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

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

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

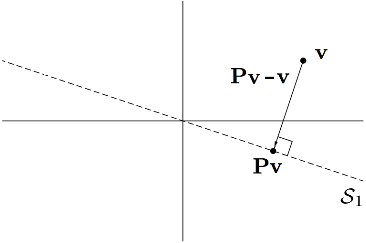
- Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be complementary subspaces. The unique projector $\mathbf{P}$ with $\text{range}(\mathbf{P}) = \mathcal{S}_1$ and $\text{null}(\mathbf{P}) = \mathcal{S}_2$ is called the *projector onto* $\mathcal{S}_1$ *along* $\mathcal{S}_2$.

1.1. Orthogonal and oblique projectors

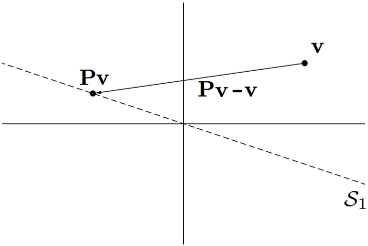
- For a projector $\mathbf{P}$, if $\text{range}(\mathbf{P})$ and $\text{null}(\mathbf{P})$ are orthogonal, then it is called an *orthogonal* projector. Otherwise, *oblique*.

  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 matrix $\mathbf{P}$ is an orthogonal projector if and only if it is idempotent ($\mathbf{P}^2 = \mathbf{P}$) and Hermitian ($\mathbf{P} = \mathbf{P}^*$).

- $\mathbf{P} = \begin{bmatrix} 0 & 0 \\ \alpha & 1 \end{bmatrix}$: 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 $\mathbf{I} - \mathbf{Q}_r\mathbf{Q}_r^*$.

- $\mathbf{a} \neq \mathbf{0}, \quad \mathbf{P}_\mathbf{a} = \dfrac{\mathbf{a}\mathbf{a}^*}{\mathbf{a}^*\mathbf{a}}, \quad \mathbf{P}_{\mathbf{a}^\perp} = \mathbf{I} - \dfrac{\mathbf{a}\mathbf{a}^*}{\mathbf{a}^*\mathbf{a}}$
- 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: $\mathbf{A}\mathbf{A}^\dagger$ onto range($\mathbf{A}$) , $\mathbf{A}^\dagger\mathbf{A}$ onto range($\mathbf{A}^*$)

1.2. General definitions

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

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

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

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

- Exercise: Prove that if $\mathbf{T}$ is self-adjoint, so is $\mathbf{I} - \mathbf{T}$ and vice versa.
- Exercise: Prove that for all $\mathbf{x}, \mathbf{y} \in \mathbb{V}$,

$$\langle \mathbf{x} - \mathbf{T}\mathbf{x}, \mathbf{T}\mathbf{y} \rangle = 0 \Leftrightarrow \mathbf{T}(\mathbf{T}\mathbf{x}) = \mathbf{T}\mathbf{x} \text{ and } \langle \mathbf{T}\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{T}\mathbf{y} \rangle.$$

  This means that

$$\text{orthogonal projector} \Leftrightarrow \text{idempotent} + \text{self-adjoint}.$$

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 span$\{\mathbf{a}_1, \ldots, \mathbf{a}_j\}$ as follows:

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

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

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

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

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

  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:

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

2.3. ClGS and MGS algorithms

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

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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

- 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

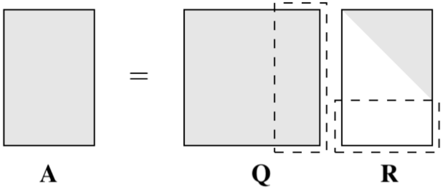
$$\mathbf{A} = \mathbf{Q}\mathbf{R}$$

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

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



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

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

  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 $\mathrm{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_{j-1}\}$, 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 $\operatorname{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n\}$. □

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

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

  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,

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

The functions $q_j(x)$ satisfy

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

Then we have "continuous QR factorization"

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

where

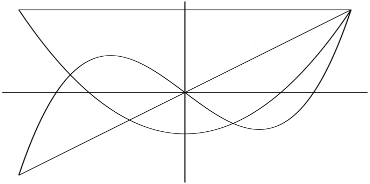
$$\mathrm{A} = \begin{bmatrix} a_1(x) & a_2(x) & \cdots & a_n(x) \end{bmatrix}$$

and

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

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

$$\mathbf{A} = \left[\begin{array}{c|c|c|c|c} 1 & x & x^2 & \cdots & x^{n-1} \end{array} \right]$$



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)
```