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 $\mathbf{v} \in \mathrm{range}(\mathbf{P})$, we have $\mathbf{P}\mathbf{v} = \mathbf{v}$;*

(2) $\mathrm{range}(\mathbf{P})$ *and* $\mathrm{null}(\mathbf{P})$ *satisfy*

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

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

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

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

Theorem 2

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

Proof.

The existence is left as an exercise. Now we prove the uniqueness. Let $\mathbf{e}_j$ denote the jth 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

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

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

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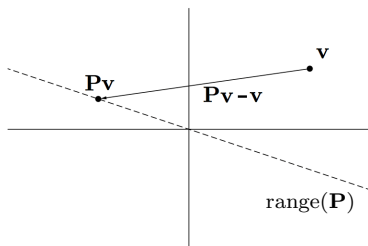
1.1. Orthogonal and oblique projectors

- For a projector **P**, if range(**P**) and null(**P**) are orthogonal, then it is called an *orthogonal* projector. Otherwise, *oblique.*

  Warning: orthogonal projectors are not orthogonal matrices!!!

- Geometric interpretation
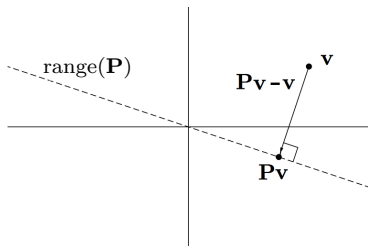
The orthogonal projection   An oblique projection

> **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 $\mathbf{I} - \mathbf{Q}_r\mathbf{Q}_r^*$.*

- $\mathbf{a} \neq \mathbf{0}, \quad \mathbf{P_a} = \dfrac{\mathbf{aa}^*}{\mathbf{a}^*\mathbf{a}}, \quad \mathbf{P_{a^{\perp}}} = \mathbf{I} - \dfrac{\mathbf{aa}^*}{\mathbf{a}^*\mathbf{a}}$
- Let $\mathbf{A} \in \mathbb{C}^{m \times n}$. The orthogonal projector onto 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: $\mathbf{AA}^{\dagger}$ onto range($\mathbf{A}$) , $\mathbf{A}^{\dagger}\mathbf{A}$ onto 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 $\mathbf{x}, \mathbf{y} \in \mathbb{C}^m$,

  $$\langle \mathbf{x} - \mathbf{Tx}, \mathbf{Ty} \rangle = 0;$$

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

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

- 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 $\forall \, \mathbf{x}, \mathbf{y} \in \mathbb{C}^m$, $\langle \mathbf{x} - \mathbf{Tx}, \mathbf{Ty} \rangle = 0$, then $\mathbf{T}^2 = \mathbf{T}$.

2. Gram–Schmidt orthogonalization (GS)

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

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

- Equivalently, Gram–Schmidt orthogonalization can be represented via projectors:

$$\widetilde{\mathbf{q}}_j = \mathbf{P}_j \mathbf{a}_j, \quad \mathbf{q}_j = \frac{\widetilde{\mathbf{q}}_j}{\|\widetilde{\mathbf{q}}_j\|_2}.$$

where $\mathbf{P}_j = \mathbf{I} - \mathbf{Q}_{j-1} \mathbf{Q}_{j-1}^*$ and $\mathbf{Q}_{j-1} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \ldots & \mathbf{q}_{j-1} \end{bmatrix}$.

2.1. Classical Gram–Schmidt orthogonalization (ClGS)

- ClGS is based on the use of

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

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

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

2.2. Modified Gram–Schmidt orthogonalization (MGS)

- MGS is based on the use of

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

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

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

2.3. ClGS and MGS algorithms

> **Algorithm**: GS for n linearly independent vectors $\{\mathbf{a}_i\}_{i=1}^n$.
>
> **for** $j = 1$ **to** n
> $\qquad \mathbf{q}_j = \mathbf{a}_j$
> $\qquad$ **for** $i = 1$ **to** $j - 1$
> $\qquad\qquad \begin{cases} r_{ij} = \mathbf{q}_i^* \mathbf{a}_j & \text{ClGS} \\ r_{ij} = \mathbf{q}_i^* \mathbf{q}_j & \text{MGS} \end{cases}$
> $\qquad\qquad \mathbf{q}_j = \mathbf{q}_j - r_{ij} \mathbf{q}_i$
> $\qquad$ **end**
> $\qquad r_{jj} = \|\mathbf{q}_j\|_2$
> $\qquad \mathbf{q}_j = \mathbf{q}_j / r_{jj}$
> **end**

- The computational cost: $\sim 2mn^2$ (leading term) for $\mathbf{a}_i \in \mathbb{C}^m$

> **Remark 5**
>
> ClGS *and* MGS *are mathematically equivalent. In finite precision arithmetic,* MGS *introduces smaller errors than* ClGS.

- Experiment: ClGS vs. MGS

```
m = 512;
n = 256;
A = rand(m,n);
[QC,RC] = clgs(A);
ClGS_error = norm(QC'*QC-eye(n))
[QM,RM] = mgs(A);
MGS_error = norm(QM'*QM-eye(n))
```

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

$$\mathbf{R}_n = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \ddots & \vdots \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}.$$

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

Theorem 6 (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 $\mathbf{A} \in \mathbb{C}^{m \times n}$:

  $$\mathbf{A}_j := \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \ldots & \mathbf{a}_j \end{bmatrix} = \mathbf{Q}_j \mathbf{R}_j, \quad j = 1\colon n.$$

  For the rank-deficient case, $\widetilde{\mathbf{q}}_j = \mathbf{0}$ 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 $\text{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_{j-1}\}$, 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

  $$\mathbf{A} = \mathbf{Q}\mathbf{R} := \begin{bmatrix} \mathbf{Q}_n & \mathbf{Q}_c \end{bmatrix} \begin{bmatrix} \mathbf{R}_n \\ \mathbf{0} \end{bmatrix},$$

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

Theorem 7

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. $\qquad\square$

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

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

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,

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

The functions $q_j(x)$ satisfy

$$\langle q_i(x), q_j(x)\rangle_{L^2} = \int_{-1}^{1} q_i(x)q_j(x)\mathrm{d}x = \delta_{ij} = \left\{ \begin{array}{ll} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{array} \right.$$

Then we have "continuous QR factorization"

$$\mathsf{A} = \mathsf{QR} = \left[\; q_1(x) \;\middle|\; q_2(x) \;\middle|\; \cdots \;\middle|\; q_n(x) \;\right] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \vdots \\ & & \ddots & \\ & & & r_{nn} \end{bmatrix}$$

where

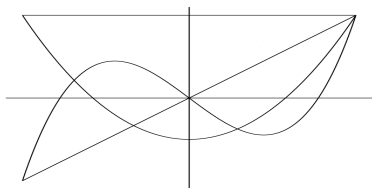$$\mathsf{A} = \begin{bmatrix} a_1(x) & a_2(x) & \cdots & a_n(x) \end{bmatrix}$$

and

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

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

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

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

$$P_1(x) = 1, \ P_2(x) = x, \ P_3(x) = \frac{3}{2}x^2 - \frac{1}{2}, \ P_4(x) = \frac{5}{2}x^3 - \frac{3}{2}x.$$

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)
```