

Projection

For any vector $\mathbf{y} \in \mathbb{R}^n$ and a subspace $\mathcal{M} \subseteq \mathbb{R}^n$, there exists a **unique** vector $\hat{\mathbf{y}}$ such that

1. $\hat{\mathbf{y}} \in \mathcal{M}$, and
2. $(\mathbf{y} - \hat{\mathbf{y}}) \perp \mathcal{M}$.

We call $\hat{\mathbf{y}}$ the **projection** of \mathbf{y} onto \mathcal{M} .

$$\mathbf{y} = \underbrace{\hat{\mathbf{y}}}_{\in \mathcal{M}} + \underbrace{(\mathbf{y} - \hat{\mathbf{y}})}_{\in \mathcal{M}^\perp}$$

How to Compute $\hat{\mathbf{y}}$?

Approach I: Suppose \mathcal{M} has an ONB $\{\mathbf{e}_1, \dots, \mathbf{e}_p\}$. Then any vector $\mathbf{v} \in \mathcal{M}$ can be uniquely expressed as

$$\mathbf{v} = a_1 \mathbf{e}_1 + \dots + a_p \mathbf{e}_p, \quad \text{with } a_j = \mathbf{v}^t \mathbf{e}_j.$$

Since $\hat{\mathbf{y}} \in \mathcal{M}$, we have

$$\hat{\mathbf{y}} = a_1 \mathbf{e}_1 + \dots + a_p \mathbf{e}_p, \quad \text{with } a_j = \hat{\mathbf{y}}^t \mathbf{e}_j.$$

Note that we can replace $\hat{\mathbf{y}}$ by \mathbf{y} when computing a_j :

$$\mathbf{y}^t \mathbf{e}_j = (\hat{\mathbf{y}} + \mathbf{y} - \hat{\mathbf{y}})^t \mathbf{e}_j = \hat{\mathbf{y}}^t \mathbf{e}_j + \underbrace{(\mathbf{y} - \hat{\mathbf{y}})^t \mathbf{e}_j}_{=0} = \hat{\mathbf{y}}^t \mathbf{e}_j.$$

So we have

$$\begin{aligned}\hat{\mathbf{y}} &= (\mathbf{e}_1^t \mathbf{y}) \mathbf{e}_1 + \cdots + (\mathbf{e}_p^t \mathbf{y}) \mathbf{e}_p \\ &= \mathbf{e}_1 (\mathbf{e}_1^t \mathbf{y}) + \cdots + \mathbf{e}_p (\mathbf{e}_p^t \mathbf{y}) \\ &= \mathbf{e}_1 \mathbf{e}_1^t \mathbf{y} + \cdots + \mathbf{e}_p \mathbf{e}_p^t \mathbf{y} \\ &= (\mathbf{e}_1 \mathbf{e}_1^t + \cdots + \mathbf{e}_p \mathbf{e}_p^t) \mathbf{y} \\ &= \mathbf{M}_{n \times 1} \mathbf{y}.\end{aligned}$$

Approach II: Suppose $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ is a basis for \mathcal{M} . Then any vector $\mathbf{v} \in \mathcal{M}$ can be expressed as a unique linear combination of \mathbf{x}_j 's. In particular, assume

$$\hat{\mathbf{y}} = b_1 \mathbf{x}_1 + \dots + b_p \mathbf{x}_p = \mathbf{X}_{n \times p} \mathbf{b}_{p \times 1}.$$

By the definition of projection, we have

$$\begin{aligned} & \mathbf{y} - \hat{\mathbf{y}} \perp \mathcal{M} \\ \iff & \mathbf{y} - \hat{\mathbf{y}} \perp \mathbf{x}_j, \quad \text{for } j = 1, \dots, p \\ \iff & \mathbf{x}_j^t (\mathbf{y} - \hat{\mathbf{y}}) = 0, \quad \text{for } j = 1, \dots, p \\ \iff & \mathbf{X}^t (\mathbf{y} - \hat{\mathbf{y}}) = \mathbf{0}_{p \times 1} \iff \mathbf{X}^t (\mathbf{y} - \mathbf{X}\mathbf{b}) = \mathbf{0} \end{aligned}$$

Solving the equation array above, we have

$$\mathbf{X}^t \mathbf{y} = (\mathbf{X}^t \mathbf{X}) \mathbf{b} \implies \mathbf{b} = (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y},$$

therefore

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = \mathbf{X}^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y} = \mathbf{M}_{n \times n} \mathbf{y}.$$

Projection Matrix

For a vector space \mathcal{M} , the projection of any vector \mathbf{y} can be computed as $\hat{\mathbf{y}} = \mathbf{M}\mathbf{y}$, and \mathbf{M} is called the **projection matrix** for \mathcal{M} .

Properties of \mathbf{M} :

- Unique; Exist
- For any vector $\mathbf{v} \in \mathcal{M}$, $\mathbf{M}\mathbf{v} = \mathbf{v}$ and for any vector $\mathbf{v} \perp \mathcal{M}$, $\mathbf{M}\mathbf{v} = \mathbf{0}$.
- **Symmetric** and **Idempotent**: $\mathbf{M}^t = \mathbf{M}$, $\mathbf{M}^2 = \mathbf{M}$. Further we have $\mathbf{M}^k = \mathbf{M}$ and $\mathbf{M}(\mathbf{I} - \mathbf{M})$.
- $\mathbf{I} - \mathbf{M}$ is the projection matrix for vector space \mathcal{M}^\perp .
- Trace of a projection matrix tells us the dim of the subspace:

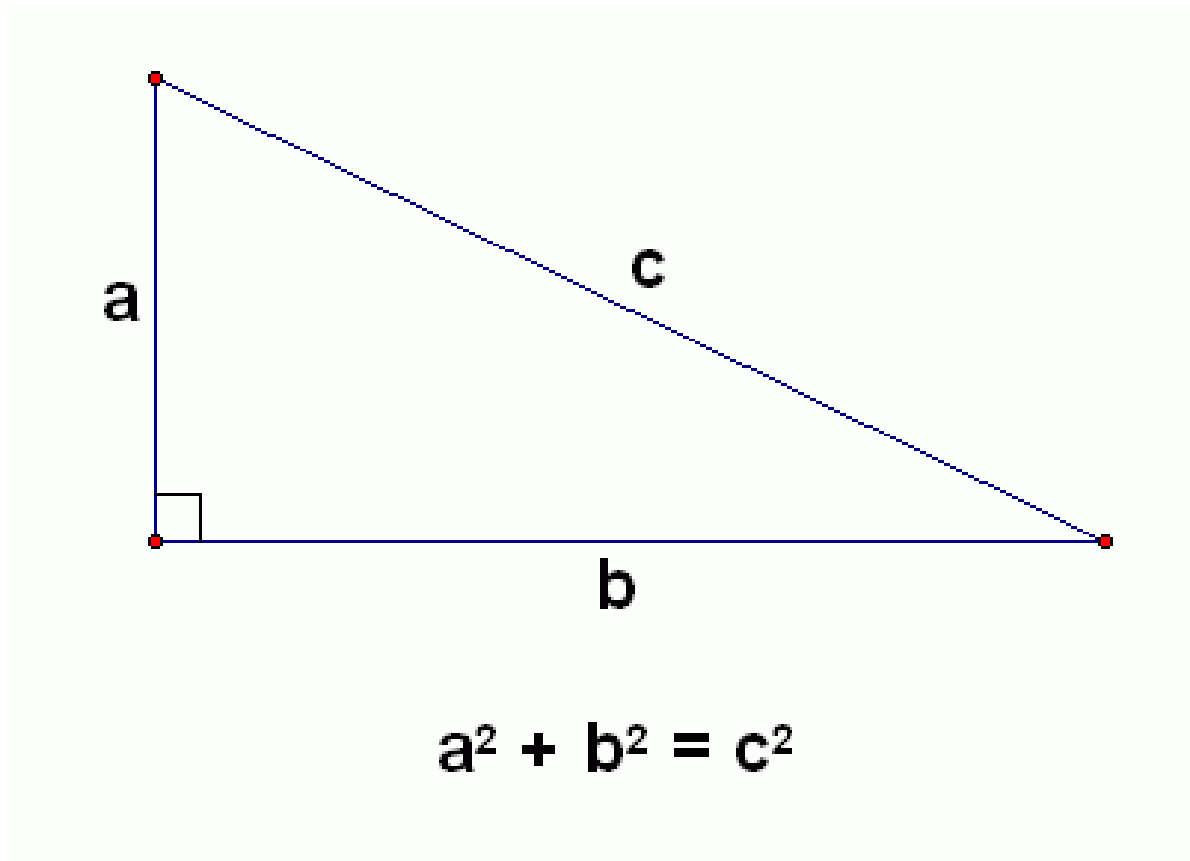
$$\text{tr}(\mathbf{M}) = p.$$

Pythagorean Theorem

If $\mathbf{v}_1 \perp \mathbf{v}_2$ then $\|\mathbf{v}_1 + \mathbf{v}_2\|^2 = \|\mathbf{v}_1\|^2 + \|\mathbf{v}_2\|^2$.

In particular

$$\|\mathbf{y}\|^2 = \|\hat{\mathbf{y}} + \mathbf{y} - \hat{\mathbf{y}}\|^2 = \|\hat{\mathbf{y}}\|^2 + \|\mathbf{y} - \hat{\mathbf{y}}\|^2$$



LS and Projection

Recall the LS problem: find a vector \mathbf{v} in $C(\mathbf{X})$, which minimizes $\|\mathbf{y} - \mathbf{v}\|^2$,
i.e.,

$$\min_{\mathbf{v} \in C(\mathbf{X})} \|\mathbf{y} - \mathbf{v}\|^2.$$

Let $\hat{\mathbf{y}}$ denote the projection of \mathbf{y} onto $C(\mathbf{X})$. We have

$$\|\mathbf{y} - \mathbf{v}\|^2 = \underbrace{\|\mathbf{y} - \hat{\mathbf{y}}\|^2}_{\in C(\mathbf{X})^\perp} + \underbrace{\|\hat{\mathbf{y}} - \mathbf{v}\|^2}_{\in C(\mathbf{X})} \geq \|\mathbf{y} - \hat{\mathbf{y}}\|^2.$$

So the LS solution is the projection of \mathbf{y} onto the space $C(\mathbf{X})$:

$$\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y} = \mathbf{H} \mathbf{y}.$$

The projection matrix \mathbf{H} is also called the hat matrix in many textbooks.

- $C(\mathbf{X})$ is often called the **estimation space**, and $C(\mathbf{X})^\perp$ the **error space**.
- $\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}} = (\mathbf{I} - \mathbf{M})\mathbf{y}$ is the projection of \mathbf{y} onto $C(\mathbf{X})^\perp$, the space orthogonal to $C(\mathbf{X})$. The corresponding projection matrix is $(\mathbf{I}_n - \mathbf{M})$ and \dim is $n - p$.
- **The essence of LS**: decompose the data vector \mathbf{y} into two **orthogonal** components

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{r},$$

where $\hat{\mathbf{y}}$ in the estimation space and \mathbf{r} in the error space.