EECS 275 Matrix Computation

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Lecture 12

Overview

- QR decomposition by Householder transformation
- QR decomposition by Givens rotation

Reading

- Chapter 10 of *Numerical Linear Algebra* by Llyod Trefethen and David Bau
- Chapter 5 of *Matrix Computations* by Gene Golub and Charles Van Loan
- Chapter 5 of *Matrix Analysis and Applied Linear Algebra* by Carl Meyer

Householder triangularization

- In Gram-Schmidt orthogonalization

$$A \underbrace{R_1 R_2 \cdots R_n}_{R^{-1}} = Q$$

  has orthonormal columns. The product $R = R_n^{-1} \cdots R_2^{-1} R_1^{-1}$ is upper triangular

- In Householder triangularization, a series of elementary orthogonal matrices Q_k is applied to the left of A, so that the resulting matrix

$$\underbrace{Q_n \cdots Q_2 Q_1}_{Q^\top} A = R$$

  is upper triangular. The product $Q = Q_1^\top Q_2^\top \cdots Q_n^\top$ is orthogonal, and therefore $A = QR$ is a QR factorization of A

- Two methods for QR factorization
  - Gram-Schmidt: triangular orthogonalization
  - Householder: orthogonal triangularization

Geometry of elementary projectors

- For $\mathbf{u}, \mathbf{x} \in \mathbb{R}^n$, s.t. $\|\mathbf{u}\| = 1$
- Orthogonal projectors onto span$\{\mathbf{u}\}$ and $\mathbf{u}^\perp$ are

$$P_{\mathbf{u}} = \frac{\mathbf{u}\mathbf{u}^\top}{\mathbf{u}^\top\mathbf{u}}, \text{ and } \quad P_{\mathbf{u}^\perp} = I - \frac{\mathbf{u}\mathbf{u}^\top}{\mathbf{u}^\top\mathbf{u}}$$

- For $\mathbf{u} \neq 0$, the Householder transformation or the elementary reflector about $\mathbf{u}^\perp$ is

$$R = I - 2\frac{\mathbf{u}\mathbf{u}^\top}{\mathbf{u}^\top\mathbf{u}}$$

or

$$R = I - 2\mathbf{u}\mathbf{u}^\top$$

when $\|\mathbf{u}\| = 1$, and

$$R = R^\top = R^{-1}$$

Triangularization by introducing zeros

- The matrix Q_k is chosen to introduce zeros below the diagonal in the k-th column while preserving all the zeros previously introduced

$$\underset{A}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}} \xrightarrow{Q_1} \underset{Q_1 A}{\begin{bmatrix} \boxtimes & \boxtimes & \boxtimes \\ \mathbf{0} & \boxtimes & \boxtimes \\ \mathbf{0} & \boxtimes & \boxtimes \\ \mathbf{0} & \boxtimes & \boxtimes \\ \mathbf{0} & \boxtimes & \boxtimes \end{bmatrix}} \xrightarrow{Q_2} \underset{Q_2 Q_1 A}{\begin{bmatrix} \times & \times & \times \\ & \boxtimes & \boxtimes \\ & \mathbf{0} & \boxtimes \\ & \mathbf{0} & \boxtimes \\ & \mathbf{0} & \boxtimes \end{bmatrix}} \xrightarrow{Q_3} \underset{Q_3 Q_2 Q_1 A}{\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \boxtimes \\ & & \mathbf{0} \\ & & \mathbf{0} \end{bmatrix}}$$

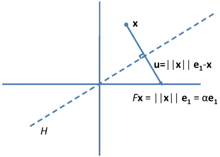
- Q_k operates on row $k, \ldots, m$ (changed entries are denoted by boldface or $\boxtimes$ and blank entries are zero)
- At beginning of step k, there is a block of zeros in the first $k-1$ columns of these rows
- The application of Q_k forms linear combinations of these rows, and the linear combination of the zero entries remain zero
- After n steps, all the entries below the diagonal have been eliminated and $Q_n \cdots Q_2 Q_1 A = R$ is upper triangular

Householder reflectors

- At beginning of step k, there is a block of zeros in the first $k-1$ columns of these rows
- Each Q_k is chosen to be

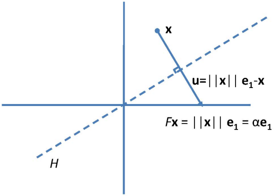
$$Q_k = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix}$$

  where I is the $(k-1) \times (k-1)$ identity matrix and F is an $(m-k+1) \times (m-k+1)$ orthogonal matrix
- Multiplication by F has to introduce zeros into the k-th column
- The Householder algorithm chooses F to be a particular matrix called Householder reflector



- At step k, the entries $k, \ldots, m$ of the k-th column are given by vector $\mathbf{x} \in \mathbb{R}^{m-k+1}$

Householder transformation (cont'd)

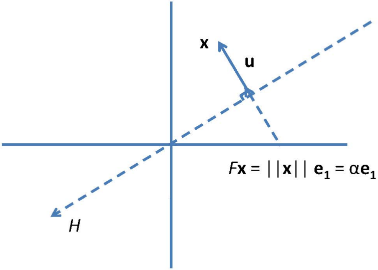


- To introduce zeros into k-th column ($\mathbf{x} \in \mathbb{R}^{m-k+1}$), the Householder transformation F should

$$\mathbf{x} = \begin{bmatrix} \times \\ \times \\ \vdots \\ \times \end{bmatrix} \xrightarrow{F} F\mathbf{x} = \begin{bmatrix} \|\mathbf{x}\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|\mathbf{x}\|\mathbf{e}_1 = \alpha\mathbf{e}_1$$

- The reflector F will reflect the space $\mathbb{R}^{m-k+1}$ across the hyperplane H orthogonal to $\mathbf{u} = \|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x}$
- A hyperplane is characterized by a vector $\mathbf{u} = \|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x}$

Householder transformation (cont'd)



- Every point $\mathbf{x} \in \mathbb{R}^m$ is mapped to a mirror point

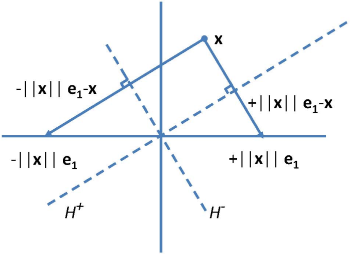
$$F\mathbf{x} = (I - 2\frac{\mathbf{u}\mathbf{u}^\top}{\mathbf{u}^\top\mathbf{u}})\mathbf{x} = \mathbf{x} - 2\mathbf{u}(\frac{\mathbf{u}^\top\mathbf{x}}{\mathbf{u}^\top\mathbf{u}})$$

  and hence

$$F = (I - 2\frac{\mathbf{u}\mathbf{u}^\top}{\mathbf{u}^\top\mathbf{u}})$$

- Will fix the $+/-$ sign in the next slide

The better of two Householder reflectors



- Two Householder reflectors (transformations)
- For numerical stability pick the one that moves reflect $\mathbf{x}$ to the vector $\|\mathbf{x}\|\mathbf{e}_1$ that is not to close to $\mathbf{x}$ itself, i.e., $-\|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x}$ in this case
- In other words, the better of the two reflectors is

$$\mathbf{u} = \text{sign}(x_1)\|\mathbf{x}\|\mathbf{e}_1 + \mathbf{x}$$

where x_1 is the first element of $\mathbf{x}$ ($\text{sign}(x_1) = 1$ if $x_1 = 0$)

Householder QR factorization

- Algorithm:

  for $k = 1$ to n **do**

  $\mathbf{x} = A_{k:m,k}$

  $\mathbf{u}_k = \text{sign}(x_1)\|\mathbf{x}\|_2\mathbf{e}_1 + \mathbf{x}$

  $\mathbf{u}_k = \frac{\mathbf{u}_k}{\|\mathbf{u}_k\|_2}$

  $A_{k:m,k:n} = (I - 2\mathbf{u}_k\mathbf{u}_k^\top)A_{k:m,k:n}$

  end for

- Recall

$$Q_k = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix}$$

- Upon completion, A has been reduced to upper triangular form, i.e., R in $A = QR$
- $Q^\top = Q_n \cdots Q_2 Q_1$ or $Q = Q_1^\top Q_2^\top \cdots Q_n^\top$

QR decomposition with Householder transformation

- Want to compute QR decomposition A with Householder transformation

$$A = \begin{bmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{bmatrix}$$

- Need to find a reflector for first column of A, $\mathbf{x} = [12, 6, -4]^\top$ to $\|\mathbf{x}\|\mathbf{e}_1 = [14, 0, 0]^\top$

$$\mathbf{u} = \|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x} = [2, -6, 4]^\top = 2[1, -3, 2]^\top$$

$$F_1 = I - 2\frac{\mathbf{u}\mathbf{u}^\top}{\mathbf{u}^\top\mathbf{u}} = \begin{bmatrix} 6/7 & 3/7 & -2/7 \\ 3/7 & -2/7 & 6/7 \\ -2/7 & 6/7 & 3/7 \end{bmatrix}, F_1 A = \begin{bmatrix} 14 & 21 & -14 \\ 0 & -49 & -14 \\ 0 & 168 & -77 \end{bmatrix}$$

- Next need to zero out A_{32} and apply the same process to

$$A' = \begin{bmatrix} -49 & -14 \\ 168 & -77 \end{bmatrix}$$

QR decomposition with Householder (cont'd)

- With the same process

$$F_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -7/25 & 24/25 \\ 0 & 24/25 & 7/25 \end{bmatrix}$$

- Thus, we have

$$\begin{aligned} Q &= Q_1 Q_2 = \begin{bmatrix} 6/7 & -69/175 & 58/175 \\ 3/7 & 158/175 & -6/175 \\ -2/7 & 6/35 & 33/35 \end{bmatrix} \\ R &= Q_2 Q_1 A = Q^\top A = \begin{bmatrix} 14 & 21 & -14 \\ 0 & 175 & -70 \\ 0 & 0 & -35 \end{bmatrix} \end{aligned}$$

- The matrix Q is orthogonal and R is upper triangular

Givens rotations

- Givens rotation: orthogonal transform to zero out elements selectively

$$G(i,k,\theta) = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & -s & \cdots & 0 \\ \vdots & & \vdots & \cdots & \vdots & & \vdots \\ 0 & \cdots & s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix} \begin{matrix} \\ \\ i \\ \\ k \\ \\ \\ \end{matrix}$$

$$\qquad\qquad\qquad\qquad i \qquad\qquad k$$

where $c = cos(\theta)$ and $s = sin(\theta)$ for some θ

- Apply G on A, only rows i and j of A are affected,

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

thus

$$r \leftarrow \sqrt{a^2 + b^2}, \quad c \leftarrow a/r, \quad s \leftarrow -b/r$$

Givens rotations (cont'd)

- Pre-multiply $G(i,k,\theta)$ amounts to a counterclockwise rotation θ in the (i,k) coordinate plane, $\mathbf{y} = G(i,k,\theta)\mathbf{x}$

$$y_j = \begin{cases} cx_i - sx_k & j = i \\ sx_i + cx_k & j = k \\ x_j & j \neq i,k \end{cases}$$

- Can zero out $y_k = sx_i + cx_k = 0$ by setting

$$c = \frac{x_i}{\sqrt{x_i^2 + x_k^2}}, \quad s = \frac{-x_k}{\sqrt{x_i^2 + x_k^2}}, \quad \theta = \arctan(x_k/x_i)$$

- QR decomposition can be computed by a series of Givens rotations
- Each rotation zeros an element in the subdiagonal of the matrix, forming R matrix, $Q = G_1 \ldots G_n$ forms the orthogonal Q matrix
- Useful for zero out few elements off diagonal (e.g., sparse matrix)
- Example If $\mathbf{x} = [1,2,3,4]^\top$, $\cos(\theta) = 1/\sqrt{5}$, and $\sin(\theta) = -2/\sqrt{5}$, then $G(2,4,\theta) = [1,\sqrt{20},3,0]^\top$.

QR factorization with Givens rotation

- Given A

$$A = \begin{bmatrix} 6 & 5 & 0 \\ 5 & 1 & 4 \\ 0 & 4 & 3 \end{bmatrix}$$

Want to zero out A_{21} with G_1

- With θ we have G_1

$$G_1 = \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 6 & 5 & 0 \\ 5 & 1 & 4 \\ 0 & 4 & 3 \end{bmatrix}$$

$$r = \sqrt{6^2 + 5^2} = 7.8102, c = 6/r = 0.7682, s = -5/r = -0.6402$$

$$G_1 A = \begin{bmatrix} 7.8102 & 4.4813 & 2.5607 \\ 0 & -2.4327 & 3.0729 \\ 0 & 4 & 3 \end{bmatrix}$$

- Continue to zero out A_{32} and form a triangular matrix R
- The orthogonal matrix $Q^\top = G_2 G_1$, and $G_2 G_1 A = Q^\top A = R$ for QR decomposition

Gram-Schmidt, Householder and Givens

- Householder QR is numerically more stable
- Gram-Schmidt computes orthonormal basis incrementally
- Givens rotation is more useful for zero out few selective elements