Column Spaces and QR

CS 205A:
Mathematical Methods for Robotics, Vision, and Graphics

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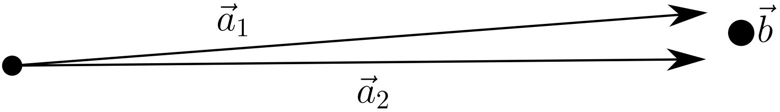
Problem

$$\operatorname{cond} A^\top A \approx (\operatorname{cond} A)^2$$

Geometric Intuition



Least-squares fit is ambiguous!

When Is $\operatorname{cond} A^\top A \approx 1$?

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

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

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(then, $\operatorname{cond} A^\top A \approx 1$!)

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

Recall: Definition of Gram matrix

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

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

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

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

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Orthonormal; orthogonal matrix

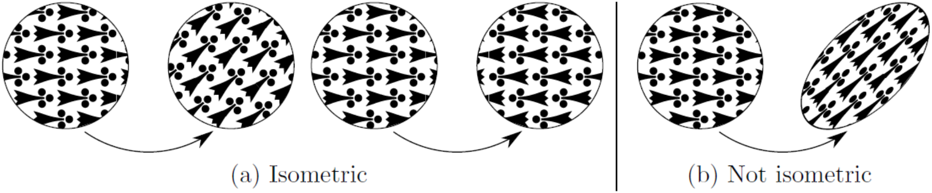
A set of vectors $\{\vec{v}_1, \cdots, \vec{v}_k\}$ is *orthonormal* if $\|\vec{v}_i\| = 1$ for all i and $\vec{v}_i \cdot \vec{v}_j = 0$ for all $i \neq j$. A square matrix whose columns are orthonormal is called an *orthogonal* matrix.

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

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

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

Observation

Lemma: Column space invariance

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

$$\mathrm{col}\ A = \mathrm{col}\ AB.$$

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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

Using QR

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

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

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

Vector Projection

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

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

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$$\mathrm{proj}_{\vec{a}}\, \vec{b} = c\vec{a} = \frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\|_2^2}\vec{a}$$

Properties of Projection

$$\operatorname{proj}_{\vec{a}} \vec{b} \parallel \vec{a}$$

$$\vec{a} \cdot (\vec{b} - \operatorname{proj}_{\vec{a}} \vec{b}) = 0$$

$$\implies (\vec{b} - \operatorname{proj}_{\vec{a}} \vec{b}) \perp \vec{a}$$

Orthonormal Projection

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

$$\text{proj}_{\hat{a}_i} \vec{b} = (\hat{a}_i \cdot \vec{b})\hat{a}_i$$

Orthonormal Projection

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

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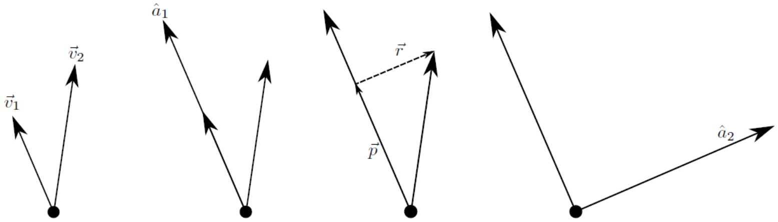
$$\implies c_i = \vec{b}\cdot\hat{a}_i$$

$$\implies \text{proj}_{\text{span }\{\hat{a}_1,\cdots,\hat{a}_k\}}\vec{b} = (\hat{a}_1\cdot\vec{b})\hat{a}_1 + \cdots + (\hat{a}_k\cdot\vec{b})\hat{a}_k$$

Geometric Strategy for Orthogonalization



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

Gram-Schmidt Orthogonalization

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

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

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Claim

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

Implementation via Column Operations

Post-multiplication!

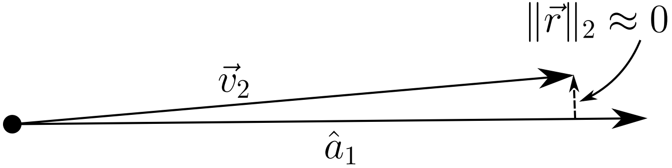
1. Rescaling to unit length: diagonal matrix
2. Subtracting off projection: upper triangular substitution matrix

New Factorization

$$A = QR$$

- Q orthogonal
- R upper-triangular

Bad Case



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

Two Strategies for QR

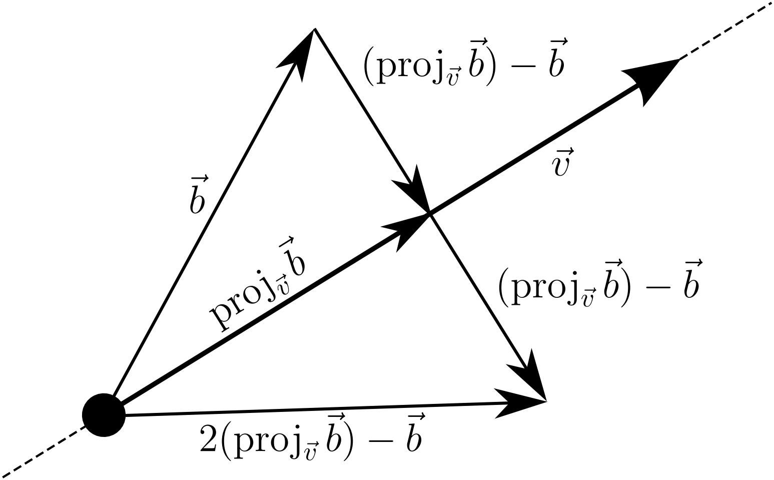
1. Post-multiply by upper triangular matrices
   Done!

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



Reflection Matrices

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

Analogy to Forward Substitution

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

$$c\vec{e}_1 = H_{\vec{v}}\vec{a}$$

$$\implies \vec{v} = (\vec{a} - c\vec{e}_1) \cdot \frac{\vec{v}^\top \vec{v}}{2\vec{v}^\top \vec{a}}$$

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

$$c\vec{e}_1 = H_{\vec{v}}\vec{a}$$

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Choose $\vec{v} = \vec{a} - c\vec{e}_1$

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

After One Step

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

Later Steps

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

Leave first k lines alone!

Householder QR

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

Householder QR

$$R = H_{\vec{v}_n} \cdots H_{\vec{v}_1} A$$
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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: $Q \in \mathbb{R}^{m\times m}$, $R \in \mathbb{R}^{m\times n}$

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

$$R = \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ \hline 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Reduced QR

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