Mathematics Methods for Computer Science

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Lecture

Column Spaces and QR

这部分主要研究 列空间

Problem

$$cond\ A^T A \approx (cond\ A)^2$$

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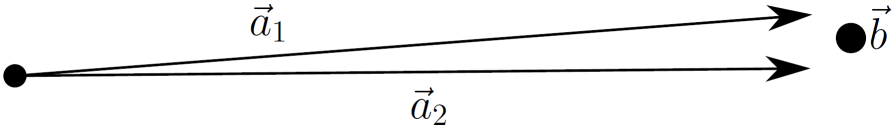
$$\begin{aligned}\text{cond } \mathrm{A}^\top A &= \|A^\top A\| \left\|(A^\top A)^{-1}\right\| \\ &\approx \|A^\top\| \, \|A\| \, \|A^{-1}\| \left\|(A^\top)^{-1}\right\| \quad \text{for many choices of } \|\cdot\| \\ &= \|A\|^2 \left\|A^{-1}\right\|^2 \\ &= (\text{ cond } A)^2\end{aligned}$$

Geometric Intuition



Least-squares fit is ambiguous!

When Is $cond\ A^T A \approx 1$?

$$cond\ I_{n\times n} = 1$$

(w.r.t. $||\cdot||_2$)

(p=2)

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$$cond\ I_{n\times n} = 1$$

(w.r.t. $||\cdot||_2$)

$$\textbf{Desirable: } A^T A \approx I_{n\times n}$$

(then, $cond\ A^T A \approx 1$!)

正交矩阵！

When Is $cond\ A^TA \approx 1$?

$$cond\ I_{n\times n} = 1$$

(w.r.t. $\|\cdot\|_2$)

Desirable: $A^TA \approx I_{n\times n}$

(then, $cond\ A^TA \approx 1$!)

Doesn't mean $A = I_{n\times n}$.

Recall: Definition of Gram matrix

$$Q^\top Q = \begin{pmatrix} - & \vec{q}_1^\top & - \\ - & \vec{q}_2 & - \\ \vdots & & \\ - & \vec{q}_n & - \end{pmatrix} \begin{pmatrix} | & | & & | \\ \vec{q}_1 & \vec{q}_2 & \cdots & \vec{q}_n \\ | & | & | & \end{pmatrix}$$

$$= \begin{pmatrix} \vec{q}_1 \cdot \vec{q}_1 & \vec{q}_1 \cdot \vec{q}_2 & \cdots & \vec{q}_1 \cdot \vec{q}_n \\ \vec{q}_2 \cdot \vec{q}_1 & \vec{q}_2 \cdot \vec{q}_2 & \cdots & \vec{q}_2 \cdot \vec{q}_n \\ \vdots & \vdots & \cdots & \vdots \\ \vec{q}_n \cdot \vec{q}_1 & \vec{q}_n \cdot \vec{q}_2 & \cdots & \vec{q}_n \cdot \vec{q}_n \end{pmatrix}$$

When $Q^T Q = I_{n \times n}$

$$\vec{q}_i \cdot \vec{q}_j = \begin{cases} 1 & \text{when } i = j \\ 0 & \text{when } i \neq j \end{cases}$$

When $Q^TQ = I_{n\times n}$

$$\vec{q}_i \cdot \vec{q}_j = \begin{cases} 1 & \text{when } i = j \\ 0 & \text{when } i \neq j \end{cases}$$

Orthonormal; orthogonal matrix

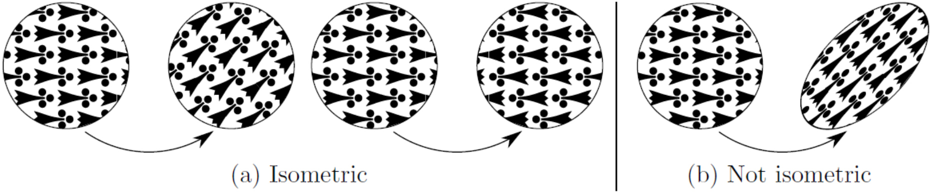
A set of vectors $\{\vec{v}_1, \cdots, \vec{v}_k\}$ is orthonormal if $||\vec{v}_i|| = 1$ for all i and $\vec{v}_i \cdot \vec{v}_j = 0$ for all $i \neq j$. A square matrix whose columns are orthonormal is called an orthogonal matrix.

Isometry Properties

$$||Q\vec{x}||^2 = ?$$

$$(Q\vec{x}) \cdot (Q\vec{y}) = ?$$

Geometric Interpretation



(a) Isometric

(b) Not isometric

Alternative Intuition for Least-Squares

$$A^T A\vec{x} = A^T\vec{b} \leftrightarrow min_{\vec{x}}||A\vec{x} - \vec{b}||_2$$

Project $\vec{b}$ onto the column space of A.

(投影)

Observation

Lemma: Column space invariance

For any $A \in \mathbb{R}^{m \times n}$ and invertible $B \in \mathbb{R}^{n \times n}$,

$$col\ A = col\ AB$$

.

(可逆的列操作不会影响列空间，同时注意矩阵列操作时操作矩阵乘在右边)

Invertible column operations do not affect column space.

New Strategy

Apply column operations to A until it is orthogonal; then, solve least-squares on the resulting orthogonal Q.

New Factorization

$$A = QR$$

- Q orthogonal
- R upper triangular

QR分解

Using QR

$$A^T A\vec{x} = A^T\vec{b}, A = QR$$

$$\rightarrow \vec{x} = R^{-1}Q^T\vec{b}$$

Using QR

$$A^T A\vec{x} = A^T\vec{b}, A = QR$$

$$\to \vec{x} = R^{-1}Q^T\vec{b}$$

Didn't need to compute $A^T A$ or $(A^T A)^{-1}$

Vector Projection

(向量投影)

"Which multiple of $\vec{a}$ is closest to $\vec{b}$?"

$$min_c||c\vec{a} - \vec{b}||_2^2$$

Vector Projection

"Which multiple of $\vec{a}$ is closest to $\vec{b}$?"

$$min_c||c\vec{a} - \vec{b}||_2^2$$

$$c = \frac{\vec{a}\cdot\vec{b}}{||\vec{a}||_2^2}$$

即b在a方向的投影长度占a总长度的比例，
因为此时c*a-b垂直于a向量，因而最短。

Vector Projection

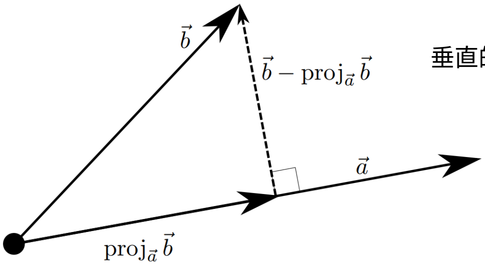
"Which multiple of $\vec{a}$ is closest to $\vec{b}$?"

$$min_c ||c\vec{a} - \vec{b}||_2^2$$

$$c = \frac{\vec{a} \cdot \vec{b}}{||\vec{a}||_2^2}$$

$$proj_{\vec{a}} \vec{b} = c\vec{a} = \frac{\vec{a} \cdot \vec{b}}{||\vec{a}||_2^2} \vec{a}$$

Properties of Projection



垂直的时候最短！

$$proj_{\vec{a}}\vec{b} \| \vec{a}$$

$$\vec{a} \cdot (\vec{b} - proj_{\vec{a}}\vec{b}) = 0$$
$$\Rightarrow (\vec{b} - proj_{\vec{a}}\vec{b}) \perp \vec{a}$$

Orthonormal Projection

Suppose $\hat{a}_1, \cdots, \hat{a}_k$ are orthonormal.

$$proj_{\hat{a}_i}\vec{b} = (\hat{a}_i \cdot \vec{b})\hat{a}_i$$

Orthonormal Projection

$$\left\| c_1\hat{a}_1 + c_2\hat{a}_2 + \cdots + c_k\hat{a}_k - \vec{b} \right\|_2^2 = \sum_{i=1}^{k} \left(c_i^2 - 2c_i\vec{b}\cdot\hat{a}_i \right) + \|\vec{b}\|_2^2$$

上式中的a_i的模均为1，且a_i为一组正交基。

Orthonormal Projection

$$\left\| c_1\hat{a}_1 + c_2\hat{a}_2 + \cdots + c_k\hat{a}_k - \vec{b} \right\|_2^2 =$$

$$\sum_{i=1}^{k} \left(c_i^2 - 2c_i\vec{b}\cdot\hat{a}_i \right) + \|\vec{b}\|_2^2$$

$$\Rightarrow c_i = \vec{b}\cdot\hat{a}_i$$

对c_i求导

Orthonormal Projection

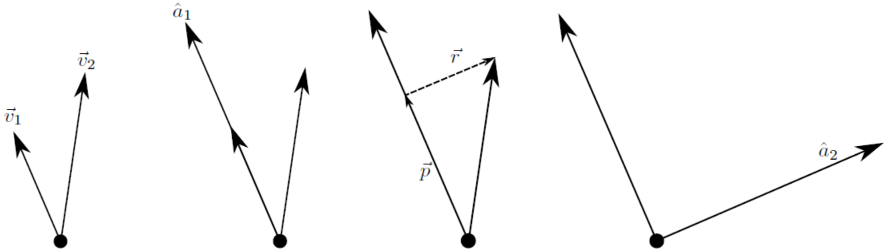
$$\left\| c_1\hat{a}_1 + c_2\hat{a}_2 + \cdots + c_k\hat{a}_k - \vec{b} \right\|_2^2 = \sum_{i=1}^{k} \left(c_i^2 - 2c_i\vec{b}\cdot\hat{a}_i \right) + \|\vec{b}\|_2^2$$

$$\Rightarrow c_i = \vec{b}\cdot\hat{a}_i$$

$$\Rightarrow \operatorname{proj}_{\operatorname{span}\{\hat{a}_1,\cdots,\hat{a}_k\}} \vec{b} = \left(\hat{a}_1\cdot\vec{b}\right)\hat{a}_1 + \cdots + \left(\hat{a}_k\cdot\vec{b}\right)\hat{a}_k$$

实际上就是使用一组正交基的线性组合来表示向量b

Geometric Strategy for Orthogonalization



(a) Input (b) Rescaling (c) Projection (d) Normalization

Gram-Schmidt Orthogonalization

To orthogonalize $\vec{v}_1, \cdots, \vec{v}_k$:

1. $\hat{a}_1 \equiv \frac{\vec{v}_1}{||\vec{v}_1||}$
2. For i from 2 to k,
   1. $\vec{p}_i \equiv \text{proj}_{\text{span}\ \{\hat{a}_1, \cdots, \hat{a}_{i-1}\}} \vec{v}_i$
   2. $\hat{a}_i \equiv \frac{\vec{v}_i - \vec{p}_i}{||\vec{v}_i - \vec{p}_i||}$

Gram-Schmidt Orthogonalization

To orthogonalize $\vec{v}_1, \cdots, \vec{v}_k$:

1. $\hat{a}_1 \equiv \frac{\vec{v}_1}{||\vec{v}_1||}$
2. For i from 2 to k,
   - 2.1 $\vec{p}_i \equiv \text{proj}_{\text{span}\ \{\hat{a}_1, \cdots, \hat{a}_{i-1}\}} \vec{v}_i$
   - 2.2 $\hat{a}_i \equiv \frac{\vec{v}_i - \vec{p}_i}{||\vec{v}_i - \vec{p}_i||}$

Claim

$span\ \{\vec{v}_1, \cdots, \vec{v}_i\} = span\ \{\hat{a}_1, \cdots, \hat{a}_i\}$ for all i.

Implementation via Column Operations

Post-multiplication!

1. Rescaling to unit length: diagonal matrix
2. Subtracting off projection: upper triangular substitution matrix

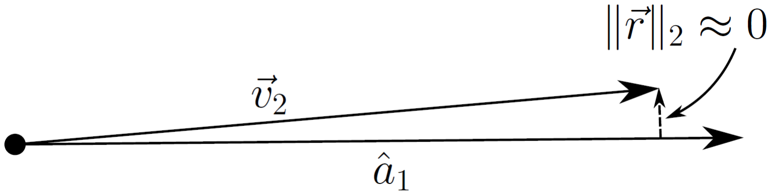
1.一个矩阵右乘一个矩阵，相当于对此矩阵的每一个列向量乘上了一个系数
2.获得垂直于投影方向的向量相当于将1个列向量乘以系数加到另外一个列向量去，故可以类比于之前的高斯消去法可知道应该是一个三角矩阵，同时由于矩阵的转置性，可知其应该是一个上三角矩阵。

New Factorization

$$A = QR$$

- Q orthogonal
- R upper-triangular

Bad Case



这里说明了施密特方法误差仍然存在

$$\vec{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} 1 \\ 1+\varepsilon \end{pmatrix}$$

Two Strategies for QR

1. Post-multiply by upper triangular matrices

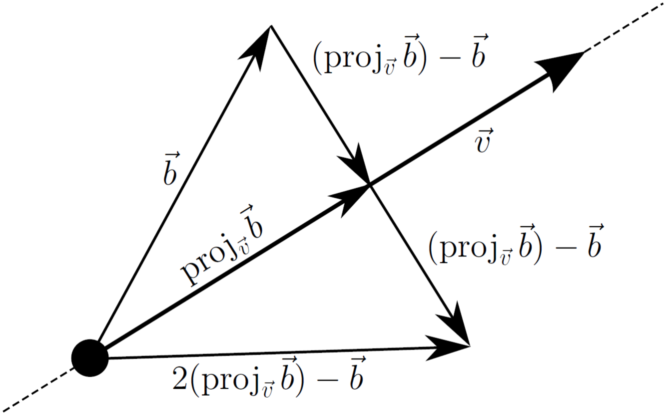
   Done!

Two Strategies for QR

1. Post-multiply by upper triangular matrices
   Done!
2. Pre-multiply by orthogonal matrices
   New idea!

"Easy" Class of Orthogonal Matrices

对称镜像法



"Easy" Class of Orthogonal Matrices

$$
\begin{aligned}
2\,\mathrm{proj}_{\vec{v}}\vec{b} - \vec{b} &= 2\frac{\vec{v}\cdot\vec{b}}{\vec{v}\cdot\vec{v}}\vec{v} - \vec{b} \text{ by definition of projection} \\
&= 2\vec{v}\cdot\frac{\vec{v}^\top\vec{b}}{\vec{v}^\top\vec{v}} - \vec{b} \text{ using matrix notation} \\
&= \left(\frac{2\vec{v}\vec{v}^\top}{\vec{v}^\top\vec{v}} - I_{n\times n}\right)\vec{b} \\
&\equiv -H_{\vec{v}}\vec{b}, \text{ where } H_{\vec{v}} \equiv I_{n\times n} - \frac{2\vec{v}\vec{v}^\top}{\vec{v}^\top\vec{v}}
\end{aligned}
$$

注：H_v显然是一个正交矩阵，使用定义容易证明

Analogy to Forward Substitution

If $\vec{a}$ is first column,

$$c\vec{e}_1 = H_{\vec{v}}\vec{a} \Rightarrow \vec{v} = (\vec{a} - c\vec{e}_1) \cdot \frac{\vec{v}^T\vec{v}}{2\vec{v}^T\vec{a}}$$

Analogy to Forward Substitution

If $\vec{a}$ is first column,

$$c\vec{e}_1 = H_{\vec{v}}\vec{a}$$
$$\Rightarrow \vec{v} = (\vec{a} - c\vec{e}_1) \cdot \frac{\vec{v}^T\vec{v}}{2\vec{v}^T\vec{a}}$$

Choose $\vec{v} = \vec{a} - c\vec{e}_1$ 此时v恰好为几何意义上的对角线

$$\Rightarrow c = \pm||\vec{a}||_2$$

因为是对称向量故模要相同

After One Step

利用对称镜像法，将第一列变为如下格式，之后则类似于高斯消去法的行操作，不过这里要改为对列的操作

$$H_{\vec{v}}A = \begin{pmatrix} c & \times & \times & \times \\ 0 & \times & \times & \times \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \times & \times & \times \end{pmatrix}$$

Later Steps

本质上都是在把原来复杂的列向量变为只有一个非零的列向量，从而使得正交化更简单

$$\vec{a} = \begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \end{pmatrix} \mapsto H_{\vec{v}}\vec{a} = \begin{pmatrix} \vec{a}_1 \\ \vec{0} \end{pmatrix}$$

Leave first k lines alone!

具体矩阵格式件上一页PPT

Householder QR

$$R = H_{\vec{v}_n} \cdots H_{\vec{v}_1} A$$

$$Q = H_{\vec{v}_1}^T \cdots H_{\vec{v}_n}^T$$

H_v为正交矩阵，则Q仍然为正交矩阵。

Householder QR

$$R = H_{\vec{v}_n} \cdots H_{\vec{v}_1} A$$

$$Q = H_{\vec{v}_1}^T \cdots H_{\vec{v}_n}^T$$

Can store Q implicitly by storing $\vec{v}_i$'s!

Slightly Different Output

- Gram-Schmidt: $Q \in \mathbb{R}^{m \times n}, R \in \mathbb{R}^{n \times n}$
- Householder: $Q \in \mathbb{R}^{m \times m}, R \in \mathbb{R}^{m \times n}$

Slightly Different Output

- Gram-Schmidt: $Q \in \mathbb{R}^{m\times n}$, $R \in \mathbb{R}^{n\times n}$
- Householder: $Q \in \mathbb{R}^{m\times m}$, $R \in \mathbb{R}^{m\times n}$

Typical least-squares case:
$A \in \mathbb{R}^{m\times n}$ has $m \gg n$.

Desired

Stability of Householder with shape of Gram-Schmidt.

Shape of R

$$R = \left(\begin{array}{ccc} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ \hline 0 & 0 & 0 \\ 0 & 0 & 0 \end{array}\right)$$

Reduced QR

$$
\begin{aligned}
A &= QR \\
&= (Q_1 Q_2) \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \\
&= Q_1 R_1
\end{aligned}
$$

分块矩阵，可以理解为作用于全零行的Q矩阵并无作用，因为使用Q的目的就是要把一列中除去一个元素之外的元素都设置为0