

# Lecture 3: Projector, Classical/Modified Gram–Schmidt orthogonalization, QR factorization



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## 1. Projector

- A square matrix  $\mathbf{P} \in \mathbb{C}^{m \times m}$  is called a *projector* if  $\mathbf{P}^2 = \mathbf{P}$ . Any projector is diagonalizable. (Eigenvalues?) **Example:**  $\mathbf{P} = \begin{bmatrix} 0 & 0 \\ \alpha & 1 \end{bmatrix}$

### Theorem 1

Let  $\mathbf{P}$  be a projector. Then,

- (1) for all  $\mathbf{v} \in \text{range}(\mathbf{P})$ , we have  $\mathbf{P}\mathbf{v} = \mathbf{v}$ ;
- (2)  $\text{range}(\mathbf{P})$  and  $\text{null}(\mathbf{P})$  satisfy

$$\text{range}(\mathbf{P}) \cap \text{null}(\mathbf{P}) = \{\mathbf{0}\}, \quad \text{range}(\mathbf{P}) + \text{null}(\mathbf{P}) = \mathbb{C}^m;$$

- (3)  $\mathbf{I} - \mathbf{P}$  is a projector, and

$$\text{range}(\mathbf{I} - \mathbf{P}) = \text{null}(\mathbf{P}), \quad \text{null}(\mathbf{I} - \mathbf{P}) = \text{range}(\mathbf{P}).$$

- (4) if  $\mathbf{P} \neq \mathbf{0}, \mathbf{I}$ , we have  $\|\mathbf{I} - \mathbf{P}\|_2 = \|\mathbf{P}\|_2$ . (See [Ref. 1](#) and [Ref. 2](#))

- Two subspaces  $\mathcal{S}_1, \mathcal{S}_2 \subseteq \mathbb{C}^m$  are called *complementary subspaces* if they satisfy

$$\mathcal{S}_1 \cap \mathcal{S}_2 = \{\mathbf{0}\}, \quad \mathcal{S}_1 + \mathcal{S}_2 = \mathbb{C}^m.$$

## Theorem 2

Let  $\mathcal{S}_1$  and  $\mathcal{S}_2$  be complementary subspaces. Then there exists a unique projector  $\mathbf{P}$  with  $\text{range}(\mathbf{P}) = \mathcal{S}_1$  and  $\text{null}(\mathbf{P}) = \mathcal{S}_2$ .

## Proof.

The existence is left as an exercise. Now we prove the uniqueness. Let  $\mathbf{e}_j$  denote the  $j$ th column of the identity matrix  $\mathbf{I}$ . Since  $\mathcal{S}_1$  and  $\mathcal{S}_2$  are complementary, we can assume  $\mathbf{e}_j = \mathbf{s}_j^1 + \mathbf{s}_j^2$ , where  $\mathbf{s}_j^1 \in \mathcal{S}_1$ , and  $\mathbf{s}_j^2 \in \mathcal{S}_2$ . Assume both  $\mathbf{P}_1$  and  $\mathbf{P}_2$  are desired projectors. Then we have

$$\begin{aligned} \forall 1 \leq j \leq m, \quad (\mathbf{P}_1 - \mathbf{P}_2)\mathbf{e}_j &= (\mathbf{P}_1 - \mathbf{P}_2)\mathbf{s}_j^1 + (\mathbf{P}_1 - \mathbf{P}_2)\mathbf{s}_j^2 \\ &= \mathbf{P}_1\mathbf{s}_j^1 - \mathbf{P}_2\mathbf{s}_j^1 = \mathbf{s}_j^1 - \mathbf{s}_j^1 = \mathbf{0}. \end{aligned}$$

Therefore,  $\mathbf{P}_1 = \mathbf{P}_2$ , i.e., uniqueness. □

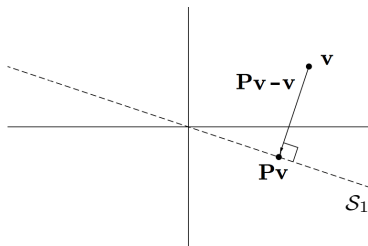
- Let  $\mathcal{S}_1$  and  $\mathcal{S}_2$  be complementary subspaces. The unique projector  $\mathbf{P}$  with  $\text{range}(\mathbf{P}) = \mathcal{S}_1$  and  $\text{null}(\mathbf{P}) = \mathcal{S}_2$  is called the *projector onto  $\mathcal{S}_1$  along  $\mathcal{S}_2$* .

### 1.1. Orthogonal and oblique projectors

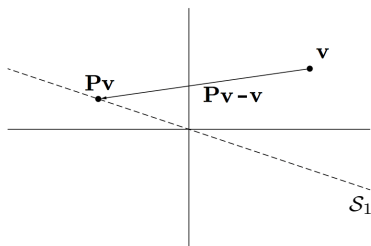
- For a projector  $\mathbf{P}$ , if  $\text{range}(\mathbf{P})$  and  $\text{null}(\mathbf{P})$  are orthogonal, then it is called an *orthogonal* projector. Otherwise, *oblique*.

**Warning:** orthogonal projector “ $\neq$ ” orthogonal matrix!!!

- Geometric interpretation: consider projector  $\mathbf{P}$  s.t.  $\text{range}(\mathbf{P}) = \mathcal{S}_1$



The orthogonal projection



An oblique projection

### Theorem 3

A projector  $\mathbf{P}$  is an orthogonal projector if and only if  $\mathbf{P} = \mathbf{P}^*$ .

- $\mathbf{P} = \begin{bmatrix} 0 & 0 \\ \alpha & 1 \end{bmatrix}$ : oblique (if  $\alpha \neq 0$ ) or orthogonal (if  $\alpha = 0$ ) projector.

### Theorem 4

Let the columns of  $\mathbf{Q}_r$  be an orthonormal basis of an  $r$ -dimensional subspace  $\mathcal{S}$ . Then the orthogonal projector onto  $\mathcal{S}$  is given by  $\mathbf{Q}_r \mathbf{Q}_r^*$ , and the orthogonal projector onto  $\mathcal{S}^\perp$  is given by  $\mathbf{I} - \mathbf{Q}_r \mathbf{Q}_r^*$ .

- $\mathbf{a} \neq \mathbf{0}$ ,  $\mathbf{P}_{\mathbf{a}} = \frac{\mathbf{a}\mathbf{a}^*}{\mathbf{a}^*\mathbf{a}}$ ,  $\mathbf{P}_{\mathbf{a}^\perp} = \mathbf{I} - \frac{\mathbf{a}\mathbf{a}^*}{\mathbf{a}^*\mathbf{a}}$
- Let  $\mathbf{A} \in \mathbb{C}^{m \times n}$ . The orthogonal projector onto  $\text{range}(\mathbf{A})$  is given by  $\mathbf{U}_r \mathbf{U}_r^*$ , where  $\mathbf{U}_r$  is the matrix in SVD of  $\mathbf{A}$ .
- Others:  $\mathbf{A}\mathbf{A}^\dagger$  onto  $\text{range}(\mathbf{A})$ ,  $\mathbf{A}^\dagger \mathbf{A}$  onto  $\text{range}(\mathbf{A}^*)$

## 1.2. General definitions

- Suppose  $\langle \cdot, \cdot \rangle$  denotes an inner product on  $\mathbb{C}^m$ . A linear mapping  $\mathbf{T} : \mathbb{C}^m \mapsto \mathbb{C}^m$  is called
  - a *projector* if it is idempotent, i.e., if  $\mathbf{T}^2 = \mathbf{T}$ ;
  - an *orthogonal projector* (with respect to  $\langle \cdot, \cdot \rangle$ ) if for all  $\mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ ,

$$\langle \mathbf{x} - \mathbf{T}\mathbf{x}, \mathbf{T}\mathbf{y} \rangle = 0;$$

- *self-adjoint* (with respect to  $\langle \cdot, \cdot \rangle$ ) if for all  $\mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ ,

$$\langle \mathbf{T}\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{T}\mathbf{y} \rangle.$$

- It is easy to see that a projector is orthogonal (with respect to  $\langle \cdot, \cdot \rangle$ ) if and only if it is self-adjoint (with respect to  $\langle \cdot, \cdot \rangle$ ).
- If  $\mathbf{T}$  is self-adjoint (with respect to  $\langle \cdot, \cdot \rangle$ ) so is  $\mathbf{I} - \mathbf{T}$  and vice versa.
- **Exercise:** Prove if  $\forall \mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ ,  $\langle \mathbf{x} - \mathbf{T}\mathbf{x}, \mathbf{T}\mathbf{y} \rangle = 0$ , then  $\mathbf{T}^2 = \mathbf{T}$ .

## 2. Gram–Schmidt orthogonalization (GS)

- For  $n$  linearly independent vectors  $\{\mathbf{a}_i\}_{i=1}^n$ : at the  $j$ th step, Gram–Schmidt orthogonalization finds a unit vector  $\mathbf{q}_j$  that is orthogonal to  $\mathbf{q}_1, \dots, \mathbf{q}_{j-1}$ , lies in  $\text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_j\}$  as follows:

$$\tilde{\mathbf{q}}_j = \mathbf{a}_j - \sum_{i=1}^{j-1} \mathbf{q}_i^* \mathbf{a}_j \mathbf{q}_i, \quad \mathbf{q}_j = \frac{\tilde{\mathbf{q}}_j}{\|\tilde{\mathbf{q}}_j\|_2}.$$

More generally, for a given inner product  $\langle \cdot, \cdot \rangle$ ,

$$\tilde{\mathbf{q}}_j = \mathbf{a}_j - \sum_{i=1}^{j-1} \langle \mathbf{a}_j, \mathbf{q}_i \rangle \mathbf{q}_i, \quad \mathbf{q}_j = \frac{\tilde{\mathbf{q}}_j}{\sqrt{\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{q}}_j \rangle}}.$$

- Gram–Schmidt orthogonalization can also be represented via orthogonal projectors. For the standard inner product, we have

$$\tilde{\mathbf{q}}_j = \mathbf{P}_j \mathbf{a}_j, \quad \mathbf{q}_j = \tilde{\mathbf{q}}_j / \|\tilde{\mathbf{q}}_j\|_2,$$

where  $\mathbf{P}_j = \mathbf{I} - \mathbf{Q}_{j-1} \mathbf{Q}_{j-1}^*$  and  $\mathbf{Q}_{j-1} = [\mathbf{q}_1 \quad \mathbf{q}_2 \quad \dots \quad \mathbf{q}_{j-1}]$ .

## 2.1. Classical Gram–Schmidt orthogonalization (ClGS)

- ClGS is based on the use of

$$\tilde{\mathbf{q}}_j = \mathbf{a}_j - \mathbf{q}_1^* \mathbf{a}_j \mathbf{q}_1 - \mathbf{q}_2^* \mathbf{a}_j \mathbf{q}_2 \cdots - \mathbf{q}_{j-1}^* \mathbf{a}_j \mathbf{q}_{j-1}$$

and calculates  $\mathbf{q}_j$  by evaluating the following formulas in order:

$$\begin{aligned}\mathbf{q}_j^{(0)} &= \mathbf{a}_j, \\ \mathbf{q}_j^{(1)} &= \mathbf{q}_j^{(0)} - \mathbf{q}_1^* \mathbf{a}_j \mathbf{q}_1, \\ \mathbf{q}_j^{(2)} &= \mathbf{q}_j^{(1)} - \mathbf{q}_2^* \mathbf{a}_j \mathbf{q}_2, \\ &\vdots \\ \mathbf{q}_j^{(j-1)} &= \mathbf{q}_j^{(j-2)} - \mathbf{q}_{j-1}^* \mathbf{a}_j \mathbf{q}_{j-1}, \\ \mathbf{q}_j &= \mathbf{q}_j^{(j-1)} / \|\mathbf{q}_j^{(j-1)}\|_2.\end{aligned}$$



## 2.2. Modified Gram–Schmidt orthogonalization (MGS)

- MGS is based on the use of

$$\tilde{\mathbf{q}}_j = \mathbf{P}_j \mathbf{a}_j = (\mathbf{I} - \mathbf{q}_{j-1} \mathbf{q}_{j-1}^*) \cdots (\mathbf{I} - \mathbf{q}_2 \mathbf{q}_2^*) (\mathbf{I} - \mathbf{q}_1 \mathbf{q}_1^*) \mathbf{a}_j$$

and calculates  $\mathbf{q}_j$  by evaluating the following formulas in order:

$$\begin{aligned} \mathbf{q}_j^{(0)} &= \mathbf{a}_j, \\ \mathbf{q}_j^{(1)} &= \mathbf{q}_j^{(0)} - \mathbf{q}_1^* \mathbf{q}_j^{(0)} \mathbf{q}_1, \\ \mathbf{q}_j^{(2)} &= \mathbf{q}_j^{(1)} - \mathbf{q}_2^* \mathbf{q}_j^{(1)} \mathbf{q}_2, \\ &\vdots \\ \mathbf{q}_j^{(j-1)} &= \mathbf{q}_j^{(j-2)} - \mathbf{q}_{j-1}^* \mathbf{q}_j^{(j-2)} \mathbf{q}_{j-1}, \\ \mathbf{q}_j &= \mathbf{q}_j^{(j-1)} / \|\mathbf{q}_j^{(j-1)}\|_2. \end{aligned}$$

## 2.3. ClGS and MGS algorithms

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**Algorithm:** GS for  $n$  linearly independent vectors  $\{\mathbf{a}_i\}_{i=1}^n$ .

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```
for  $j = 1$  to  $n$ 
     $\mathbf{q}_j = \mathbf{a}_j$ 
    for  $i = 1$  to  $j - 1$ 
         $\begin{cases} r_{ij} = \mathbf{q}_i^* \mathbf{a}_j & \text{ClGS} \\ r_{ij} = \mathbf{q}_i^* \mathbf{q}_j & \text{MGS} \end{cases}$ 
         $\mathbf{q}_j = \mathbf{q}_j - r_{ij} \mathbf{q}_i$ 
    end
     $r_{jj} = \|\mathbf{q}_j\|_2$ 
     $\mathbf{q}_j = \mathbf{q}_j / r_{jj}$ 
end
```

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- The computational cost:  $\sim 2mn^2$  (leading term) for  $\mathbf{a}_i \in \mathbb{C}^m$
- ClGS and MGS are mathematically equivalent. In finite precision arithmetic, MGS introduces smaller errors than ClGS.

### 3. QR factorization

- **Definition:** Let  $m$  and  $n$  be arbitrary positive integers ( $m \geq n$  or  $m < n$ ). Given  $\mathbf{A} \in \mathbb{C}^{m \times n}$ , not necessarily of full rank, a *full QR factorization* of  $\mathbf{A}$  is a factorization

$$\mathbf{A} = \mathbf{Q}\mathbf{R}$$

where  $\mathbf{Q} \in \mathbb{C}^{m \times m}$  is unitary, and  $\mathbf{R} \in \mathbb{C}^{m \times n}$  is upper triangular. For  $m \geq n$ , a *reduced QR factorization* of  $\mathbf{A}$  is a factorization

$$\mathbf{A} = \mathbf{Q}_n \mathbf{R}_n$$

where  $\mathbf{Q}_n \in \mathbb{C}^{m \times n}$  has orthonormal columns, and

$$\mathbf{R}_n = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \ddots & \vdots \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix} \cdot \begin{array}{c} \text{[Gray Box]} \\ \mathbf{A} \end{array} = \begin{array}{c} \text{[Gray Box]} \\ \mathbf{Q} \end{array} \cdot \begin{array}{c} \text{[Upper Triangular Box]} \\ \mathbf{R} \end{array}$$

## Theorem 5 (Existence of QR)

*Every matrix  $\mathbf{A} \in \mathbb{C}^{m \times n} (m \geq n)$  has a reduced QR factorization and a full QR factorization.*

*Proof.*

- Existence of reduced QR factorization.

For the full column rank case, Gram–Schmidt orthogonalization produces a sequence of reduced QR factorizations for  $\mathbf{A} \in \mathbb{C}^{m \times n}$ :

$$\mathbf{A}_j := [\mathbf{a}_1 \quad \mathbf{a}_2 \quad \dots \quad \mathbf{a}_j] = \mathbf{Q}_j \mathbf{R}_j, \quad j = 1:n.$$

For the rank-deficient case,  $\tilde{\mathbf{q}}_j = \mathbf{0}$  at one or more steps  $j$ , GS fails to produce  $\mathbf{q}_j$ . At this moment, we pick  $\mathbf{q}_j$  arbitrarily to be any unit vector orthogonal to  $\text{span}\{\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_{j-1}\}$ , set  $r_{jj} = 0$ , and then continue the Gram–Schmidt orthogonalization until we obtain a reduced QR factorization.

- Existence of full QR factorization.

Let  $\mathbf{A} = \mathbf{Q}_n \mathbf{R}_n$  be a reduced QR factorization of  $\mathbf{A}$ . A full QR factorization can be constructed via

$$\mathbf{A} = \mathbf{QR} := [\mathbf{Q}_n \quad \mathbf{Q}_c] \begin{bmatrix} \mathbf{R}_n \\ \mathbf{0} \end{bmatrix},$$

where  $\mathbf{Q}_c \in \mathbb{C}^{m \times (m-n)}$  has orthonormal columns orthogonal to  $\text{span}\{\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n\}$ . □

### Theorem 6

*Every matrix  $\mathbf{A} \in \mathbb{C}^{m \times n}$  ( $m \geq n$ ) of full column rank has a unique reduced QR factorization  $\mathbf{A} = \mathbf{Q}_n \mathbf{R}_n$  with  $r_{jj} > 0$ .*

### Proof.

$r_{11}\mathbf{q}_1 = \mathbf{a}_1$  and  $r_{11} > 0 \Rightarrow r_{11}$  and  $\mathbf{q}_1$  unique  $\Rightarrow r_{12}$  and  $r_{22}\mathbf{q}_2$  unique, by  $r_{22} > 0 \Rightarrow r_{22}$  and  $\mathbf{q}_2$  unique, and so on. □

### 3.1. When vectors become continuous functions

- Replace  $\mathbb{C}^m$  by  $C[-1, 1]$ , a linear space of real-valued continuous functions on  $[-1, 1]$  with the  $L^2$  inner product

$$\forall f(x), g(x) \in C[-1, 1], \quad \langle f(x), g(x) \rangle_{L^2} = \int_{-1}^1 f(x)g(x)dx,$$

and the norm

$$\|f(x)\|_{L^2} = \sqrt{\langle f(x), f(x) \rangle_{L^2}}.$$

Gram–Schmidt orthogonalization (GS) with respect to the  $L^2$  inner product  $\langle f(x), g(x) \rangle_{L^2}$  is: At step  $j$ ,

$$\begin{aligned}\tilde{q}_j(x) &= a_j(x) - \sum_{i=1}^{j-1} \langle a_j(x), q_i(x) \rangle_{L^2} q_i(x), \\ q_j(x) &= \tilde{q}_j(x) / \|\tilde{q}_j(x)\|_{L^2}.\end{aligned}$$

The functions  $q_j(x)$  satisfy

$$\langle q_i(x), q_j(x) \rangle_{L^2} = \int_{-1}^1 q_i(x) q_j(x) dx = \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

Then we have “continuous QR factorization”

$$A = QR = \left[ \begin{array}{c|c|c|c} & & & \\ \hline & & & \\ \hline q_1(x) & q_2(x) & \cdots & q_n(x) \\ \hline & & & \end{array} \right] \left[ \begin{array}{cccc} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \\ & & \ddots & \vdots \\ & & & r_{nn} \end{array} \right]$$

where

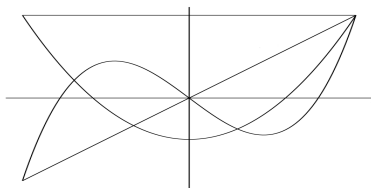
$$A = [a_1(x) \quad a_2(x) \quad \cdots \quad a_n(x)]$$

and

$$r_{jj} = \|\tilde{q}_j(x)\|_{L^2}, \quad r_{ij} = \langle a_j(x), q_i(x) \rangle_{L^2}.$$

- **Example:**  $a_j(x) = x^{j-1}$ ,  $j = 1, 2, \dots, n$

$$\mathbf{A} = \begin{bmatrix} 1 & x & x^2 & \dots & x^{n-1} \end{bmatrix}$$



*Legendre polynomials*  $P_j(x) = q_j(x)/q_j(1)$ :

$$P_1(x) = x, \quad P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}, \quad P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x.$$

**Experiment:** Discrete Legendre polynomials

```
x = (-128:128)'/128;
A = [x.^0 x.^1 x.^2 x.^3]
[Q,R] = qr(A,0);
scale = Q(257,:);
Q = Q*diag(1./scale);
plot(x,Q)
```

