Orthogonality

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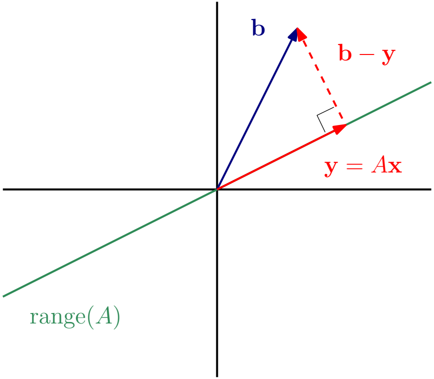
Normal Equation Revisited

Alternate perspective on the "normal equation":

$$A^{\mathrm{T}}(\mathbf{b} - A\mathbf{x}) = \mathbf{0} \quad \iff \quad \mathbf{z}^{\mathrm{T}}(\underbrace{\mathbf{b} - A\mathbf{x}}_{\text{residual } = \mathbf{r}}) = 0 \quad \text{for all } \mathbf{z} \in \mathcal{R}(A)\,,$$

i.e., $\mathbf{x}$ solves the normal equation if and only if the residual is orthogonal to the range of A.



Orthogonal Vectors

Recall that the angle θ between two vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ satisfies

$$\cos(\theta) = \frac{\mathbf{u}^{\mathrm{T}}\mathbf{v}}{\|\mathbf{u}\|_2 \|\mathbf{v}\|_2}.$$

Definition 1

- Two vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ are **orthogonal** if $\mathbf{u}^{\mathrm{T}}\mathbf{v} = 0$.
- Vectors $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_k \in \mathbb{R}^n$ are **orthogonal** if $\mathbf{q}_i^{\mathrm{T}}\mathbf{q}_j = 0$ for all $i \neq j$.
- Vectors $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_k \in \mathbb{R}^n$ are **orthonormal** if $\mathbf{q}_i^{\mathrm{T}}\mathbf{q}_j = \delta_{i,j}$.

Notation. (Kronecker delta function)

$$\delta_{i,j} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Matrices with Orthogonal Columns

Let $Q = \left[\ \mathbf{q}_1 \mid \mathbf{q}_2 \mid \cdots \mid \mathbf{q}_k\ \right] \in \mathbb{R}^{n \times k}$. Note that

$$Q^{\mathrm{T}} Q = \begin{bmatrix} \mathbf{q}_1^{\mathrm{T}} \\ \hline \mathbf{q}_2^{\mathrm{T}} \\ \hline \vdots \\ \hline \mathbf{q}_k^{\mathrm{T}} \end{bmatrix} \left[\begin{array}{c|c|c|c} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_k \end{array}\right] = \begin{bmatrix} \mathbf{q}_1^{\mathrm{T}}\mathbf{q}_1 & \mathbf{q}_1^{\mathrm{T}}\mathbf{q}_2 & \cdots & \mathbf{q}_1^{\mathrm{T}}\mathbf{q}_k \\ \mathbf{q}_2^{\mathrm{T}}\mathbf{q}_1 & \mathbf{q}_2^{\mathrm{T}}\mathbf{q}_2 & \cdots & \mathbf{q}_2^{\mathrm{T}}\mathbf{q}_k \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{q}_k^{\mathrm{T}}\mathbf{q}_1 & \mathbf{q}_k^{\mathrm{T}}\mathbf{q}_2 & \cdots & \mathbf{q}_k^{\mathrm{T}}\mathbf{q}_k \end{bmatrix}.$$

Therefore,

- $\mathbf{q}_1, \ldots, \mathbf{q}_k$ are orthogonal. $\iff$ $Q^{\mathrm{T}} Q$ is a $k \times k$ diagonal matrix.
- $\mathbf{q}_1, \ldots, \mathbf{q}_k$ are orthonormal. $\iff$ $Q^{\mathrm{T}} Q$ is the $k \times k$ identity matrix.

Matrices with Orthonormal Columns

Theorem 2

Let $Q = \left[\, \mathbf{q}_1 \mid \mathbf{q}_2 \mid \cdots \mid \mathbf{q}_k \,\right] \in \mathbb{R}^{n\times k}$ *and suppose that* $\mathbf{q}_1, \ldots, \mathbf{q}_k$ *are orthonormal. Then*

1. $Q^{\mathrm{T}}Q = I \in \mathbb{R}^{k\times k}$;
2. $\|Q\mathbf{x}\|_2 = \|\mathbf{x}\|_2$ *for all* $\mathbf{x} \in \mathbb{R}^k$;
3. $\|Q\|_2 = 1$.

Orthogonal Matrices

Definition 3

We say that $Q \in \mathbb{R}^{n\times n}$ is an **orthogonal matrix** if $Q^{\mathrm{T}}Q = I \in \mathbb{R}^{n\times n}$.

- A square matrix with orthogonal columns is not, in general, an orthogonal matrix!

Properties of Orthogonal Matrices

Theorem 4

Let $Q \in \mathbb{R}^{n\times n}$ be orthogonal. Then

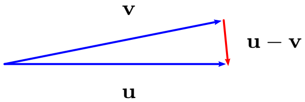
1. $Q^{-1} = Q^{\mathrm{T}}$;
2. Q^{T} *is also an orthogonal matrix;*
3. $\kappa_2(Q) = 1$;
4. *For any* $A \in \mathbb{R}^{n\times n}$, $\|AQ\|_2 = \|A\|_2$;
5. *if* $P \in \mathbb{R}^{n\times n}$ *is another orthogonal matrix, then* PQ *is also orthogonal.*

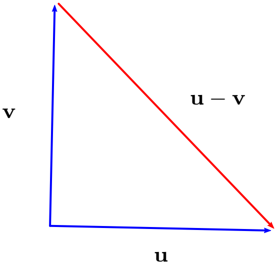
Why Do We Like Orthogonal Vectors?

- If $\mathbf{u}$ and $\mathbf{v}$ are orthogonal, then

$$\|\mathbf{u} \pm \mathbf{v}\|_2^2 =$$

- Without orthogonality, it is possible that $\|\mathbf{u} - \mathbf{v}\|_2$ is much smaller than $\|\mathbf{u}\|_2$ and $\|\mathbf{v}\|_2$.
- The addition and subtraction of orthogonal vectors are guaranteed to be well-conditioned.





Appendix: Projection and Reflection

Projection and Reflection Operators

Let $\mathbf{u}, \mathbf{v} \in \mathbb{R}^m$ be nonzero vectors.

- Projection of $\mathbf{u}$ onto $\langle \mathbf{v} \rangle = \text{span}(\mathbf{v})$:

$$\frac{\mathbf{v}^{\mathrm{T}}\mathbf{u}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\mathbf{v} = \underbrace{\left(\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\right)}_{=:P}\mathbf{u} =: P\mathbf{u}.$$

- Projection of $\mathbf{u}$ onto $\langle \mathbf{v} \rangle^{\perp}$, the orthogonal complement of $\langle \mathbf{v} \rangle$:

$$\mathbf{u} - \frac{\mathbf{v}^{\mathrm{T}}\mathbf{u}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\mathbf{v} = \left(I - \frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\right)\mathbf{u} =: (I - P)\mathbf{u}.$$

- Reflection of $\mathbf{u}$ across $\langle \mathbf{v} \rangle^{\perp}$:

$$\mathbf{u} - 2\frac{\mathbf{v}^{\mathrm{T}}\mathbf{u}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\mathbf{v} = \left(I - 2\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\right)\mathbf{u} =: (I - 2P)\mathbf{u}.$$

Projection and Reflection Operators (cont')

Summary: for given $\mathbf{v} \in \mathbb{R}^m$, a nonzero vector, let

$$P = \frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}} \in \mathbb{R}^{m \times m}.$$

Then the following matrices carry out geometric transformations

- Projection onto $\langle \mathbf{v} \rangle$: P
- Projection onto $\langle \mathbf{v} \rangle$: $I - P$
- Reflection across $\langle \mathbf{v} \rangle^{\perp}$: $I - 2P$

Note. If $\mathbf{v}$ were a unit vector, the definition of P simplifies to $P = \mathbf{v}\mathbf{v}^{\mathrm{T}}$.