy of problem statement).

- If $\mathbf{R}$ is used to solve linear least squares problem, result is highly sensitive to perturbations in right-hand side.
- For practical purposes, $\operatorname{rank}(\mathbf{A}) = 1$ rather than 2, because columns are nearly linearly dependent.

QR with Column Pivoting

- Instead of processing columns in natural order, select for reduction at each stage column of remaining unreduced submatrix having maximum Euclidean norm.
- If $\mathrm{rank}(\mathbf{A}) = k < n$, then after k steps, norms of remaining unreduced columns will be zero (or "negligible" in finite-precision arithmetic) below row k.
- Yields orthogonal factorization of form

$$\mathbf{Q}^T\mathbf{A}\mathbf{P} = \begin{bmatrix} \mathbf{R} & \mathbf{S} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where $\mathbf{R}$ is $k \times k$, upper triangular, and nonsingular, and permutation matrix $\mathbf{P}$ performs column interchanges.

QR with Column Pivoting

- Instead of processing columns in natural order, select for reduction at each stage column of remaining unreduced submatrix having maximum Euclidean norm.
- If $\mathrm{rank}(\mathbf{A}) = k < n$, then after k steps, norms of remaining unreduced columns will be zero (or "negligible" in finite-precision arithmetic) below row k.
- Yields orthogonal factorization of form

$$\mathbf{Q}^T\mathbf{A}\mathbf{P} = \begin{bmatrix} \mathbf{R} & \mathbf{S} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where $\mathbf{R}$ is $k \times k$, upper triangular, and nonsingular, and permutation matrix $\mathbf{P}$ performs column interchanges.

QR with Column Pivoting

- Instead of processing columns in natural order, select for reduction at each stage column of remaining unreduced submatrix having maximum Euclidean norm.
- If $\mathrm{rank}(\mathbf{A}) = k < n$, then after k steps, norms of remaining unreduced columns will be zero (or "negligible" in finite-precision arithmetic) below row k.
- Yields orthogonal factorization of form

$$\mathbf{Q}^T\mathbf{A}\mathbf{P} = \begin{bmatrix} \mathbf{R} & \mathbf{S} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where $\mathbf{R}$ is $k \times k$, upper triangular, and nonsingular, and permutation matrix $\mathbf{P}$ performs column interchanges.

Basic solution to least squares problem $\mathbf{Ax} \cong \mathbf{b}$ can now be computed by solving triangular system $\mathbf{Rz} = \mathbf{c}_1$, where $\mathbf{c}_1$ contains first k components of $\mathbf{Q}^T\mathbf{b}$, and then taking

$$\mathbf{x} = \mathbf{P}\begin{bmatrix} \mathbf{z} \\ \mathbf{0} \end{bmatrix}$$

- Minimum-norm solution can be computed, if desired, at expense of additional processing to annihilate $\mathbf{S}$.
- $\mathrm{rank}(\mathbf{A})$ is usually unknown, so rank is determined by monitoring norms of remaining unreduced columns and terminating factorization when maximum value falls below chosen tolerance .

- **Singular Value Decomposition (SVD)** of $m \times n$ matrix $\mathbf{A}$ has form

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$$

- Where
  - $\mathbf{U}$ is $m \times m$ orthogonal matrix， $\mathbf{U}^T\mathbf{U} = \mathbf{I}$.
  - $\mathbf{V}$ is $n \times n$ orthogonal matrix, $\mathbf{V}\mathbf{V}^T = \mathbf{I}$
  - $\Sigma = (\sigma_{ij})_{m\times n}$ is $m \times n$ diagonal matrix, with

$$\sigma_{ij} = \begin{cases} 0, & i \neq j; \\ \sigma_i > 0, & i = j. \end{cases}$$

- Diagonal entries σ_i, called **Singular Values** of $\mathbf{A}$, are usually ordered so that

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$$

思考：为什么要排序？如何实现排序？

- Columns $\mathbf{u}_i$ of $\mathbf{U}$ are called **left singular vectors**.
- Columns $\mathbf{v}_i$ of $\mathbf{V}$ are called **right singular vectors**.

- If $\mathbf{A}$ is $m \times n$ with $\mathbf{rank}(\mathbf{A}) = n$, then

$$\begin{aligned} \mathbf{A} &= \mathbf{U}\Sigma\mathbf{V}^T \\ &= [\mathbf{U}_1 \ \mathbf{U}_2] \begin{bmatrix} \Sigma_1 \\ \mathbf{0} \end{bmatrix} \mathbf{V}^T \\ &= \mathbf{U}_1\Sigma_1\mathbf{V}^T \end{aligned}$$

  where $\mathbf{U}_1$ is $m \times n$ matrix with **orthonormal** columns, and Σ_1 is an $n \times n$ **diagonal** matrix and nonsingular, $\mathbf{V}$ is an $n \times n$ **orthonormal** matrix.
- $\mathbf{A} = \mathbf{U}_1 \sum_1 \mathbf{V}^T$ is called reduced **SVD** of A.

- For least square problem $\mathbf{A}\mathbf{x} = \mathbf{b}$, it can be solved with normal equations with the form

$$\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$$

- If $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ has a SVD form, then

$$\begin{aligned}
(\mathbf{U}\Sigma\mathbf{V}^T)^T\mathbf{U}\Sigma\mathbf{V}^T\mathbf{x} &= (\mathbf{U}\Sigma\mathbf{V}^T)^T\mathbf{b} \\
\mathbf{V}\Sigma^T\mathbf{U}^T\mathbf{U}\Sigma\mathbf{V}^T\mathbf{x} &= \mathbf{V}\Sigma^T\mathbf{U}^T\mathbf{b} \\
\mathbf{V}\Sigma^T\Sigma\mathbf{V}^T\mathbf{x} &= \mathbf{V}\Sigma^T\mathbf{U}^T\mathbf{b} \\
\mathbf{V}^T\mathbf{V}\Sigma^T\Sigma\mathbf{V}^T\mathbf{x} &= \mathbf{V}^T\mathbf{V}\Sigma^T\mathbf{U}^T\mathbf{b} \\
\Sigma^T\Sigma\mathbf{V}^T\mathbf{x} &= \Sigma^T\mathbf{U}^T\mathbf{b} \\
\Sigma\mathbf{V}^T\mathbf{x} &= \mathbf{U}^T\mathbf{b} \\
\mathbf{x} &= \mathbf{V}\Sigma^{-1}\mathbf{U}^T\mathbf{b}.
\end{aligned}$$

- More generally, for $\mathbf{A}$ of any shape or rank, the least squares solution to $\mathbf{A}\mathbf{x} \cong \mathbf{b}$ of minimum norm is given by

$$\mathbf{x} = \sum_{\sigma_i \neq 0} \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i$$

- For ill-conditioned or rank deficient problems, "small" singular values can be omitted from summation to stabilize solution.
- Euclidean matrix norm: $\|\mathbf{A}\|_2 = \sigma_{\max}$.
- Euclidean condition number of matrix : $\mathrm{cond}(\mathbf{A}) = \frac{\sigma_{\max}}{\sigma_{\min}}$.
- Rank of matrix: number of nonzero singular values.

Pseudoinverse (广义逆)

- Define pseudoinverse of scalar σ to be $1/\sigma$ if $\sigma \neq 0$, zero otherwise.
- Define **pseudoinverse of (possibly rectangular) diagonal matrix** by transposing and taking scalar pseudoinverse of each entry.
- Then pseudoinverse of general real $m \times n$ matrix $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ is given by

$$\mathbf{A}^+ = \mathbf{V}\Sigma^+\mathbf{U}^T.$$

- Pseudoinverse always exists whether or not matrix is square or has full rank
- If $\mathbf{A}$ is square and nonsingular, then $\mathbf{A}^+ = \mathbf{A}^{-1}$.
- In all cases, minimum-norm solution to $\mathbf{Ax} \cong \mathbf{b}$ is given by

$$\mathbf{x} = \mathbf{A}^+\mathbf{b}.$$

Orthogonal Bases

- SVD of matrix, $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$, provides orthogonal bases for subspaces relevant to $\mathbf{A}$.
- Columns of $\mathbf{U}$ corresponding to nonzero singular values form orthonormal basis for $\mathbf{span}(\mathbf{A})$.
- Remaining columns of $\mathbf{U}$ form orthonormal basis for orthogonal complement $\mathbf{span}(\mathbf{A})^\perp$.
- Columns of $\mathbf{V}$ corresponding to zero singular values form orthonormal basis for null space of $\mathbf{A}$.
- Remaining columns of $\mathbf{V}$ form orthonormal basis for orthogonal complement of null space of $\mathbf{A}$.

- Another way to write **SVD** is

$$\mathbf{A} = \mathbf{U} \sum \mathbf{V}^T = \sigma_1 \mathbf{E}_1 + \sigma_2 \mathbf{E}_2 + \cdots + \sigma_n \mathbf{E}_n$$

with $\mathbf{E}_i = \mathbf{u}_i \mathbf{v}_i^T$.

- $\mathbf{E}_i$ has rank 1 and can be stored using only $m + n$ storage locations.
- Product $\mathbf{E}_i \mathbf{x}$ can be computed using only $m + n$ multiplications.

- Condensed approximation to $\mathbf{A}$ is obtained by omitting from summation terms corresponding to small singular values.
- Approximation using k largest singular values is closest matrix of rank k to $\mathbf{A}$.
- Approximation is useful in
  image processing(图像处理),
  data compression(数据压缩),
  information retrieval(信息检索),
  cryptography(加密), etc.

Total Least Squares

- Ordinary least squares is applicable when right-hand side $\mathbf{b}$ is subject to random error but matrix $\mathbf{A}$ is known accurately.
- When all data, including $\mathbf{A}$, are subject to error, then total least squares is more appropriate.
- Total least squares minimizes orthogonal distances, rather than vertical distances, between model and data.
- Total least squares solution can be computed from **SVD** of $[\mathbf{A}, \mathbf{b}]$.

已知矩阵

$$\mathbf{A} = \begin{bmatrix} 4 & -1 & 1 \\ -1 & 3 & -2 \\ 1 & -2 & 3 \end{bmatrix}$$

是一个对称矩阵，且其特征值为 $\lambda_1 = 6$, $\lambda_2 = 3$, $\lambda_3 = 1$.

分别利用幂法、对称幂法、反幂法求其最大特征值和特征向量.

注意：可取初始向量$\mathbf{x}^{(0)} = (1\ 1\ 1)^T$.