



## Classical Numerical Analysis, Chapter 05

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# Chapter 05, Part 1 of 2

## Linear Least Squares Problem



## Data Fitting

Suppose that we are given a table of values

$$(x_k, y_k), \quad k = 1, \dots, n,$$

that is obtained, say, by a series of measurements.

Find a simple function — a linear function, for example,  $y = c_1x + c_0$ , where  $c_0, c_1 \in \mathbb{C}$  — that *fits* the data in some exact or approximate sense. If we demand that it matches the data exactly, then

$$y_k = c_1x_k + c_0, \quad k = 1, \dots, n.$$

This can also be expressed in vector form as

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_0 \end{bmatrix}.$$



## Data Fitting

This is equivalent to the system of linear equations of the form  $\mathbf{A}\mathbf{c} = \mathbf{y}$  with

$$\mathbf{A} = \begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \in \mathbb{C}^{n \times 2}, \quad \mathbf{c} = \begin{bmatrix} c_1 \\ c_0 \end{bmatrix} \in \mathbb{C}^2, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{C}^n.$$

Usually  $n$  is much larger than 2, so that we end up with an *overdetermined* system of equations, i.e., there are more equations than unknowns. There is no solution in general.

On the other hand, if we only approximately enforce the matching conditions

$$y_k \approx c_1 x_k + c_0, \quad k = 1, \dots, n,$$

then it is not clear how to proceed.



# Linear Least Squares: Full Rank Setting



## Generalized and Least Squares Solutions

Idea: There may be no solution to  $A\mathbf{x} = \mathbf{f}$ . So, let us find  $\mathbf{x}$  so that  $\mathbf{f} - A\mathbf{x}$  is as small as possible in some norm.

### Definition

Suppose that  $\|\cdot\| : \mathbb{C}^m \rightarrow \mathbb{R}$  is a norm. Given  $A \in \mathbb{C}^{m \times n}$ ,  $m \geq n$ , and  $\mathbf{f} \in \mathbb{C}^m$  we say that  $\mathbf{x} \in \mathbb{C}^n$  is a **weak** or **generalized** solution of the system  $A\mathbf{x} = \mathbf{f}$  iff

$$\mathbf{x} \in \operatorname{argmin}_{\mathbf{w} \in \mathbb{C}^n} \|\mathbf{r}(\mathbf{w})\| = \operatorname{argmin}_{\mathbf{w} \in \mathbb{C}^n} \|\mathbf{f} - A\mathbf{w}\|.$$

We say that  $\mathbf{x} \in \mathbb{C}^n$  is a **least squares** solution of the system  $A\mathbf{x} = \mathbf{f}$  iff

$$\mathbf{x} \in \operatorname{argmin}_{\mathbf{w} \in \mathbb{C}^n} \|\mathbf{r}(\mathbf{w})\|_{\ell^2(\mathbb{C}^m)}^2 = \operatorname{argmin}_{\mathbf{w} \in \mathbb{C}^n} \|\mathbf{f} - A\mathbf{w}\|_{\ell^2(\mathbb{C}^m)}^2.$$

When these minima exist and are unique, we replace  $\in$  with  $=$ .

Full-Rank Coefficient Matrix  $A \in \mathbb{C}^{m \times n}$ ,  $m \geq n$ 

## Lemma

Let  $A \in \mathbb{C}^{m \times n}$  with  $m \geq n$ , then  $A^H A$  is Hermitian positive definite (HPD) iff  $A$  is full rank, i.e.,  $\text{rank}(A) = n$ .

## Proof.

Clearly the matrix  $A^H A$  is Hermitian. By construction this matrix is also nonnegative definite since, for any  $\mathbf{x} \in \mathbb{C}^n$ ,

$$(A^H A \mathbf{x}, \mathbf{x})_2 = (A \mathbf{x}, A \mathbf{x})_2 = \|A \mathbf{x}\|_2^2 \geq 0.$$

( $\implies$ ): Suppose that  $A^H A$  is HPD and, to reach a contradiction, that  $\text{rank}(A) < n$ . This is equivalent to say that there is a nonzero  $\mathbf{x} \in \mathbb{C}^n$  such that  $A \mathbf{x} = \mathbf{0}$ . But then we must have  $A^H A \mathbf{x} = \mathbf{0}$  and  $(A^H A \mathbf{x}, \mathbf{x})_2 = 0$ , contradicting the assumption that  $A^H A$  is positive definite.



## Proof, Cont.

( $\Leftarrow$ ): Let us now assume that  $A$  is of full rank. To reach a contradiction, suppose that  $A^H A$  is not positive definite. There must be a nonzero  $\mathbf{x} \in \mathbb{C}_*^n$  for which

$$0 = (A^H A \mathbf{x}, \mathbf{x})_2 = (A \mathbf{x}, A \mathbf{x})_2 = \|A \mathbf{x}\|_2^2,$$

which implies that

$$A \mathbf{x} = \mathbf{0} \implies \mathbf{x} \in \ker(A).$$

This contradicts the assumption that  $A$  has full rank. □





## Theorem (least squares: real case)

Let  $A \in \mathbb{R}^{m \times n}$ , with  $m \geq n$  and  $\text{rank}(A) = n$ , and let  $\mathbf{f} \in \mathbb{R}^m$ . The vector  $\mathbf{x} \in \mathbb{R}^n$  is the unique least squares solution to  $A\mathbf{x} = \mathbf{f}$ , i.e.,

$$\mathbf{x} = \underset{\mathbf{w} \in \mathbb{R}^n}{\text{argmin}} \|\mathbf{f} - A\mathbf{w}\|_{\ell^2(\mathbb{R}^m)}^2, \quad (1)$$

iff  $\mathbf{x}$  is the unique solution to the normal equation

$$A^T A \mathbf{x} = A^T \mathbf{f}. \quad (2)$$

## Proof.

( $\implies$ ): Suppose that  $\mathbf{x} \in \mathbb{R}^n$  solves the least squares problem and set  $\mathbf{r} = \mathbf{f} - A\mathbf{x}$ . Now fix  $\mathbf{y} \in \mathbb{R}^n$ , and define

$$g(s) = \Phi(\mathbf{x} + s\mathbf{y}),$$

for all  $s \in \mathbb{R}$ , where

$$\Phi(\mathbf{z}) = \|\mathbf{r}(\mathbf{z})\|_{\ell^2(\mathbb{C}^m)}^2, \quad \mathbf{r}(\mathbf{z}) = \mathbf{f} - A\mathbf{z}, \quad \forall \mathbf{z} \in \mathbb{C}^n.$$



## Proof, Cont.

Then, for any  $s \in \mathbb{R}$ ,

$$g(0) = \Phi(\mathbf{x}) \leq \Phi(\mathbf{x} + s\mathbf{y}) = g(s),$$

since  $\mathbf{x}$  is a least squares solution. Calculating, we find

$$\begin{aligned} g(s) &= (\mathbf{r} - s\mathbf{A}\mathbf{y})^\top (\mathbf{r} - s\mathbf{A}\mathbf{y}) \\ &= \mathbf{r}^\top \mathbf{r} - s\mathbf{y}^\top \mathbf{A}^\top \mathbf{r} - s\mathbf{r}^\top \mathbf{A}\mathbf{y} + s^2 \mathbf{y}^\top \mathbf{A}^\top \mathbf{A}\mathbf{y} \\ &= g(0) - 2s\mathbf{r}^\top \mathbf{A}\mathbf{y} + s^2 \mathbf{y}^\top \mathbf{A}^\top \mathbf{A}\mathbf{y}. \end{aligned}$$

Since  $\mathbf{A}^\top \mathbf{A}$  is symmetric positive definite,  $g$  is a positive quadratic function of one variable, with a global minimum at  $s = 0$ . Hence,

$$0 = \left. \frac{dg}{ds} \right|_{s=0} = -2\mathbf{r}^\top \mathbf{A}\mathbf{y},$$

for arbitrary  $\mathbf{y} \in \mathbb{R}^n$ . From this condition we conclude that  $\mathbf{r}^\top \mathbf{A} = \mathbf{0}^\top$ . This is equivalent to (2).



## Proof, Cont.

( $\Leftarrow$ ): Now, suppose  $\mathbf{x} \in \mathbb{R}^n$  solves the normal equation (2), and set  $\mathbf{r} = \mathbf{f} - \mathbf{A}\mathbf{x}$ . This implies that  $\mathbf{r}^T \mathbf{A}\mathbf{y} = 0$ , for all  $\mathbf{y} \in \mathbb{R}^n$ , or, equivalently,  $\mathbf{r} \in \text{im}(\mathbf{A})^\perp$ . Then

$$\begin{aligned}\Phi(\mathbf{x} + \mathbf{y}) &= (\mathbf{r} - \mathbf{A}\mathbf{y})^T (\mathbf{r} - \mathbf{A}\mathbf{y}) \\ &= \Phi(\mathbf{x}) - \mathbf{r}^T \mathbf{A}\mathbf{y} - \mathbf{y}^T \mathbf{A}^T \mathbf{r} + \mathbf{y}^T \mathbf{A}^T \mathbf{A} \mathbf{y} \\ &= \Phi(\mathbf{x}) + \mathbf{y}^T \mathbf{A}^T \mathbf{A} \mathbf{y} \\ &\geq \Phi(\mathbf{x}),\end{aligned}$$

since  $\mathbf{y}^T \mathbf{A}^T \mathbf{A} \mathbf{y} \geq 0$  for any  $\mathbf{y}$ . More importantly, since  $\mathbf{A}^T \mathbf{A}$  is symmetric positive definite (SPD),

$$\Phi(\mathbf{x} + \mathbf{y}) > \Phi(\mathbf{x}), \quad \forall \mathbf{y} \in \mathbb{R}_*^n.$$

Thus  $\mathbf{x} \in \mathbb{R}^n$  is a least squares solution. □



## Theorem (least squares: complex case)

Let  $A \in \mathbb{C}^{m \times n}$ , with  $m \geq n$  and  $\text{rank}(A) = n$ , and let  $\mathbf{f} \in \mathbb{C}^m$ . The vector  $\mathbf{x} \in \mathbb{C}^n$  is the unique least squares solution to  $A\mathbf{x} = \mathbf{f}$ , i.e.,

$$\mathbf{x} = \underset{\mathbf{w} \in \mathbb{C}^n}{\text{argmin}} \|\mathbf{f} - A\mathbf{w}\|_{\ell^2(\mathbb{C}^m)}^2, \quad (3)$$

iff  $\mathbf{x}$  is the unique solution to the normal equation

$$A^H A \mathbf{x} = A^H \mathbf{f}. \quad (4)$$

## Proof.

( $\Rightarrow$ ): Suppose that  $\mathbf{x} \in \mathbb{C}^n$  solves the least squares problem and set  $\mathbf{r} = \mathbf{f} - A\mathbf{x}$ . Now fix  $\mathbf{y} \in \mathbb{C}^n$ , and define

$$g(s, t) = \Phi(\mathbf{x} + z\mathbf{y}) = \|\mathbf{r} - zA\mathbf{y}\|_2^2,$$

for all  $z = s + it \in \mathbb{C}$ , with  $s, t \in \mathbb{R}$ ,  $i = \sqrt{-1}$ . Then, for any  $s, t \in \mathbb{R}$ ,

$$g(0, 0) = \Phi(\mathbf{x}) \leq \Phi(\mathbf{x} + z\mathbf{y}) = g(s, t),$$

since  $\mathbf{x}$  is a least squares solution.



## Proof, Cont.

Calculating, we find

$$\begin{aligned}
 g(s, t) &= (\mathbf{r} - z\mathbf{A}\mathbf{y})^H (\mathbf{r} - z\mathbf{A}\mathbf{y}) \\
 &= \mathbf{r}^H \mathbf{r} - \bar{z} \mathbf{y}^H \mathbf{A}^H \mathbf{r} - z \mathbf{r}^H \mathbf{A} \mathbf{y} + |z|^2 \mathbf{y}^H \mathbf{A}^H \mathbf{A} \mathbf{y} \\
 &= g(0, 0) - 2 \Re \left( z \mathbf{r}^H \mathbf{A} \mathbf{y} \right) + (s^2 + t^2) \mathbf{y}^H \mathbf{A}^H \mathbf{A} \mathbf{y} \\
 &= g(0, 0) - 2s \Re \left( \mathbf{r}^H \mathbf{A} \mathbf{y} \right) + 2t \Im \left( \mathbf{r}^H \mathbf{A} \mathbf{y} \right) + (s^2 + t^2) \mathbf{y}^H \mathbf{A}^H \mathbf{A} \mathbf{y} .
 \end{aligned}$$

Since  $\mathbf{A}^H \mathbf{A}$  is Hermitian positive definite,  $g$  is a positive quadratic function of two variables. Hence,

$$0 = \left. \frac{\partial g}{\partial s} \right|_{s,t=0} = -2 \Re \left( \mathbf{r}^H \mathbf{A} \mathbf{y} \right), \quad 0 = \left. \frac{\partial g}{\partial t} \right|_{s,t=0} = 2 \Im \left( \mathbf{r}^H \mathbf{A} \mathbf{y} \right),$$

for arbitrary  $\mathbf{y} \in \mathbb{C}^n$ . From these two conditions we conclude that  $\mathbf{r}^H \mathbf{A} = \mathbf{0}^T$ . Hence  $\mathbf{r} \in \text{im}(\mathbf{A})^\perp$ , as desired.



## Proof, Cont.

( $\Leftarrow$ ): This step is more or less the same as in the real case. Suppose  $\mathbf{x} \in \mathbb{C}^n$  satisfies  $\mathbf{r} \in \text{im}(\mathbf{A})^\perp$ , and set  $\mathbf{r} = \mathbf{f} - \mathbf{A}\mathbf{x}$ . Then

$$\begin{aligned}\Phi(\mathbf{x} + \mathbf{y}) &= (\mathbf{r} + \mathbf{A}\mathbf{y})^H (\mathbf{r} + \mathbf{A}\mathbf{y}) \\ &= \Phi(\mathbf{x}) + \mathbf{r}^H \mathbf{A}\mathbf{y} + \mathbf{y}^H \mathbf{A}^H \mathbf{r} + \mathbf{y}^H \mathbf{A}^H \mathbf{A}\mathbf{y} \\ &= \Phi(\mathbf{x}) + \mathbf{y}^H \mathbf{A}^H \mathbf{A}\mathbf{y} \\ &\geq \Phi(\mathbf{x}),\end{aligned}$$

since  $\mathbf{y}^H \mathbf{A}^H \mathbf{A}\mathbf{y} \geq 0$  for any  $\mathbf{y}$ . And, since  $\mathbf{A}^H \mathbf{A}$  is HPD,

$$\Phi(\mathbf{x} + \mathbf{y}) > \Phi(\mathbf{x}), \quad \forall \mathbf{y} \in \mathbb{C}_*^n.$$

Thus  $\mathbf{x} \in \mathbb{C}^n$  is a least squares solution. □



## Least Squares in Other Inner Products

Instead of doing our least squares computations using the norm  $\|\cdot\|_{\ell^2(\mathbb{C}^m)}$ , we could, in fact, use any norm that on  $\mathbb{C}^n$  that arises from an inner product. Suppose that  $(\cdot, \cdot)_w : \mathbb{C}^n \times \mathbb{C}^n \rightarrow \mathbb{C}$  is an inner product and  $\|\cdot\|_w$  is the norm induced by this inner product. We could pose the least squares problem with respect to this inner product.

As an example, suppose that  $B \in \mathbb{C}^{n \times n}$  is HPD, and consider the inner product  $(\cdot, \cdot)_B$ , defined by

$$(\mathbf{x}, \mathbf{y})_B = \mathbf{y}^H B \mathbf{x}, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{C}^n.$$

Define

$$\Phi_B(\mathbf{z}) = \|\mathbf{r}(\mathbf{z})\|_B^2, \quad \mathbf{r}(\mathbf{z}) = \mathbf{f} - A\mathbf{z}, \quad \forall \mathbf{z} \in \mathbb{C}^n. \quad (5)$$

What is the analogue of the normal equations for this case?



# Projection Matrices





# Projection Matrices

To study the least squares problem in the case that the coefficient matrix  $A \in \mathbb{C}^{m \times n}$ ,  $m \geq 0$  is rank-deficient, that is,  $\text{rank}(A) = r < n$ , it helps to introduce projection matrices.

## Definition

The square matrix  $P \in \mathbb{C}^{n \times n}$  is called a **projection matrix** iff it is idempotent, that is,

$$P^2 = P.$$



## The Image of a Projection Matrix $P$

### Proposition

Let  $P \in \mathbb{C}^{n \times n}$  be a projection matrix and  $\mathbf{v} \in \text{im}(P)$ . Then

$$P\mathbf{v} = \mathbf{v}.$$

### Proof.

If  $\mathbf{v} \in \text{im}(P)$ , then there is a vector  $\mathbf{w} \in \mathbb{C}^n$  such that  $P\mathbf{w} = \mathbf{v}$ . Then

$$P\mathbf{v} = P(P\mathbf{w}) = P^2\mathbf{w} = P\mathbf{w} = \mathbf{v}.$$





## Theorem (properties of a projection matrix)

*Suppose that  $P \in \mathbb{C}^{n \times n}$  is a projection matrix. Then  $I_n - P$  is also a projection matrix and*

- ❶  $\text{im}(I_n - P) = \ker(P)$ ;
- ❷  $\ker(I_n - P) = \text{im}(P)$ ;
- ❸  $\text{im}(P) \cap \ker(P) = \{\mathbf{0}\}$ ;
- ❹  $\text{im}(I_n - P) \cap \ker(I_n - P) = \{\mathbf{0}\}$ .

## Proof.

We will prove the first property and leave the remaining ones as an exercise. Suppose that  $\mathbf{x} \in \text{im}(I_n - P)$ . Then there is a vector  $\mathbf{y} \in \mathbb{C}^n$  such that  $(I_n - P)\mathbf{y} = \mathbf{x}$ . So,

$$P\mathbf{x} = P(I_n - P)\mathbf{y} = P\mathbf{y} - P^2\mathbf{y} = \mathbf{0}$$

Consequently  $P\mathbf{x} = \mathbf{0}$ , and  $\mathbf{x} \in \ker(P)$ .



## Proof, Cont.

Suppose now that  $\mathbf{x} \in \ker(P)$ . Then  $P\mathbf{x} = \mathbf{0}$ . Therefore,

$$(I_n - P)\mathbf{x} = \mathbf{x},$$

which implies that  $\mathbf{x} \in \text{im}(I_n - P)$ .





# Sums of Subspaces

## Definition

Let  $S_1, S_2 \subseteq \mathbb{C}^n$  be subspaces. Recall, that we write  $S_1, S_2 \leq \mathbb{C}^n$ , for short. Then,

$$S_1 + S_2 = \{\mathbf{w} \in \mathbb{C}^n \mid \mathbf{w} = \mathbf{v}_1 + \mathbf{v}_2, \exists \mathbf{v}_i \in S_i, i = 1, 2\}.$$

## Proposition (property of the sum)

*Let  $S_1, S_2 \leq \mathbb{C}^n$ . Then  $S_1 + S_2 \leq \mathbb{C}^n$ .*

## Proof.

Exercise. □



## Complementary Subspaces

### Definition

Suppose  $S_1, S_2 \leq \mathbb{C}^n$ . If  $S_1 + S_2 = \mathbb{C}^n$  and  $S_1 \cap S_2 = \{\mathbf{0}\}$ , then we call  $S_1$  and  $S_2$  **complementary** subspaces, and we write  $S_1 \oplus S_2 = \mathbb{C}^n$ .

### Theorem (decomposition)

*Suppose that  $P \in \mathbb{C}^{n \times n}$  is a projection matrix. Then  $\text{im}(P) \oplus \text{ker}(P) = \mathbb{C}^n$ , i.e.,  $\text{im}(P)$  and  $\text{ker}(P)$  are complementary.*

### Proof.

This follows from a previous theorem and the trivial decomposition

$$\mathbf{v} = P\mathbf{v} + \mathbf{v} - P\mathbf{v} = \underbrace{P\mathbf{v}}_{\in \text{im}(P)} + \underbrace{(I - P)\mathbf{v}}_{\in \text{ker}(P)}.$$





# Constructing a Projection

## Theorem

*Let  $S_1, S_2 \leq \mathbb{C}^n$  be complementary subspaces. Then, there is a projection matrix  $P \in \mathbb{C}^{n \times n}$  such that*

$$S_1 = \text{im}(P) \quad \text{and} \quad S_2 = \text{ker}(P).$$

## Proof.

Suppose that

$$B_i = \{\mathbf{w}_1^{(i)}, \dots, \mathbf{w}_{k_i}^{(i)}\} \subset S_i,$$

is a basis for  $S_i$ ,  $i = 1, 2$ . Then, it is left to the reader to prove that the set

$$B = B_1 \cup B_2$$

is a basis for  $\mathbb{C}^n = S_1 \oplus S_2$ .



## Proof, Cont.

Now, define a mapping  $P : \mathbb{C}^n \rightarrow \mathbb{C}^n$  such that

$$P(\mathbf{w}_j^{(1)}) = \mathbf{w}_j^{(1)}, \quad j = 1, \dots, k_1,$$

and

$$P(\mathbf{w}_j^{(2)}) = \mathbf{0}, \quad j = 1, \dots, k_2.$$

We require  $P$  to be linear, so that

$$\begin{aligned} P\left(\sum_{j=1}^{k_1} c_j^{(1)} \mathbf{w}_j^{(1)} + \sum_{j=1}^{k_2} c_j^{(2)} \mathbf{w}_j^{(2)}\right) &= \sum_{j=1}^{k_1} c_j^{(1)} P(\mathbf{w}_j^{(1)}) + \sum_{j=1}^{k_2} c_j^{(2)} P(\mathbf{w}_j^{(2)}) \\ &= \sum_{j=1}^{k_1} c_j^{(1)} \mathbf{w}_j^{(1)}. \end{aligned}$$

It is now straightforward to prove that  $P^2 = P$  and  $\text{im}(P) = S_1$  and  $\text{ker}(P) = S_2$ , as required. □





## Orthogonal Subspaces

### Definition

Two subspaces  $S_1, S_2 \leq \mathbb{C}^n$  are called **orthogonal** iff

$$(\mathbf{v}_1, \mathbf{v}_2)_{\ell^2(\mathbb{C}^n)} = (\mathbf{v}_1, \mathbf{v}_2)_2 = \mathbf{v}_2^H \mathbf{v}_1 = 0,$$

for all  $\mathbf{v}_1 \in S_1$  and  $\mathbf{v}_2 \in S_2$ .

### Proposition (orthogonality)

*If  $S_1, S_2 \leq \mathbb{C}^n$  are orthogonal subspaces, then  $S_1 \cap S_2 = \{\mathbf{0}\}$ .*

### Proof.

To get a contradiction, suppose there is a non-zero vector,  $\mathbf{v}$  in the intersection. Thus,

$$\|\mathbf{v}\|_2^2 = \mathbf{v}^H \mathbf{v} > 0.$$

But, since  $\mathbf{v} \in S_1$  and  $\mathbf{v} \in S_2$ , the orthogonality property demands that  $\mathbf{v}^H \mathbf{v} = 0$ , a contradiction. □



# Orthogonal Decomposition

## Proposition

*Suppose that  $L \leq \mathbb{C}^n$  has dimension  $1 \leq k < n$ . Then  $L^\perp$  is a complementary subspace of dimension  $n - k$ :*

$$L \oplus L^\perp = \mathbb{C}^n.$$

*Furthermore, the decomposition of any  $\mathbf{w} \in \mathbb{C}^n$  into*

$$\mathbf{w} = \mathbf{x} + \mathbf{y}, \quad \mathbf{x} \in L, \quad \mathbf{y} \in L^\perp,$$

*is unique.*

## Proof.

$L$  and  $L^\perp$  are orthogonal subspaces, and therefore  $L \cap L^\perp = \{\mathbf{0}\}$ . Let  $B = \{\mathbf{w}_1, \dots, \mathbf{w}_k\}$  be an orthonormal basis for  $L$ . Using basis completion and the Gram-Schmidt process, we can find the orthonormal set  $T = \{\mathbf{w}_{k+1}, \dots, \mathbf{w}_n\}$ , such that  $B \cup T$  is an orthonormal basis for  $\mathbb{C}^n$ . We claim that  $T$  is an orthonormal basis for  $L^\perp$ .



## Proof, Cont.

Now, let  $\mathbf{w} \in \mathbb{C}^n$  be arbitrary. Define

$$\mathbf{x} = \sum_{i=1}^k \alpha_i \mathbf{w}_i \quad \text{and} \quad \mathbf{y} = \sum_{i=k+1}^n \alpha_i \mathbf{w}_i,$$

where

$$\alpha_i = \mathbf{w}_i^H \mathbf{w} = (\mathbf{w}, \mathbf{w}_i)_{\ell^2(\mathbb{C}^n)}, \quad i = 1, \dots, n.$$

It is not too hard to see that  $\mathbf{w} = \mathbf{x} + \mathbf{y}$ . To see that such decompositions are unique. Suppose that

$$\mathbf{w} = \mathbf{x}_1 + \mathbf{y}_1 = \mathbf{x}_2 + \mathbf{y}_2, \quad \mathbf{x}_i \in L, \quad \mathbf{y}_i \in L^\perp, \quad i = 1, 2.$$

Then

$$L \ni \mathbf{x}_1 - \mathbf{x}_2 = \mathbf{y}_2 - \mathbf{y}_1 \in L^\perp.$$

This implies that, since  $L \cap L^\perp = \{\mathbf{0}\}$ ,

$$\mathbf{0} = \mathbf{x}_1 - \mathbf{x}_2 = \mathbf{y}_2 - \mathbf{y}_1 = \mathbf{0}.$$





## Definition (orthogonal projection)

The matrix  $P \in \mathbb{C}^{n \times n}$  is called an **orthogonal projection** iff  $P = P^2$  and  $\text{im}(P)$  and  $\text{ker}(P)$  are orthogonal subspaces.

## Theorem (characterization of orthogonal projection)

*Let  $P \in \mathbb{C}^{n \times n}$  be a projection matrix. Then  $P$  is an orthogonal projection iff  $P = P^H$ .*

## Proof.

Suppose that  $P^H = P$ . Let  $\mathbf{v}_1 \in \text{ker}(P)$  and  $\mathbf{v}_2 \in \text{im}(P)$  be arbitrary. Then

$$P\mathbf{v}_2 = \mathbf{v}_2, \quad (I_n - P)\mathbf{v}_1 = \mathbf{v}_1,$$

and

$$\mathbf{v}_2^H \mathbf{v}_1 = (P\mathbf{v}_2)^H (I_n - P)\mathbf{v}_1 = \mathbf{v}_2^H P^H (I_n - P)\mathbf{v}_1 = \mathbf{v}_2^H (P - P^2)\mathbf{v}_1 = 0.$$

Thus  $\text{im}(P)$  and  $\text{ker}(P)$  are orthogonal subspaces, which implies that  $P$  is an orthogonal projection.



## Proof, Cont.

Suppose now that  $P$  is an orthogonal projection. Set

$$S_1 = \text{im}(P), \quad S_2 = \text{ker}(P),$$

with

$$\dim(S_1) = k < n, \quad \dim(S_2) = n - k.$$

We want to prove that  $P^H = P$ , using the fact that  $S_1$  and  $S_2$  are orthogonal subspaces of  $\mathbb{C}^n$ . Let

$$B_1 = \{\mathbf{q}_1, \dots, \mathbf{q}_k\} \subset S_1, \quad B_2 = \{\mathbf{q}_{k+1}, \dots, \mathbf{q}_n\} \subset S_2,$$

be orthonormal bases for the respective spaces. This is always possible thanks to basis completion and the Gram–Schmidt process. We leave it as an exercise for the reader to prove that  $B = B_1 \cup B_2$  is an orthonormal basis for  $\mathbb{C}^n$ . (Use the fact that  $S_1$  and  $S_2$  are complementary orthogonal subspaces.)



## Proof, Cont.

By our construction,

$$P\mathbf{q}_j = \begin{cases} \mathbf{q}_j & j = 1, \dots, k, \\ \mathbf{0} & j = k + 1, \dots, n. \end{cases}$$

Set

$$Q = \begin{bmatrix} | & & | \\ \mathbf{q}_1 & \cdots & \mathbf{q}_n \\ | & & | \end{bmatrix} \in \mathbb{C}^{n \times n}.$$

Then

$$PQ = \begin{bmatrix} | & & | & | & & | \\ \mathbf{q}_1 & \cdots & \mathbf{q}_k & \mathbf{0} & \cdots & \mathbf{0} \\ | & & | & | & & | \end{bmatrix} \in \mathbb{C}^{n \times n},$$

and

$$Q^H PQ = \begin{bmatrix} I_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{n-k} \end{bmatrix} = \Sigma \in \mathbb{C}^{n \times n}.$$



## Proof, Cont.

Consequently,

$$P = Q\Sigma Q^H,$$

and  $P^H = P$ .



## Theorem (special projectors)

Let  $k \in \{1, \dots, n\}$  and suppose that the collection of vectors  $\{\mathbf{q}_1, \dots, \mathbf{q}_k\} \subset \mathbb{C}^n$  is orthonormal. Define

$$\hat{Q} = \begin{bmatrix} | & & | \\ \mathbf{q}_1 & \cdots & \mathbf{q}_k \\ | & & | \end{bmatrix} \in \mathbb{C}^{n \times k},$$

then the matrices

$$P = \hat{Q}\hat{Q}^H, \quad I_n - P = I_n - \hat{Q}\hat{Q}^H$$

are orthogonal projectors.



## Rank-one Projections

### Definition

Suppose that  $\mathbf{q} \in \mathbb{C}^n$ ,  $\|\mathbf{q}\|_2 = 1$ . The matrix  $P = \mathbf{q}\mathbf{q}^H$  is called a **rank-one orthogonal projection**. The complement,  $I_n - \mathbf{q}\mathbf{q}^H$ , is called a **rank- $(n-1)$  orthogonal projection**.

### Theorem

*The identity matrix  $I_n \in \mathbb{C}^{n \times n}$  is a sum of  $n$  rank-one orthogonal projection matrices.*

### Proof.

Write  $I_n = UU^H$ , where  $U$  is unitary. Then,

$$I_n = UI_nU^H = \sum_{i=1}^n U\mathbf{e}_i\mathbf{e}_i^T U^H = \sum_{i=1}^n \mathbf{u}_i\mathbf{u}_i^H.$$







## The 2-Norm of a Projection Matrix

### Theorem

*Let  $P \in \mathbb{C}^{n \times n}$  be a non-zero projection matrix. Then  $\|P\|_2 \geq 1$ . Moreover,  $\|P\|_2 = 1$  iff  $P$  is an orthogonal projection, that is  $P^H = P$ .*

### Proof.

Suppose that  $P$  is a projection matrix, that is,  $P^2 = P$ . Then, using the sub-multiplicativity of the 2-norm

$$\|P\|_2 = \|P^2\|_2 \leq \|P\|_2 \|P\|_2.$$

Since  $P$  is not the zero matrix,  $\|P\|_2 > 0$ , and  $\|P\|_2 \geq 1$ .

Now, for the second part, we have two directions to prove. Assume first that  $P^2 = P$  and  $P^H = P$ .



## Proof, Cont.

In the proof of a previous theorem, we showed that

$$P = Q\Sigma Q^H,$$

where  $Q = [\mathbf{q}_1, \dots, \mathbf{q}_n] \in \mathbb{C}^{n \times n}$  is unitary and

$$\Sigma = \begin{bmatrix} I_k & O \\ O & O_{n-k} \end{bmatrix},$$

for some  $1 \leq k < n$ . In other words,  $\Sigma = \text{diag}[\sigma_1, \dots, \sigma_k, 0, \dots, 0]$ , where  $\sigma_i = 1$ ,  $1 \leq i \leq k$ . Recall that  $\{\mathbf{q}_1, \dots, \mathbf{q}_k\}$  is a basis for  $\text{im}(P)$  and  $\{\mathbf{q}_{k+1}, \dots, \mathbf{q}_n\}$  is a basis for  $\text{ker}(P)$ . In any case,  $P$  is Hermitian positive semi-definite,  $P = Q\Sigma Q^H$  is a unitary diagonalization of  $P$ , and

$$\|P\|_2 = \sigma_1 = \rho(P) = 1.$$



## Proof, Cont.

The other implication is proved by contrapositive. Let us assume that  $P^2 = P$ , but  $P^H \neq P$ . We want to show that this implies that

$$\|P\|_2 > 1.$$

Since  $P^H \neq P$ ,  $\ker(P) \cap \text{im}(P) = \{\mathbf{0}\}$ , but

$$\ker(P) \not\perp \text{im}(P).$$

So, there is some non-zero vector  $\mathbf{v}_1 \in \text{im}(P)$  and some non-zero vector  $\mathbf{v}_2 \in \ker(P)$  such that

$$(\mathbf{v}_1, \mathbf{v}_2)_2 = \mathbf{v}_2^H \mathbf{v}_1 \neq 0.$$

Set

$$\mathbf{v} = \mathbf{v}_1 + \alpha \mathbf{v}_2, \quad \alpha \in \mathbb{C}.$$

Then  $P\mathbf{v} = \mathbf{v}_1$ . Now, we want to choose  $\alpha \in \mathbb{C}$  so that

$$\|P\mathbf{v}\|_2 > \|\mathbf{v}\|_2 > 0.$$



## Proof, Cont.

Indeed, if such an  $\alpha \in \mathbb{C}$  exists, then

$$\|P\|_2 = \sup_{\mathbf{x} \in \mathbb{C}_*^n} \frac{\|P\mathbf{x}\|_2}{\|\mathbf{x}\|_2} \geq \frac{\|P\mathbf{v}\|_2}{\|\mathbf{v}\|_2} > 1.$$

Since

$$P\mathbf{v} = P(\mathbf{v}_1 + \alpha\mathbf{v}_2) = P\mathbf{v}_1 + \alpha P\mathbf{v}_2 = \mathbf{v}_1,$$

it follows that

$$\|\mathbf{v}_1\|_2^2 = \|P\mathbf{v}\|_2^2$$

and

$$\|\mathbf{v}\|_2^2 = \|\mathbf{v}_1 + \alpha\mathbf{v}_2\|_2^2 = \|P\mathbf{v}\|_2^2 + 2\Re(\alpha\mathbf{v}_1^H\mathbf{v}_2) + |\alpha|^2\|\mathbf{v}_2\|_2^2 = \|P\mathbf{v}\|_2^2 + T,$$

where

$$T = 2\Re(\alpha\mathbf{v}_1^H\mathbf{v}_2) + |\alpha|^2\|\mathbf{v}_2\|_2^2.$$



## Proof, Cont.

Therefore, it suffices to choose  $\alpha \in \mathbb{C}$  so that  $T < 0$  for, in that case,

$$\|\mathbf{v}\|_2^2 < \|\mathbf{P}\mathbf{v}\|_2^2.$$

The key is to choose  $\alpha \in \mathbb{C}$  such that  $\mathbf{v} \perp \mathbf{v}_2$ , that is,  $\mathbf{v}_2^H \mathbf{v} = 0$ . This is equivalent to

$$\begin{aligned}\mathbf{v}_2^H (\mathbf{v}_1 + \alpha \mathbf{v}_2) &= 0 \\ \iff \mathbf{v}_2^H \mathbf{v}_1 &= -\alpha \mathbf{v}_2^H \mathbf{v}_2 \\ \iff \bar{\alpha} \mathbf{v}_2^H \mathbf{v}_1 &= -|\alpha|^2 \|\mathbf{v}_2\|_2^2 \in \mathbb{R} \\ \iff \bar{\alpha} \overline{\mathbf{v}_1^H \mathbf{v}_2} &= -|\alpha|^2 \|\mathbf{v}_2\|_2^2 \in \mathbb{R} \\ \iff \alpha \mathbf{v}_1^H \mathbf{v}_2 &= -|\alpha|^2 \|\mathbf{v}_2\|_2^2 \in \mathbb{R}.\end{aligned}$$

In this case,

$$T = -|\alpha|^2 \|\mathbf{v}_2\|_2^2 \in \mathbb{R}.$$

Thus, the result follows upon choosing  $\alpha = -\frac{\mathbf{v}_2^H \mathbf{v}_1}{\|\mathbf{v}_2\|_2^2}$ .





# Rank-Deficient Case



## Theorem (general least squares)

*Suppose that  $m \geq n$ , and the matrix  $A \in \mathbb{C}^{m \times n}$  is such that  $\text{rank}(A) \leq n$ , i.e.,  $A$  may be rank deficient. Let  $\mathbf{f} \in \mathbb{C}^m$  be given. Then the normal equations,*

$$A^H A \mathbf{x} = A^H \mathbf{f}, \quad (6)$$

*always have at least one solution, and, for any two solutions,  $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{C}^n$  — in the case that there are multiple solutions — we find that*

$$\mathbf{r}(\mathbf{x}_1) = \mathbf{r}(\mathbf{x}_2),$$

*where, for  $\mathbf{w} \in \mathbb{C}^n$ , we defined*

$$\mathbf{r}(\mathbf{w}) = \mathbf{f} - A\mathbf{w}.$$

*In other words, the residual is always unique.*



## Theorem (Cont.)

*Furthermore, the following are equivalent*

- ❶  $\mathbf{x}_o \in \mathbb{C}^n$  is a solution to

$$\mathbf{x} \in \underset{\mathbf{w} \in \mathbb{C}^n}{\operatorname{argmin}} \Phi(\mathbf{w}), \quad \Phi(\mathbf{w}) = \|\mathbf{r}(\mathbf{w})\|_2^2. \quad (7)$$

- ❷  $\mathbf{x}_o \in \mathbb{C}^n$  is a solution to the normal equations (6).

- ❸  $\mathbf{x}_o \in \mathbb{C}^n$  has the property that

$$\mathbf{r}(\mathbf{x}_o) \perp \operatorname{im}(\mathbf{A}).$$





## Proof.

First, let us prove that the normal equations (6) have a solution. Set  $L = \text{im}(A)$ . Then  $L$  and  $L^\perp$  are complementary, orthogonal, subspaces of  $\mathbb{C}^m$ :

$$\mathbb{C}^m = L \oplus L^\perp.$$

Therefore the decomposition

$$\mathbf{f} = \mathbf{s} + \mathbf{r}, \quad \mathbf{s} \in L = \text{im}(A), \quad \mathbf{r} \in L^\perp$$

is unique. Since  $\mathbf{s} \in \text{im}(A)$ , there is at least one vector  $\mathbf{x}_o \in \mathbb{C}^n$  such that

$$A\mathbf{x}_o = \mathbf{s}.$$

Since  $\mathbf{r} \in L^\perp$ ,  $\mathbf{r}^H A\mathbf{x} = 0$ , for all  $\mathbf{x} \in \mathbb{C}^n$ . This implies that

$$A^H \mathbf{r} = \mathbf{0} \in \mathbb{C}^n.$$



## Proof, Cont.

Recall that,

$$\mathbf{f} = A\mathbf{x}_o + \mathbf{r},$$

which implies that

$$\mathbf{r} = \mathbf{f} - A\mathbf{x}_o = \mathbf{r}(\mathbf{x}_o).$$

Hence

$$A^H \mathbf{r}(\mathbf{x}_o) = \mathbf{0} \in \mathbb{C}^n,$$

which is equivalent to the normal equations. Thus, the normal equations have at least one solution.

Suppose that  $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{C}^n$  are solutions to the normal equations (6). Recall that the decomposition

$$\mathbf{f} = \mathbf{s} + \mathbf{r}, \quad \mathbf{s} \in L = \text{im}(A), \quad \mathbf{r} \in L^\perp$$

is unique. But

$$\mathbf{f} = A\mathbf{x}_1 + \mathbf{r}(\mathbf{x}_1) = A\mathbf{x}_2 + \mathbf{r}(\mathbf{x}_2)$$

So  $\mathbf{s} = A\mathbf{x}_1 = A\mathbf{x}_2$  and  $\mathbf{r} = \mathbf{r}(\mathbf{x}_1) = \mathbf{r}(\mathbf{x}_2)$ .



## Proof, Cont.

(2  $\iff$  3): This follows from the calculations we carried out above.

(2  $\implies$  1): This argument is similar to previous ones. Suppose that  $\mathbf{x}_o \in \mathbb{C}^n$  is a solution to the normal equation (6). Let  $\mathbf{w} \in \mathbb{C}^n$  be arbitrary. Then

$$\begin{aligned}\Phi(\mathbf{x}_o + \mathbf{w}) &= (\mathbf{r}(\mathbf{x}_o) - A\mathbf{w})^H (\mathbf{r}(\mathbf{x}_o) - A\mathbf{w}) \\ &= \Phi(\mathbf{x}_o) - (\mathbf{r}(\mathbf{x}_o))^H A\mathbf{w} - \mathbf{w}^H A^H \mathbf{r}(\mathbf{x}_o) + \mathbf{w}^H A^H A\mathbf{w} \\ &= \Phi(\mathbf{x}_o) + \mathbf{w}^H A^H A\mathbf{w} \\ &\geq \Phi(\mathbf{x}_o),\end{aligned}$$

since  $A^H A$  is Hermitian positive semi-definite. Note that we cannot claim that  $\Phi(\mathbf{x}_o + \mathbf{w}) > \Phi(\mathbf{x}_o)$ , for all  $\mathbf{w} \in \mathbb{C}_*^n$ , since we do not know that  $A^H A$  is HPD. However, we can still assert that  $\mathbf{x}_o$  is a minimizer, though it might not be unique.



## Proof, Cont.

(1  $\implies$  3): Suppose that  $\mathbf{x}_o \in \mathbb{C}^n$  is a solution to (7). We want to show that  $\mathbf{r}(\mathbf{x}_o) \perp \text{im}(A)$ . To get a contradiction, suppose that  $\mathbf{r}(\mathbf{x}_o) \not\perp \text{im}(A)$ . If this is the case, there is some  $\mathbf{q} \in \text{im}(A)$ ,  $\mathbf{q} \neq \mathbf{0}$ , such that  $\mathbf{q}^H \mathbf{r}(\mathbf{x}_o) \neq 0$ . Since  $\mathbf{q} \in \text{im}(A)$ , there is a vector  $\mathbf{w} \in \mathbb{C}^n$  such that  $A\mathbf{w} = \mathbf{q}$ . Since  $\mathbf{x}_o$  is a minimizer of  $\Phi$ , for any  $\alpha \in \mathbb{C}$

$$\begin{aligned}\|\mathbf{r}(\mathbf{x}_o)\|_2^2 &= \Phi(\mathbf{x}_o) \\ &\leq \Phi(\mathbf{x}_o + \alpha \mathbf{w}) \\ &= \Phi(\mathbf{x}_o) - \alpha(\mathbf{r}(\mathbf{x}_o))^H A\mathbf{w} - \bar{\alpha} \mathbf{w}^H A^H \mathbf{r}(\mathbf{x}_o) + |\alpha|^2 \mathbf{w}^H A^H A \mathbf{w} \\ &= \|\mathbf{r}(\mathbf{x}_o)\|_2^2 - 2\Re\left(\bar{\alpha} \mathbf{q}^H \mathbf{r}(\mathbf{x}_o)\right) + |\alpha|^2 \mathbf{q}^H \mathbf{q}.\end{aligned}$$

Thus, for all  $\alpha \in \mathbb{C}$ ,

$$2\Re\left(\bar{\alpha} \mathbf{q}^H \mathbf{r}(\mathbf{x}_o)\right) \leq |\alpha|^2 \mathbf{q}^H \mathbf{q}.$$

Now, set

$$\alpha = \frac{\mathbf{q}^H \mathbf{r}(\mathbf{x}_o)}{\mathbf{q}^H \mathbf{q}}$$

to get a contradiction. □