Math 381 - Fall 2022

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Week 9

Last Time

1. LU decomposition (Cholesky decomposition)
2. QR decomposition
3. SVD ~~decomposition~~

Today

1. QR decomposition
2. Gram-Schmidt orthogonalization
3. Householder reflections

Reduced QR decomposition

Definition: reduced QR decomposition

Let $A \in \mathbb{R}^{m\times n}$ be a full rank matrix (with $m > n$). We have that

$$A = QR = \hat{Q}\hat{R},$$

where $Q \in \mathbb{R}^{m\times m}$ is an orthogonal matrix, $\cancel{R\mathbb{R}^{m\times n}}$ $R \in \mathbb{R}^{m\times n}$ is upper triangular, and

$$Q = \begin{bmatrix} \hat{Q} & Q_0 \end{bmatrix}, \qquad Q = \begin{bmatrix} \hat{R} \\ \mathbf{0} \end{bmatrix}$$

, for $\hat{Q} \in \mathbb{R}^{m\times n}$ and $\hat{R} \in \mathbb{R}^{n\times n}$.

$$\boxed{A} = \underbrace{\begin{bmatrix} \hat{Q} & Q_0 \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}}_{R} = \hat{Q}\hat{R} + Q_0 \cdot 0 = \hat{Q}\hat{R}$$

Example:

Example: Reduced QR decomposition

$$
\text{Full rank} \rightarrow
\overset{A}{\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}}
=
\overset{\hat{Q}}{\begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \\ q_{31} & q_{32} \end{bmatrix}}
\overset{\hat{R}}{\begin{bmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{bmatrix}}
$$

$a_1 \quad a_2 \qquad q_1 \quad q_2$

$a_1 = r_{11} q_1$

$\Rightarrow \boxed{q_1 = \frac{1}{r_{11}} a_1}$

Orthonormal q_j

$1 = \|q_1\|_2 = \frac{1}{r_{11}} \|a_1\|_2$

$\Rightarrow r_{11} = \|a_1\|_2$

$a_2 = r_{12} q_1 + r_{22} q_2 \Rightarrow q_2 = \frac{1}{r_{22}}(a_2 - r_{12} q_1)$

Orthogonality

$q_1^T a_2 = r_{12} q_1^T q_1 + r_{22} \underbrace{q_1^T q_2}_{0}$

$\Rightarrow r_{12} = q_1^T a_2$

$\|q_2\|_2 = 1$

$\Rightarrow r_{22} = \|a_2 - (q_1^T a_2) q_1\|_2$

Gram-Schmidt Orthogonalization

Let $a_j \in \mathbb{R}^m$, $j = 1, \ldots, n$, be a set of linearly independent column vectors, and let $q_j \in \mathbb{R}^m$, $j = 1, \ldots, n$, be an orthonormal set of vectors such that

$$a_j = \sum_{k=1}^{j} r_{kj} q_k.$$

$$a_j = \sum_{k=1}^{j-1} r_{kj} q_k + r_{jj} q_j$$

$$\Rightarrow \boxed{q_j = \frac{1}{r_{jj}}\left(a_j - \sum_{k=1}^{j-1} r_{kj} q_k\right)}$$

$$\boxed{r_{jj} = \left\| a_j - \sum_{k=1}^{j-1} r_{kj} q_k \right\|_2}$$

$$q_i^T a_j = \sum_{k=1}^{j} r_{kj} q_i^T q_k = r_{ij} \cdot 1$$

$$\boxed{r_{ij} = q_i^T a_j}$$

Gram-Schmidt Orthogonalization

Let $A \in \mathbb{R}^{m \times n}$ be a full rank matrix (with $m > n$)

Algorithm: Gram-Schmidt Orthogonalization (unstable)

for j in $1, 2, \ldots, n$:

  $q_j = a_j$

  for i in $1, 2, \ldots, j-1$:

    $r_{ij} = q_i^T a_j$

    $q_j = q_j - r_{ij} q_i$

  $r_{jj} = \|q_j\|_2$

  $q_j = q_j / r_{jj}$

Modified Gram-Schmidt Orthogonalization

Let $A \in \mathbb{R}^{m \times n}$ be a full rank matrix (with $m > n$)

Algorithm: Modified Gram-Schmidt Orthogonalization

for i in $1, 2, \dots, n$:
    $v_i = a_i$
for i in $1, 2, \dots, n$:
    $r_{ii} = \|v_i\|_2$
    $q_i = v_i / r_{ii}$
    for j in $i + 1, \dots, n$:
        $r_{ij} = q_i^T v_j$
        $v_j = v_j - r_{ij} q_i$

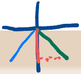
Householder reflections: Motivation

$$\underset{A}{\begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}} \quad \underset{Q_1 A = \hat{A}^{(1)}}{\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{bmatrix}} \quad \underset{Q_2 Q A = \hat{A}^{(2)}}{\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \end{bmatrix}} \quad \underset{Q_3 Q_2 Q A = R}{\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \end{bmatrix}}$$

$$Q_n Q_{n-1} \cdots Q_2 Q_1 A = R$$

$$A = (Q_n \cdots Q_1)^{-1} R$$

Householder reflections



Complementary projection

$P = I - uu^T$

Canonical vectors

We typically write the *jth* column vector of the identity matrix I as e_j where

$$e_j = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{bmatrix}^T$$

Definition: Reflector matrix

For a unit vector $u \in \mathbb{R}^n$ with $\|u\|_2 = 1$. The reflector matrix is given by

$$F = I - 2uu^T.$$

$z = Fx$

$x = Fz$

$\Rightarrow FFx = x$

$\Rightarrow FF = I$

$F^T = [I - 2uu^T]^T = I - 2[uu^T]^T$

$= I - 2uu^T$

$= F$

Orthogonal Matrix

$FF^T = I$

Householder reflections

Definition: Householder reflector

Given a nonzero vector $z \in \mathbb{R}^n$, the Householder reflector is given by

$e_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$

$$Fz = \alpha e_1,$$

for some unit vector $u \in \mathbb{R}^n$.

$[I - 2uu^T]z = \alpha e_1$

$\Rightarrow z - 2u(u^T z) = \alpha e_1$

$\Rightarrow u = \frac{1}{2u^T z}(\alpha e_1 - z)$

Reflection

$\|Fz\|_2 = \|z\|_2$

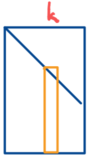
$\Rightarrow \|\alpha e_1\|_2 = |\alpha| \cdot 1 = \|z\|_2$

$\Rightarrow \alpha = \pm \frac{1}{\|z\|_2}$

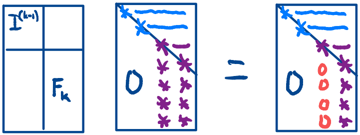
Householder reflections

Define the matrices

$$Q_k = \begin{bmatrix} I^{(k-1)} & \mathbf{0} \\ \mathbf{0} & F_k \end{bmatrix},$$



where F_k are the Housholder reflectors for $\hat{A}^{(k)}_{k:m,k}$. z from prev slide



Householder reflections

The following modifies the elements of A in place and stores the vectors $v_1, \dots, v_n$.

Algorithm: Householder QR decomposition

for k in $1, 2, \dots, n$:

$x = A_{k:m,k}$
$v_k = \mathrm{sign}(x_1)\|x\|_2 e_1 + x$
$v_k = v_k / \|v_k\|_2$
$A_{k:m,k:n} = A_{k:m,k:n} - 2v_k(v_k^T A_{k:m,k:n})$

The vectors v_k are stored instead of forming Q explicitly (expensive). They can be used in an algorithm to compute $Q^T b$ for some vector b or Qx for some vector x. If forming Q is needed, then this algorithm can be applied to the canonical vectors e_j that form the columns of the identity matrix.