Solving the Least-Squares Problem Using Geometry

Objectives

- develop orthogonality condition for the least-squares problem
- find the least-squares problem solution
- introduce matrix inversion

The Least-Squares Problem

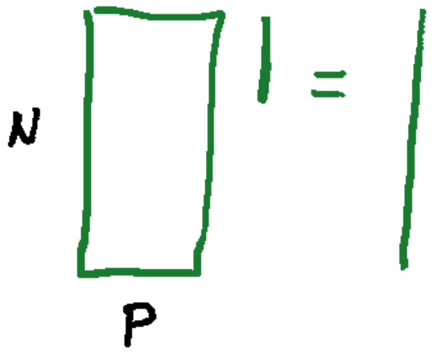
N feature vectors

$$\begin{bmatrix} \cdots \underline{x}_1^T \cdots \\ \cdots \underline{x}_2^T \cdots \\ \vdots \\ \cdots \underline{x}_N^T \cdots \end{bmatrix}\begin{bmatrix} w_1\\ w_2\\ \vdots\\ w_p\end{bmatrix} = \begin{bmatrix} d_1\\ d_2\\ \vdots\\ d_N\end{bmatrix}$$

labels

p model parameters

$$\underline{A}\,\underline{w} = \underline{d}$$



Assume:

- $N \geq P$
- $\text{rank}(\underline{A}) = P$

$$\min_{\underline{w}} \|\underline{A}\underline{w} - \underline{d}\|_2^2 \qquad \text{Let } \hat{\underline{d}} = \underline{A}\underline{w}$$

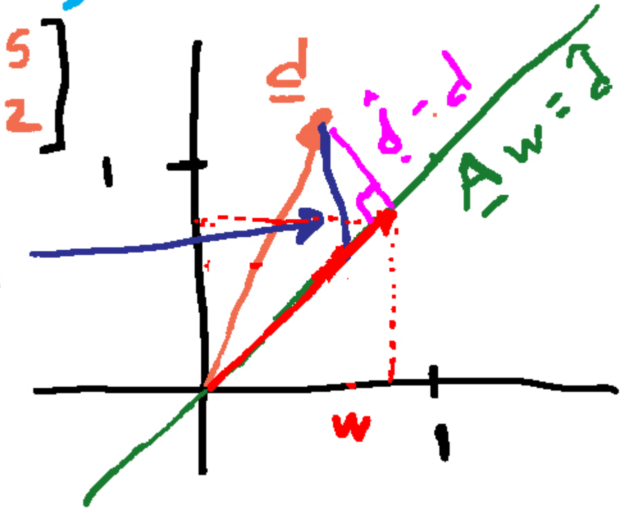
- $\hat{\underline{d}}$ lies in p-dim subspace spanned by columns of $\underline{A}$

Example $(P=1, N=2)$

$$\underline{A} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \underline{d} = \begin{bmatrix} 0.5 \\ 1.2 \end{bmatrix}$$

$$\hat{\underline{d}} = \begin{bmatrix} w \\ w \end{bmatrix} \qquad \hat{\underline{d}} - \underline{d}$$

Soln: $\hat{\underline{d}} - \underline{d} \perp \underline{A}$

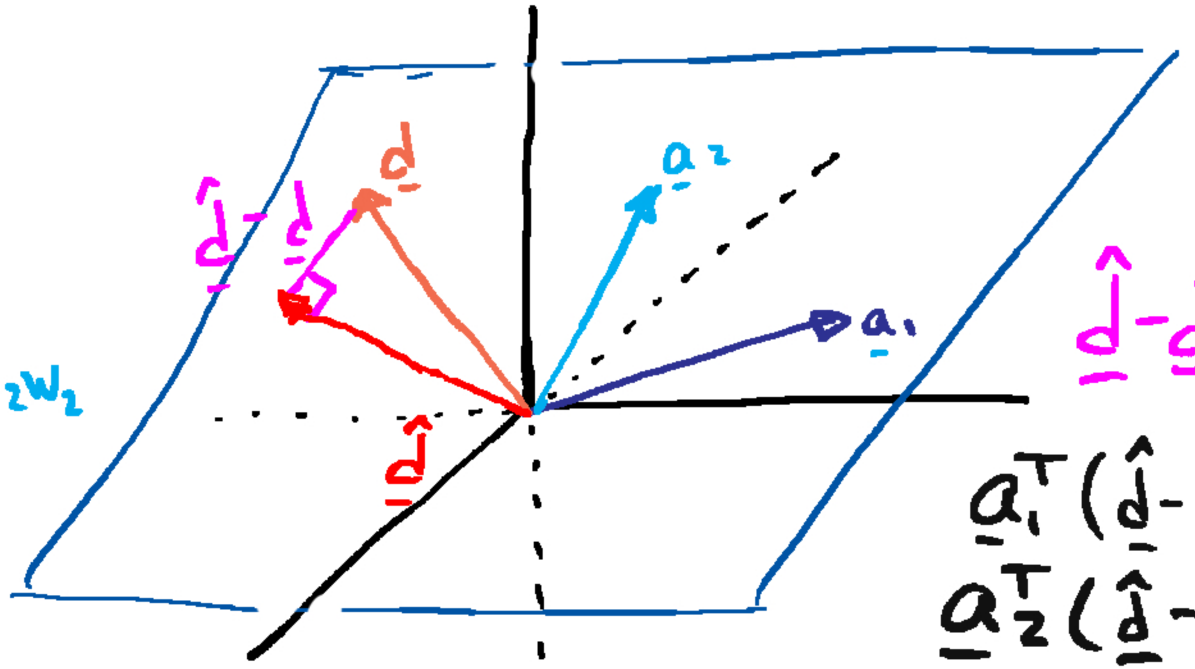


Orthogonality: $\underline{A} \perp (\hat{\underline{d}} - \underline{d})$

$N=3,\ P=2$

$\underline{A} = [\underline{a}_1 \ \ \underline{a}_2] \qquad \underline{d}$

$\hat{\underline{d}} = \underline{A}\,\underline{w} = \underline{a}_1 w_1 + \underline{a}_2 w_2$



$\hat{\underline{d}} - \underline{d} \perp \mathrm{span}\{\underline{a}_1, \underline{a}_2\}$

$\underline{a}_1^T(\hat{\underline{d}} - \underline{d}) = 0$

$\underline{a}_2^T(\hat{\underline{d}} - \underline{d}) = 0$

In general

$\underline{A}^T(\hat{\underline{d}} - \underline{d}) = \underline{0}$ "orthognality condition"

Solution: $\underline{A}^T(\underline{A}\,\underline{w} - \underline{d}) = \underline{0} \Rightarrow \underline{A}^T\underline{A}\,\underline{w} = \underline{A}^T\underline{d}$

$(\underline{A}^T\underline{A})^{-1}(\underline{A}^T\underline{A})\underline{w} = (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d} \Rightarrow \underline{w} = (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$ (matrix inverse)

Matrix Inversion

Let $\underline{B}$ be a $P \times P$ invertible matrix. $\underline{B}^{-1}$ satisfies

$$\underline{B}^{-1}\underline{B} = \underline{\underline{I}} = \begin{bmatrix} 1 & & 0 \\ & 1 & \\ & & \ddots & \\ 0 & & & 1 \end{bmatrix} \quad \text{(identity matrix: } \underline{\underline{I}}\,\underline{v} = \underline{v}\text{)}$$

$$\underline{B}\,\underline{B}^{-1} = \underline{I}$$

Examples:

$$\underline{B} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}, \quad \underline{B}^{-1} = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix} \Rightarrow \underline{B}\,\underline{B}^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\underline{B} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \quad \underline{B}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \Rightarrow \underline{B}\,\underline{B}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} ad-bc & 0 \\ 0 & ad-bc \end{bmatrix}$$

Not all matrices have inverses

$$\underline{B} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \underline{B}^{-1} = \frac{1}{0} \times$$

Full rank (P) square matrices are invertible!

(proof in notes)

A few conditions for invertibility

- $\underline{A}^T\underline{A}$ is invertible iff $\underline{A}$ ($N \times P$, $P \leq N$) is rank P
- Positive definite $\Rightarrow$ invertible. $\underline{Q}$ is positive definite ($\underline{Q} > 0$) iff $\underline{v}^T\underline{Q}\underline{v} > 0 \;\forall\; \underline{v} \neq 0$ "for all"

(proofs in notes)

$\underline{A}^T\underline{A}$ is positive definite:

Let $\underline{y} = \underline{A}\underline{v}$. $\text{rank}(\underline{A}) = P \Rightarrow \underline{y} \neq \underline{0}$ for $\underline{v} \neq \underline{0}$

$$(\underline{A}\underline{v})^T\underline{A}\underline{v} = \underline{v}^T\underline{A}^T\underline{A}\underline{v} = \underline{y}^T\underline{y} = \sum_i y_i^2 > 0 \quad (\underline{v} \neq \underline{0})$$

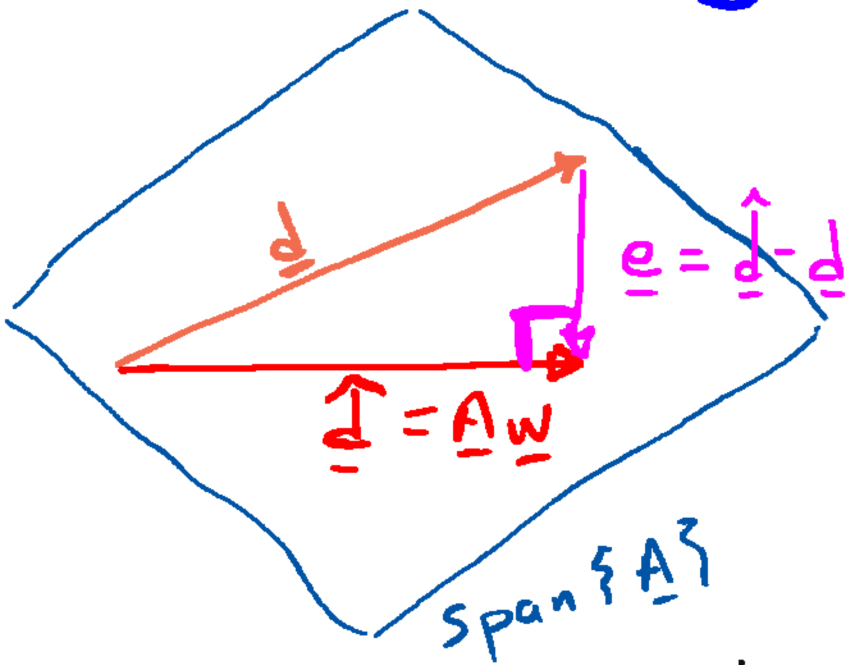
$\Rightarrow (\underline{A}^T\underline{A})^{-1}$ exists

Note: $\underline{Q}$ is positive semidefinite iff $\underline{v}^T\underline{Q}\underline{v} \geq 0 \;\forall\; \underline{v} \neq \underline{0}$

Summary

$$\min_{\underline{w}} \|\underline{A}\,\underline{w}-\underline{d}\|_2^2 \Rightarrow \min_{\underline{w}} \|\underline{e}\|_2^2$$

$$\Rightarrow \underline{e} \perp \text{span}\{\underline{A}\} \qquad \underline{A}^T\underline{e} = \underline{0}$$



$$\underset{P\times N}{\underline{A}^T}\Big(\underset{N\times P}{\underline{A}}\;\underset{P}{\underline{w}} - \underset{N}{\underline{d}}\Big) = \underline{0}$$

$$\underset{P\times P}{\underline{A}^T\underline{A}}\;\underset{P\times 1}{\underline{w}} = \underset{P\times 1}{\underline{A}^T\underline{d}}$$

$$\boxed{\underline{w} = (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}}$$

$$\underline{A}\,\underline{w} \rightarrow (\underline{A}^T\underline{A})^{-1}\underline{A}^T\;\underline{A}\;\underline{w} = \underline{w}$$

$$\hat{\underline{d}} = \underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$$