

Linear Algebra Refresher

Source: Guillaume Rabusseau Lecture Notes

These are heavily based on lecture notes by Guillaume Rabusseau [2].

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1 Basic Definitions

Definition 1 (Vector Space). A vector space $(V, +, \cdot)$ over a field \mathbb{F} (e.g. \mathbb{R}, \mathbb{C}) is a set V with two operations:

- Addition: if $\mathbf{u}, \mathbf{v} \in V$ then $\mathbf{u} + \mathbf{v} \in V$
- Scalar multiplication: if $\alpha \in \mathbb{F}, \mathbf{v} \in V$, then $\alpha \mathbf{v} \in V$

A vector space V satisfies the following properties: for $\forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in V, \forall \alpha, \beta \in \mathbb{F}$

- Commutativity: $\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$
- Associativity: $(\mathbf{u} + \mathbf{v}) + \mathbf{w} = \mathbf{u} + (\mathbf{v} + \mathbf{w})$
- Additive identity: $\exists \mathbf{0} \in V, \mathbf{u} + \mathbf{0} = \mathbf{u}$
- Additive inverse: $\exists -\mathbf{u} \in V, \mathbf{u} + (-\mathbf{u}) = \mathbf{0}$
- Distributive properties: $\alpha(\mathbf{u} + \mathbf{v}) = \alpha\mathbf{u} + \alpha\mathbf{v}$
- Distributive properties: $(\alpha + \beta)\mathbf{u} = \alpha\mathbf{u} + \beta\mathbf{u}$
- Multiplicative identity: $1\mathbf{v} = \mathbf{v}$ (where 1 is the identity of \mathbb{F})

Definition 2 (Subspace). Given a vector space V , a subset of V , $W \subseteq V$ is a subspace of V iff:

- $\mathbf{0} \in W$
- $\forall \mathbf{u}, \mathbf{v} \in W: \mathbf{u} + \mathbf{v} \in W$
- $\forall \alpha \in \mathbb{F}, \forall \mathbf{v} \in W: \alpha \mathbf{v} \in W$

Definition 3 (Sum, Direct Sum). If W_1, W_2 are two vector spaces, denote sum of W_1, W_2 by $W_1 + W_2$ and it is defined by:

$$W_1 + W_2 = \{\mathbf{w}_1 + \mathbf{w}_2 \mid \mathbf{w}_1 \in W_1, \mathbf{w}_2 \in W_2\}$$

In addition, if $W_1 \subseteq V, W_2 \subseteq V$, then $W_1 + W_2$ is a subspace of V . Moreover, if $V = W_1 + W_2$ and $W_1 \cap W_2 = \{\mathbf{0}\}$, we call the sum of W_1 and W_2 as the direct sum and is denoted by $W_1 \oplus W_2$.

Definition 4 (Linear Combination). A linear combination of $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k \in V$ is defined by:

$$\mathbf{v} = \sum_{i=1}^k \alpha_i \mathbf{v}_i$$

where $\alpha_1, \alpha_2, \dots, \alpha_k \in \mathbb{F}$

In fact, we can stack all the vector in a column-wise fashion, i.e.

$$\mathbf{V} = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_k \\ | & | & \cdots & | \end{bmatrix}$$

Then the linear combination $\mathbf{v} = \sum_{i=1}^k \alpha_i \mathbf{v}_i$ can be written in its matrix form: $\mathbf{v} = \mathbf{V}\mathbf{a}$, where $\mathbf{a}^\top = [\alpha_1, \alpha_2, \dots, \alpha_k]$

Definition 5 (Span). The span of a set of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k \in V$ is defined as:

$$\text{span}(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k) = \left\{ \sum_{i=1}^k \alpha_i \mathbf{v}_i \mid \alpha_1, \alpha_2, \dots, \alpha_k \in \mathbb{F} \right\}$$

Note from the above definition, $\text{span}(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k)$ is in fact a vector space. Moreover, it is a subspace of V , i.e. $\text{span}(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k) \subseteq V$. We can also write Definition 5 in its matrix form. Following the matrix format above, we have:

$$\text{span}(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k) = \{\mathbf{V}\mathbf{a} \mid \mathbf{a} \in \mathbb{F}^k\}$$

Definition 6 (Linearly Independent). *A set of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k \in V$ is linearly independent if and only if (iff):*

$$\sum_{i=1}^k \alpha_i \mathbf{v}_i = \mathbf{0} \Rightarrow \alpha_1 = \alpha_2 = \dots = \alpha_k = 0$$

That is:

$$\mathbf{V}\mathbf{a} = \mathbf{0} \Rightarrow \mathbf{a} = \mathbf{0}$$

in the matrix form, where $\mathbf{0} \in \mathbb{F}^k$ is an all zero vector.

Definition 7 (Basis). *Let $W \subseteq V$ be a subspace of V , $w_1, w_2, \dots, w_k \in W$ form a basis of W iff:*

- $\text{span}(w_1, w_2, \dots, w_k) = W$.
- w_1, w_2, \dots, w_k are linearly independent.

Definition 8 (Dimension). *The dimension of a subspace $W \subseteq V$, denoted by $\dim(W)$, is the number of vectors in any basis of W .*

Take the most common Euclidean 3-D space as an example. Let us denote $\mathbf{e}_1 = [1, 0, 0]^\top$, $\mathbf{e}_2 = [0, 1, 0]^\top$, $\mathbf{e}_3 = [0, 0, 1]^\top$ and denote the Euclidean 3-D space by D_3 . One can easily check that $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are a set of basis for D_3 . In addition, $\text{span}(\mathbf{e}_1, \mathbf{e}_2) = D_2$ is a subspace of D_3 . Note that for any vector space, it is closed under the operation addition and scalar multiplication.

2 Four Subspaces of a Matrix

From this section on, we will focus on the field of real numbers (i.e. \mathbb{R}) instead of any arbitrary field. Since we will be introducing matrix in this section, it is good to clarify some notations beforehand.

As we did in the previous section, we will use bold lower case letters to denote vectors while bold capital letters to denote matrices. For $\mathbf{v} \in \mathbb{R}^n$, $\mathbf{M} \in \mathbb{R}^{m \times n}$, we use \mathbf{v}_i to denote the i th entry of the vector \mathbf{v} and $\mathbf{M}_{i,j}$ to denote the (i, j) th entry of the matrix \mathbf{M} , where $i \in [n]$, $j \in [m]$ and $[n] = \{1, 2, \dots, n\}$. Similar to Python's notation, We denote the i th row of \mathbf{M} by $\mathbf{M}_{i,:} \in \mathbb{R}^{1 \times n}$ and the j th column of \mathbf{M} by $\mathbf{M}_{:,j} \in \mathbb{R}^{m \times 1}$ (by convention, a vector $\mathbf{v} \in \mathbb{R}^m$ will always denote a column vector).

Definition 9 (Matrix Product). For $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times p}$, the matrix product $\mathbf{AB} \in \mathbb{R}^{m \times p}$ is defined by:

$$(\mathbf{AB})_{i,j} = \sum_{k=1}^n \mathbf{A}_{i,k} \mathbf{B}_{k,j} \quad \forall i \in [m], \forall j \in [p]$$

Definition 10 (Transpose). For a matrix $\mathbf{M} \in \mathbb{R}^{m \times n}$, the transpose of the matrix \mathbf{M} , \mathbf{M}^\top is defined by:

$$(\mathbf{M}^\top)_{i,j} = \mathbf{M}_{j,i} \quad \forall i \in [m], \forall j \in [n]$$

Definition 11 (Inner Product). For $\mathbf{a} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^n$, the inner product of \mathbf{a} and \mathbf{b} is defined by:

$$\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a}^\top \mathbf{b} = \sum_{i=1}^n \mathbf{a}_i \mathbf{b}_i$$

Definition 12 (Outer Product). For $\mathbf{a} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^n$, the outer product of \mathbf{a} and \mathbf{b} is defined by:

$$\mathbf{a} \otimes \mathbf{b} = \mathbf{ab}^\top$$

That is, for $i, j \in [n]$:

$$(\mathbf{a} \otimes \mathbf{b})_{i,j} = \mathbf{a}_i \mathbf{b}_j$$

In fact, we can also define the matrix product in terms of inner product and outer product between vectors. We can view each matrix $\mathbf{M} \in \mathbb{R}^{m \times n}$ as either a stack of row vectors or a stack of column vectors, that is:

$$\mathbf{M} = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{M}_{:,1} & \mathbf{M}_{:,2} & \cdots & \mathbf{M}_{:,n} \\ | & | & \cdots & | \end{bmatrix} = \begin{bmatrix} -\mathbf{M}_{1,:} - \\ -\mathbf{M}_{2,:} - \\ \vdots \\ -\mathbf{M}_{m,:} - \end{bmatrix}$$

Then for the matrix product, we can either have the inner product view:

$$(\mathbf{AB})_{i,j} = \left(\begin{bmatrix} -\mathbf{A}_{1,:} - \\ -\mathbf{A}_{2,:} - \\ \vdots \\ -\mathbf{A}_{m,:} - \end{bmatrix} \begin{bmatrix} | & | & \cdots & | \\ \mathbf{B}_{:,1} & \mathbf{B}_{:,2} & \cdots & \mathbf{B}_{:,p} \\ | & | & \cdots & | \end{bmatrix} \right)_{i,j} = \langle \mathbf{A}_{i,:}^\top, \mathbf{B}_{:,j} \rangle$$

or we can have the outer product view:

$$\mathbf{AB} = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{A}_{:,1} & \mathbf{A}_{:,2} & \cdots & \mathbf{A}_{:,n} \\ | & | & \cdots & | \end{bmatrix} \begin{bmatrix} -\mathbf{B}_{1,:} - \\ -\mathbf{B}_{2,:} - \\ \vdots \\ -\mathbf{B}_{n,:} - \end{bmatrix} = \sum_{i=1}^n \mathbf{A}_{:,i} \otimes \mathbf{B}_{i,:}^\top$$

Now we can finally define the four subspaces of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$.

Definition 13 (Range). *The range (image, column space) of \mathbf{A} is the span of its columns, i.e*

$$\mathcal{R}(\mathbf{A}) = \text{span}(\mathbf{A}_{:,1}, \mathbf{A}_{:,2}, \dots, \mathbf{A}_{:,n}) = \{\mathbf{Ax} \mid \mathbf{x} \in \mathbb{R}^n\} \subseteq \mathbb{R}^m$$

Definition 14 (Nullspace). *The nullspace (kernel) of \mathbf{A} is defined by:*

$$\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{Ax} = \mathbf{0}\} \subseteq \mathbb{R}^n$$

Definition 15 (Row Space). *The row space of \mathbf{A} is the span of its rows, i.e.*

$$\mathcal{R}(\mathbf{A}^\top) \subseteq \mathbb{R}^n$$

Definition 16 (Left Nullspace). *The left nullspace of \mathbf{A} is defined by:*

$$\mathcal{N}(\mathbf{A}^\top) \subseteq \mathbb{R}^m$$

Note that all these four subspaces are vector subspaces (they are closed under addition and scalar multiplication).

Theorem 17. *The nullspace of a matrix is orthogonal to its row space: $\mathcal{N}(\mathbf{A}) \perp \mathcal{R}(\mathbf{A}^\top)$. That is, for all $\mathbf{u} \in \mathcal{N}(\mathbf{A})$, $\mathbf{v} \in \mathcal{R}(\mathbf{A}^\top)$ we have $\langle \mathbf{u}, \mathbf{v} \rangle = 0$*

Proof. We want to show for all $\mathbf{u} \in \mathcal{N}(\mathbf{A})$ and all $\mathbf{v} \in \mathcal{R}(\mathbf{A}^\top)$, we have $\langle \mathbf{u}, \mathbf{v} \rangle = 0$. By Definition 15, there exists $\mathbf{x} \in \mathbb{R}^m$ such that $\mathbf{v} = \mathbf{A}^\top \mathbf{x}$. Then we have $\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^\top \mathbf{A}^\top \mathbf{x} = (\mathbf{Au})^\top \mathbf{x}$. Note by Definition 14, we have $\mathbf{Au} = \mathbf{0}$. Thus $\langle \mathbf{u}, \mathbf{v} \rangle = (\mathbf{Au})^\top \mathbf{x} = 0$ and $\mathcal{N}(\mathbf{A}) \perp \mathcal{R}(\mathbf{A}^\top)$. \square

Definition 18 (Rank). *The rank of $\mathbf{A} \in \mathbb{R}^{m \times n}$ is the dimension of the range of \mathbf{A} :*

$$\text{rank}(\mathbf{A}) = \dim(\mathcal{R}(\mathbf{A}))$$

Definition 19 (Factorization). *A factorization $\mathbf{A} = \mathbf{BC}$, where $\mathbf{B} \in \mathbb{R}^{m \times r}$, $\mathbf{C} \in \mathbb{R}^{r \times n}$ and $r = \text{rank}(\mathbf{A})$, is called a rank factorization. A graphical illustration of matrix factorization can be found in Figure 2.*

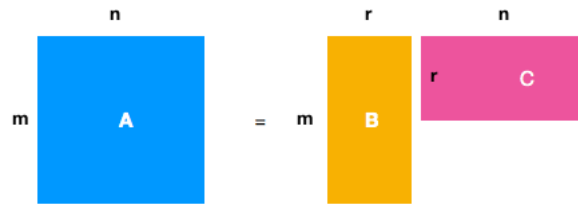


Figure 1: Illustration of matrix factorization

Theorem 20. For a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, all the followings are equivalent:

(1) $\text{rank}(\mathbf{A}) \leq r$

(2) $\dim(\mathcal{R}(\mathbf{A})) \leq r$

(3) $\exists \mathbf{B} \in \mathbb{R}^{m \times r}, \exists \mathbf{C} \in \mathbb{R}^{r \times n}$ such that:

$$\mathbf{A} = \mathbf{BC}$$

(4) $\exists \mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_r \in \mathbb{R}^m, \exists \mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_r \in \mathbb{R}^n$ such that:

$$\mathbf{A} = \sum_{k=1}^r \mathbf{b}_k \mathbf{c}_k^\top$$

(5) $\dim(\mathcal{R}(\mathbf{A}^\top)) \leq r$

Proof. (1) \Leftrightarrow (2), by Definition 18.

(2) \Rightarrow (3): By Definition 8, $\dim(\mathcal{R}(\mathbf{A})) \leq r$ indicates that there exists a basis $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r \in \mathbb{R}^m$ of $\mathcal{R}(\mathbf{A})$. Therefore, for $i \in [n]$, $\mathbf{A}_{:,i}$ can be written as a linear combination of $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r$. More precisely, $\forall i \in [n]$, there exists $\gamma_{i,1}, \gamma_{i,2}, \dots, \gamma_{i,r}$ such that $\mathbf{A}_{:,i} = \sum_{j=1}^r \gamma_{i,j} \mathbf{v}_j$. Define the following matrices:

$$\mathbf{B} = \begin{bmatrix} | & | & | & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_r \\ | & | & | & | \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} \gamma_{1,1} & \gamma_{2,1} & \cdots & \gamma_{n,1} \\ \gamma_{1,2} & \gamma_{2,2} & \cdots & \gamma_{n,2} \\ \cdots & \cdots & \cdots & \cdots \\ \gamma_{1,r} & \gamma_{2,r} & \cdots & \gamma_{n,r} \end{bmatrix}$$

Then we have $\mathbf{A} = \mathbf{BC}$, where $\mathbf{B} \in \mathbb{R}^{m \times r}$ and $\mathbf{C} \in \mathbb{R}^{r \times n}$.

(3) \Leftrightarrow (4): It is easy to check from the inner product, outer product views of the matrix product we mentioned earlier.

(4) \Rightarrow (5): If $\mathbf{A} = \mathbf{BC}$, where $\mathbf{B} \in \mathbb{R}^{m \times r}$ and $\mathbf{C} \in \mathbb{R}^{r \times n}$, then it is easy to check by Definition 15, we have:

$$\text{span}(\mathbf{C}_{1,:}, \mathbf{C}_{2,:}, \dots, \mathbf{C}_{r,:}) = \mathcal{R}(\mathbf{A}^\top)$$

To see this, for $i \in [m]$, we have $\mathbf{A}_{i,:} = \mathbf{B}_{i,:} \mathbf{C} = \sum_{k=1}^r \mathbf{B}_{i,k} \mathbf{C}_{k,:}$. Thus $\mathcal{R}(\mathbf{A}^\top) = \text{span}(\mathbf{C}_{1,:}, \mathbf{C}_{2,:}, \dots, \mathbf{C}_{r,:})$ and $\dim(\mathcal{R}(\mathbf{A}^\top)) \leq r$.

(5) \Rightarrow (1): The implication (5) \Rightarrow (3) \Rightarrow (2) follows from the exact same arguments reasoning by replacing \mathbf{A} with \mathbf{A}^\top . Since we have proved (1) \Leftrightarrow (2), we have (5) \Rightarrow (3) \Rightarrow (2) \Rightarrow (1) holds. \square

Theorem 21 (Rank Nullity). Let $\mathbf{A} \in \mathbb{R}^{m \times n}$, then $n = \text{rank}(\mathbf{A}) + \dim(\mathcal{N}(\mathbf{A}))$.

Proof. Let $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r \in \mathbb{R}^m$ be a basis of $\mathcal{R}(\mathbf{A})$. Then, there exists $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r \in \mathbb{R}^n$ such that $\forall i \in [r], \mathbf{u}_i = \mathbf{A}\mathbf{x}_i$. Let $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k \in \mathbb{R}^n$ be a basis of $\mathcal{N}(\mathbf{A})$. We want to show that $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ is a basis of \mathbb{R}^n .

First we show that $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ spans \mathbb{R}^n . For all $\mathbf{y} \in \mathbb{R}^n$, there exists $\alpha_1, \alpha_2, \dots, \alpha_r$ such that $\mathbf{A}\mathbf{y} = \sum_{i=1}^r \alpha_i \mathbf{u}_i = \sum_{i=1}^r \alpha_i \mathbf{A}\mathbf{x}_i$, hence

$$\mathbf{A}(\mathbf{y} - \sum_{i=1}^r \alpha_i \mathbf{x}_i) = \mathbf{0}$$

Therefore, we have $(\mathbf{y} - \sum_{i=1}^r \alpha_i \mathbf{x}_i) \in \mathcal{N}(\mathbf{A})$ and $(\mathbf{y} - \sum_{i=1}^r \alpha_i \mathbf{x}_i) = \sum_{j=1}^k \beta_j \mathbf{v}_j$ for some scalars β_1, \dots, β_k . It follows that

$$\mathbf{y} = (\mathbf{y} - \sum_{i=1}^r \alpha_i \mathbf{x}_i) + \sum_{i=1}^r \alpha_i \mathbf{x}_i = \sum_{j=1}^k \beta_j \mathbf{v}_j + \sum_{i=1}^r \alpha_i \mathbf{x}_i$$

Therefore, $\mathbb{R}^n = \text{span}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k)$.

It remains to show that $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ are linearly independent. Suppose that $\sum_{j=1}^k \beta_j \mathbf{v}_j + \sum_{i=1}^r \alpha_i \mathbf{x}_i = \mathbf{0}$. This implies that $\mathbf{A}(\sum_{j=1}^k \beta_j \mathbf{v}_j + \sum_{i=1}^r \alpha_i \mathbf{x}_i) = \mathbf{0}$ and thus that $\mathbf{A} \sum_{i=1}^r \alpha_i \mathbf{x}_i = \sum_{i=1}^r \alpha_i \mathbf{u}_i = \mathbf{0}$ since $\sum_{j=1}^k \beta_j \mathbf{v}_j \in \mathcal{N}(\mathbf{A})$. Consequently $\alpha_1 = \alpha_2 = \dots = \alpha_r = 0$ since the \mathbf{u}_i are linearly independent. To conclude, since $\alpha_1 = \alpha_2 = \dots = \alpha_r = 0$, we have $\mathbf{0} = \sum_{j=1}^k \beta_j \mathbf{v}_j + \sum_{i=1}^r \alpha_i \mathbf{x}_i = \sum_{j=1}^k \beta_j \mathbf{v}_j$, hence $\beta_1 = \beta_2 = \dots = \beta_k = 0$ since the \mathbf{v}_j are linearly independent. Hence $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ form a basis of \mathbb{R}^n . Therefore, $n = r + k = \text{rank}(\mathbf{A}) + \dim(\mathcal{N}(\mathbf{A}))$ \square

Definition 22 (Linear Map). A map $f : \mathbb{R}^n \mapsto \mathbb{R}^m$ is linear, if $\forall \alpha, \beta \in \mathbb{R}, \forall \mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, we have:

$$f(\alpha \mathbf{u} + \beta \mathbf{v}) = \alpha f(\mathbf{u}) + \beta f(\mathbf{v})$$

Remark 23 (Matrices and Linear Maps).

- (1) Let $\mathbf{A} \in \mathbb{R}^{m \times n}$, then the map $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ defined by $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$ for all $\mathbf{x} \in \mathbb{R}^n$ is a linear map.
- (2) Let $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a linear map and let $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$ be the canonical basis of \mathbb{R}^n . Construct the matrix $\mathbf{M} \in \mathbb{R}^{m \times n}$ such that:

$$\mathbf{M} = \begin{bmatrix} | & | & & | \\ f(\mathbf{e}_1) & f(\mathbf{e}_2) & \cdots & f(\mathbf{e}_n) \\ | & | & & | \end{bmatrix}$$

then we have $f(\mathbf{x}) = \mathbf{M}\mathbf{x}$ for all $\mathbf{x} \in \mathbb{R}^n$.

Proof. (1) is trivial to show.

(2) For all vectors $\mathbf{x} \in \mathbb{R}^n$, we have $\mathbf{x} = \sum_{i=1}^n x_i \mathbf{e}_i$ (where x_i is the i th component of the vector \mathbf{x}). Then $\mathbf{M}\mathbf{x} = \sum_{i=1}^n x_i f(\mathbf{e}_i) = f(\sum_{i=1}^n x_i \mathbf{e}_i) = f(\mathbf{x})$ where we crucially used the linearity of f for the second equality. \square

Definition 24 (Kernel, Image). Given a linear map $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, the kernel of f is defined by:

$$\text{Ker}(f) = \{\mathbf{x} \in \mathbb{R}^n \mid f(\mathbf{x}) = \mathbf{0}\}$$

The image of f is defined by:

$$\text{Im}(f) = \{f(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\}$$

Remark 25. Given a matrix $\mathbf{M} \in \mathbb{R}^{m \times n}$, if $f(\mathbf{x}) = \mathbf{M}\mathbf{x}$ for $\mathbf{x} \in \mathbb{R}^n$, then $\text{Ker}(f) = \mathcal{N}(\mathbf{M})$ and $\text{Im}(f) = \mathcal{R}(\mathbf{M})$

3 Orthogonality and Projections

Definition 26 (The dot product). *The dot product on \mathbb{R}^n has the following properties:*

- The dot product $\langle \mathbf{a}, \mathbf{b} \rangle := \mathbf{a}^T \mathbf{b}$ is an inner product on \mathbb{R}^n
- The inner product induces a norm on \mathbb{R}^n : $\|\mathbf{v}\| = \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle}$

Definition 27 (Orthogonal vectors). *We say that $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$ are orthogonal if $\langle \mathbf{a}, \mathbf{b} \rangle = 0$.*

Definition 28 (Orthogonal basis). *A basis $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k \in \mathbb{R}^n$ of a sub-space \mathcal{U} is orthonormal iff*

$$\langle \mathbf{u}_i, \mathbf{u}_j \rangle = \begin{cases} 1 & \forall i = j \\ 0 & \forall i \neq j \end{cases} ; \text{ for all } i, j \in \{1, 2, \dots, k\}$$

This means the vectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ are all of norm 1 and pairwise orthogonal.

Definition 29 (Orthogonal matrix). *A matrix $\mathbf{U} \in \mathbb{R}^{n \times k}$ is orthogonal if its columns form an orthonormal basis of $\mathcal{R}(\mathbf{U})$. Equivalently, \mathbf{U} is orthogonal if and only if $\mathbf{U}^T \mathbf{U} = \mathbf{I}$.*

$\mathbf{U} \mathbf{U}^T$ is not necessarily equal to the identity matrix: $\mathbf{U} \mathbf{U}^T \neq \mathbf{I}$. However, if the matrix \mathbf{U} is square i.e. $\mathbf{U} \in \mathbb{R}^{n \times n}$, then $\mathbf{U}^T \mathbf{U} = \mathbf{I}$ implies $\mathbf{U} \mathbf{U}^T = \mathbf{I}$

Definition 30 (Orthogonal complement). *If \mathcal{U} is a subspace of \mathbb{R}^n , the orthogonal complement of \mathcal{U} is defined as*

$$\mathcal{U}^\perp = \{\mathbf{v} \in \mathbb{R}^n \mid \langle \mathbf{u}, \mathbf{v} \rangle = 0 \quad \forall \mathbf{u} \in \mathcal{U}\}$$

\mathcal{U}^\perp is the set of vectors that are orthogonal to every vector in \mathcal{U} . A graphical illustration of the orthogonal complement can be found in figure 2.

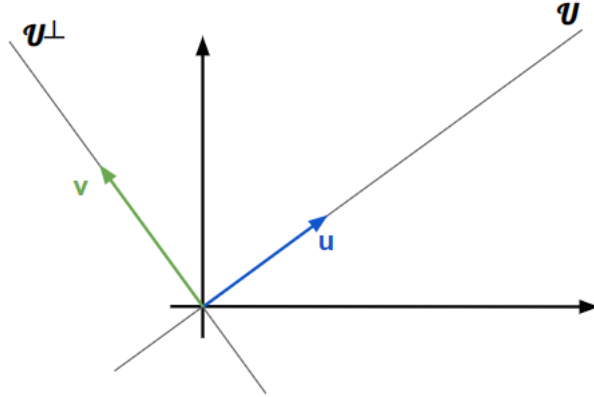


Figure 2: Illustration of the orthogonal complement of \mathcal{U}

Property 31. \mathcal{U}^\perp is a sub-space of \mathbb{R}^n .

Proof. \mathcal{U}^\perp will be a subspace of \mathbb{R}^n if and only if \mathcal{U}^\perp is closed under addition and scalar multiplication, and that it contains the $\mathbf{0}$ vector. Let $\mathbf{v}_1, \mathbf{v}_2 \in \mathcal{U}^\perp$, $\mathbf{u} \in \mathcal{U}$, and c be a constant, then

$$(1) (\mathbf{v}_1 + \mathbf{v}_2) \cdot \mathbf{u} = \mathbf{v}_1 \cdot \mathbf{u} + \mathbf{v}_2 \cdot \mathbf{u} = 0, \text{ hence } \mathbf{v}_1 + \mathbf{v}_2 \in \mathcal{U}^\perp.$$

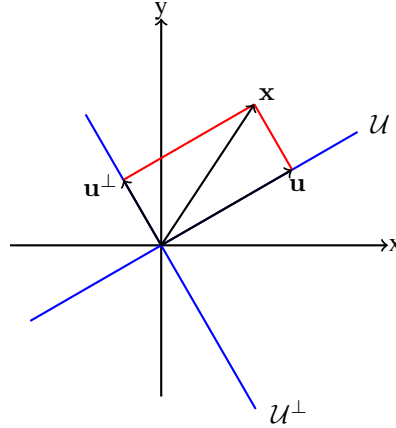
$$(2) (c\mathbf{v}_1) \cdot \mathbf{u} = c(\mathbf{v}_1 \cdot \mathbf{u}) = c(0) = 0, \text{ hence } c\mathbf{v}_1 \in \mathcal{U}^\perp.$$

(3) $\mathbf{0} \cdot \mathbf{u} = 0$, hence $\mathbf{0} \in \mathcal{U}^\perp$.

□

Property 32. $\mathbb{R}^n = \mathcal{U} \oplus \mathcal{U}^\perp$, i.e. every vector in \mathbb{R}^n can be decomposed uniquely into a sum of two vectors, one belonging to \mathcal{U} and the other to \mathcal{U}^\perp .

Figure 3: Splitting a vector into its components on two sub-spaces \mathcal{U} and \mathcal{U}^\perp



Proof. We know that both \mathcal{U} and \mathcal{U}^\perp are sub-spaces of \mathbb{R}^n , and that zero is an element of every sub-space. It is easily seen that zero is the only common element of these two sub-spaces (assuming that there is a non-zero vector \mathbf{w} that belongs to both of the sub-spaces \mathcal{U} and \mathcal{U}^\perp , using the above definition of \mathcal{U}^\perp , we can prove that the inner product of \mathbf{w} with itself must be 0 i.e. $\langle \mathbf{w}, \mathbf{w} \rangle = 0$ which is contradictory to the assumption that $\mathbf{w} \neq 0$).

Any vector $\mathbf{x} \in \mathbb{R}^n$ can be written as $\mathbf{x} = \Pi_{\mathcal{U}}(\mathbf{x}) + \mathbf{v}$. It can be proven (see property 36 below) that the vector $\mathbf{v} = \mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x})$ must be orthogonal to $\Pi_{\mathcal{U}}(\mathbf{x}) \in \mathcal{U}$ and so it must belong to the orthogonal complement of \mathcal{U} .

We conclude that $\mathbb{R}^n = \mathcal{U} \oplus \mathcal{U}^\perp$, i.e. every vector in \mathbb{R}^n can be decomposed uniquely into a sum of two vectors, one belonging to \mathcal{U} and the other to \mathcal{U}^\perp . □

Property 33. Let $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k \in \mathbb{R}^n$ be an orthonormal basis of a sub-space \mathcal{U} , and let

$$\mathbf{U} = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_k \\ | & | & \cdots & | \end{bmatrix} \in \mathbb{R}^{n \times k}$$

Then, for all $\mathbf{x} \in \mathcal{U}$,

$$\mathbf{U}\mathbf{U}^T\mathbf{x} = \mathbf{x}$$

and consequently,

$$\|\mathbf{x}\| = \|\mathbf{U}^T\mathbf{x}\|.$$

Note: Even though $\mathbf{U}\mathbf{U}^T$ is not the identity matrix, it acts as such on the sub-space \mathcal{U} .

Proof. A vector \mathbf{x} in the sub-space \mathcal{U} can, by definition, be written as a linear combination of its basis vectors. $\mathbf{x} \in \mathcal{U} \Rightarrow \exists \mathbf{a} \in \mathbb{R}^k : \mathbf{x} = \mathbf{U}\mathbf{a}$. To prove that $\mathbf{U}\mathbf{U}^T$ acts as an identity matrix, we look at what it does to \mathbf{x} . Using the fact that \mathbf{x} can be written as a linear combination of the basis vectors of the sub-space \mathcal{U} , and that \mathbf{U} is defined as an orthogonal matrix, we have:

$$\mathbf{U}\mathbf{U}^T\mathbf{x} = \mathbf{U}\mathbf{U}^T\mathbf{U}\mathbf{a} = \mathbf{U}\mathbf{a} = \mathbf{x}$$

A consequence of this property is that \mathbf{x} and $\mathbf{U}^T \mathbf{x}$ have the same norm (even though they are not of the same dimension):

$$\|\mathbf{x}\|^2 = \mathbf{x}^T \mathbf{x} = (\mathbf{U} \mathbf{U}^T \mathbf{x})^T \mathbf{x} = \mathbf{x}^T \mathbf{U} \mathbf{U}^T \mathbf{x} = (\mathbf{U}^T \mathbf{x})^T (\mathbf{U}^T \mathbf{x}) = \|\mathbf{U}^T \mathbf{x}\|^2$$

so,

$$\|\mathbf{x}\| = \|\mathbf{U}^T \mathbf{x}\|$$

□

Definition 34 (Linear map). A function $f : V \rightarrow W$ is said to be a linear map if for any two vectors $\mathbf{u}, \mathbf{v} \in V$ and any scalar $c \in \mathbb{F}$ the following two conditions are satisfied:

- Additivity: $f(\mathbf{u} + \mathbf{v}) = f(\mathbf{u}) + f(\mathbf{v})$
- homogeneity (of degree 1): $f(c\mathbf{u}) = cf(\mathbf{u})$

Given a linear map $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$, the kernel of f and the image of f are defined by:

- $\text{Ker}(f)$: $\{\mathbf{x} \in \mathbb{R}^n \mid f(\mathbf{x}) = \mathbf{0}\}$
- $\text{Im}(f)$: $\{f(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\}$

If $f : \mathbf{x} \mapsto \mathbf{M}\mathbf{x}$, then $\mathcal{R}(\mathbf{M}) = \text{Im}(f)$ and $\mathcal{N}(\mathbf{M}) = \text{ker}(f)$

Definition 35 (Orthogonal projection). Let $\mathbf{u}_1, \dots, \mathbf{u}_k \in \mathbb{R}^n$ an orthonormal basis of a subspace \mathcal{U} and $\mathbf{U} \in \mathbb{R}^{n \times k}$ such that

$$\mathbf{U} = \begin{bmatrix} | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_k \\ | & & | \end{bmatrix}$$

The orthogonal projection onto \mathcal{U} is defined as:

$$\begin{aligned} \Pi_u : \mathbb{R}^n &\rightarrow \mathbb{R}^n \\ \mathbf{x} &\mapsto \mathbf{U} \mathbf{U}^T \mathbf{x} \end{aligned}$$

A graphical illustration of the orthogonal projection can be found in figure 4.

Proof. We need to show that Π_u does not depend on the particular choice of an orthonormal basis of \mathcal{U} , that is, we need to show that Π_u is well-defined, i.e, if $\mathbf{V} \in \mathbb{R}^{n \times k}$ is orthogonal and $\mathcal{R}(\mathbf{V}) = \mathcal{R}(\mathbf{U})$ then $\mathbf{U} \mathbf{U}^T = \mathbf{V} \mathbf{V}^T$. Let $\mathbf{v}_1, \dots, \mathbf{v}_k$ be another orthogonal basis of \mathcal{U} and $\mathbf{V} \in \mathbb{R}^{n \times k}$ such that

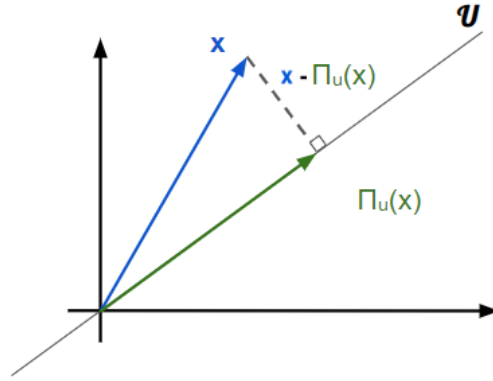
$$\mathbf{V} = \begin{bmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_k \\ | & & | \end{bmatrix}$$

Since $\mathcal{R}(\mathbf{V}) = \mathcal{R}(\mathbf{U})$ then there exists $\mathbf{P} \in \mathbb{R}^{k \times k}$ such that $\mathbf{V} = \mathbf{U} \mathbf{P}$. Since:

- \mathbf{P} is square
- $\mathbf{I} = \mathbf{V}^T \mathbf{V} = \mathbf{P}^T \underbrace{\mathbf{U}^T \mathbf{U}}_{\mathbf{I}} \mathbf{P} = \mathbf{P}^T \mathbf{P}$

we have $\mathbf{P} \mathbf{P}^T = \mathbf{I}$. Thus, $\mathbf{V} \mathbf{V}^T = \mathbf{U} \mathbf{P} \mathbf{P}^T \mathbf{U}^T = \mathbf{U} \mathbf{U}^T$

□

Figure 4: Illustration of the orthogonal projection of \mathbf{x} onto \mathcal{U}

Property 36. Based on the above definitions of orthogonality and orthogonal complement, we can summarize the following properties of orthogonal projection:

- $\Pi_{\mathcal{U}}^2 = \Pi_{\mathcal{U}}$
- $\forall \mathbf{x} : \langle \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x}) \rangle = 0$
- $\text{Im}(\Pi_{\mathcal{U}}) = \mathcal{U}$
- $\text{Ker}(\Pi_{\mathcal{U}}) = \mathcal{U}^\perp$
- $\forall \mathbf{x} : \|\Pi_{\mathcal{U}}(\mathbf{x})\| \leq \|\mathbf{x}\|$

Proof. These properties can be proven as follows :

- $\Pi_{\mathcal{U}}^2 = \Pi_{\mathcal{U}}$.

To prove this we use the definition of projection in terms of matrices and the fact that $\mathbf{U}^T \mathbf{U} = \mathbf{I}$ when \mathbf{U} is an orthogonal matrix. Knowing that $\Pi_{\mathcal{U}}(\mathbf{x}) = \mathbf{U} \mathbf{U}^T \mathbf{x}$, we evaluate the expression $\Pi_{\mathcal{U}}^2(\mathbf{x})$:

$$\Pi_{\mathcal{U}}^2(\mathbf{x}) = \Pi_{\mathcal{U}}(\Pi_{\mathcal{U}}(\mathbf{x})) = \Pi_{\mathcal{U}}(\mathbf{U} \mathbf{U}^T \mathbf{x}) = \mathbf{U} \underbrace{(\mathbf{U}^T \mathbf{U})}_{\mathbf{I}} \mathbf{U}^T \mathbf{x} = \mathbf{U} \mathbf{U}^T \mathbf{x} = \Pi_{\mathcal{U}}(\mathbf{x}).$$

- $\forall \mathbf{x} : \langle \Pi_{\mathcal{U}}(\mathbf{x}), \Pi_{\mathcal{U}}(\mathbf{x}) - \mathbf{x} \rangle = 0.$

To prove this we use the definition of projection in terms of matrices and the fact that $\mathbf{U}^T \mathbf{U} = \mathbf{I}$ when \mathbf{U} is an orthogonal matrix. Knowing that $\Pi_{\mathcal{U}}(\mathbf{x}) = \mathbf{U} \mathbf{U}^T \mathbf{x}$, we evaluate the expression:

$$\begin{aligned} \langle \Pi_{\mathcal{U}}(\mathbf{x}), \Pi_{\mathcal{U}}(\mathbf{x}) - \mathbf{x} \rangle &= \langle \mathbf{U} \mathbf{U}^T \mathbf{x}, \mathbf{U} \mathbf{U}^T \mathbf{x} - \mathbf{x} \rangle \\ &= \mathbf{x}^T \mathbf{U} \underbrace{(\mathbf{U}^T \mathbf{U})}_{\mathbf{I}} \mathbf{U}^T \mathbf{x} - \mathbf{x}^T \mathbf{U} \mathbf{U}^T \mathbf{x} \\ &= \mathbf{x}^T \mathbf{U} \mathbf{U}^T \mathbf{x} - \mathbf{x}^T \mathbf{U} \mathbf{U}^T \mathbf{x} \\ &= 0 \end{aligned}$$

- $\text{Im}(\Pi_{\mathcal{U}}) = \mathcal{U}.$

We first show that $\text{Im}(\Pi_{\mathcal{U}}) \subset \mathcal{U}$. Let $\mathbf{v} \in \text{Im}(\Pi_{\mathcal{U}})$, this means that there exists \mathbf{x} such that $\mathbf{v} = \Pi_{\mathcal{U}}(\mathbf{x}) = \mathbf{U} \mathbf{U}^T \mathbf{x} = \mathbf{U}(\mathbf{U}^T \mathbf{x})$, showing that \mathbf{v} is a linear combination of the columns of \mathbf{U} , hence $\mathbf{v} \in \mathcal{U}$ since $\mathcal{R}(\mathbf{U}) = \mathcal{U}$ by definition.

The inclusion $\text{Im}(\Pi_{\mathcal{U}}) \supset \mathcal{U}$ directly follows for Property 33: for all $\mathbf{x} \in \mathcal{U}$, we have $\mathbf{x} = \mathbf{U} \mathbf{U}^T \mathbf{x} = \Pi_{\mathcal{U}}(\mathbf{x}) \in \text{Im}(\Pi_{\mathcal{U}})$.

- $\text{Ker}(\Pi_{\mathcal{U}}) = \mathcal{U}_{\perp}$.

Let $\mathbf{x} \in \text{Ker}(\Pi_{\mathcal{U}})$, and $\mathbf{u} \in \mathcal{U}$, we first show that their dot product is 0:

$$\begin{aligned}
 \langle \mathbf{x}, \mathbf{u} \rangle &= \mathbf{x}^T \mathbf{u} \\
 &= \mathbf{x}^T (\mathbf{U} \mathbf{U}^T \mathbf{u}) \\
 &= (\mathbf{x}^T \mathbf{U} \mathbf{U}^T) \mathbf{u} \\
 &= (\mathbf{U} \mathbf{U}^T \mathbf{x})^T \mathbf{u} \\
 &= \langle \mathbf{U} \mathbf{U}^T \mathbf{x}, \mathbf{u} \rangle \\
 &= \langle \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{u} \rangle \\
 &= \langle \mathbf{0}, \mathbf{u} \rangle \\
 &= 0.
 \end{aligned}$$

This shows that $\text{Ker}(\Pi_{\mathcal{U}})$ is a subspace of the orthogonal complement of \mathcal{U} .

To show that \mathcal{U}_{\perp} is a subspace of $\text{Ker}(\Pi_{\mathcal{U}})$, we need to show that if $\langle \mathbf{x}, \mathbf{u} \rangle = 0$ for all $\mathbf{u} \in \mathcal{U}$, then $\mathbf{x} \in \text{Ker}(\Pi_{\mathcal{U}})$:

$$\langle \mathbf{x}, \mathbf{u} \rangle = 0 \text{ for all } \mathbf{u} \in \mathcal{U} \Rightarrow \mathbf{U}^T \mathbf{x} = \mathbf{0} \Rightarrow \mathbf{U} \mathbf{U}^T \mathbf{x} = \mathbf{0} \Rightarrow \mathbf{x} \in \text{Ker}(\Pi_{\mathcal{U}})$$

- $\forall \mathbf{x} : \|\Pi_{\mathcal{U}}(\mathbf{x})\| \leq \|\mathbf{x}\|$.

We know that any vector \mathbf{x} can be uniquely decomposed into two components: one is $\Pi_{\mathcal{U}}(\mathbf{x}) \in \mathcal{U}$, and the other is in \mathcal{U}_{\perp} . For simplicity we call the other component \mathbf{v} , which gives us $\mathbf{x} = \Pi_{\mathcal{U}}(\mathbf{x}) + \mathbf{v}$. Developing the expression of the norm of \mathbf{x} we find:

$$\|\mathbf{x}\|^2 = \|\Pi_{\mathcal{U}}(\mathbf{x}) + \mathbf{v}\|^2 = \langle \Pi_{\mathcal{U}}(\mathbf{x}) + \mathbf{v}, \Pi_{\mathcal{U}}(\mathbf{x}) + \mathbf{v} \rangle = \langle \Pi_{\mathcal{U}}(\mathbf{x}), \Pi_{\mathcal{U}}(\mathbf{x}) \rangle + \langle \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{v} \rangle + \langle \mathbf{v}, \Pi_{\mathcal{U}}(\mathbf{x}) \rangle + \langle \mathbf{v}, \mathbf{v} \rangle$$

Since the vector \mathbf{v} is in the orthogonal complement of \mathcal{U} , it must be orthogonal to all the vectors on \mathcal{U} , therefore

$$\langle \mathbf{v}, \Pi_{\mathcal{U}}(\mathbf{x}) \rangle = \langle \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{v} \rangle = 0$$

$$\text{and } \|\mathbf{x}\|^2 = \|\Pi_{\mathcal{U}}(\mathbf{x})\|^2 + \underbrace{\|\mathbf{v}\|^2}_{\geq 0} \Rightarrow \|\Pi_{\mathcal{U}}(\mathbf{x})\|^2 \leq \|\mathbf{x}\|^2 \Rightarrow \|\Pi_{\mathcal{U}}(\mathbf{x})\| \leq \|\mathbf{x}\|$$

□

Property 37. Let \mathcal{U} be a subspace of \mathbb{R}^n . Then, for any $\mathbf{x} \in \mathbb{R}^n$ we have

$$\arg \min_{\mathbf{u} \in \mathcal{U}} \|\mathbf{u} - \mathbf{x}\| = \Pi_{\mathcal{U}}(\mathbf{x}).$$

Which means the orthogonal projection of \mathbf{x} onto \mathcal{U} is the closest point to \mathbf{x} in \mathcal{U} .

Proof. We want to show that for all $\mathbf{x} \in \mathbb{R}^n$, we have $\arg \min_{\mathbf{v} \in \mathcal{U}} \|\mathbf{x} - \mathbf{v}\| = \Pi_{\mathcal{U}}(\mathbf{x})$, where $\mathbf{v} \in \mathcal{U}$.

We first show that the vectors $\mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x})$ and $\mathbf{v} - \Pi_{\mathcal{U}}(\mathbf{x})$ are orthogonal.

$$\begin{aligned}
 \langle \mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{v} - \Pi_{\mathcal{U}}(\mathbf{x}) \rangle &= \langle \mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{v} \rangle - \langle \mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x}), \Pi_{\mathcal{U}}(\mathbf{x}) \rangle \\
 &= \langle \mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{v} \rangle - 0 && \text{Using 2nd element of property 36} \\
 &= \langle \mathbf{x}, \mathbf{v} \rangle - \langle \Pi_{\mathcal{U}}(\mathbf{x}), \mathbf{v} \rangle \\
 &= \mathbf{x}^T \mathbf{v} - (\mathbf{U} \mathbf{U}^T \mathbf{x})^T \mathbf{v} \\
 &= \mathbf{x}^T \mathbf{v} - \mathbf{x}^T \mathbf{U} \mathbf{U}^T \mathbf{v} \\
 &= 0
 \end{aligned}$$

Note that the last equality is due to the fact that vectors in \mathcal{U} are projected onto themselves ($\mathbf{u} = \mathbf{U} \mathbf{U}^T \mathbf{u}$).

Knowing that $\mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x})$ and $\mathbf{v} - \Pi_{\mathcal{U}}(\mathbf{x})$ are orthogonal, we can then use the Pythagorean theorem to express $\|\mathbf{x} - \mathbf{v}\|^2$ as $\|\mathbf{x} - \mathbf{v}\|^2 = \|\mathbf{x} - \Pi_{\mathcal{U}}(\mathbf{x})\|^2 + \|\mathbf{v} - \Pi_{\mathcal{U}}(\mathbf{x})\|^2$. Therefore, the minimum distance between \mathbf{x} and \mathbf{v} is when \mathbf{v} is the orthogonal projection of \mathbf{x} onto \mathcal{U} which gives us $\|\mathbf{v} - \Pi_{\mathcal{U}}(\mathbf{x})\|^2 = 0$ as shown in figure 5. □

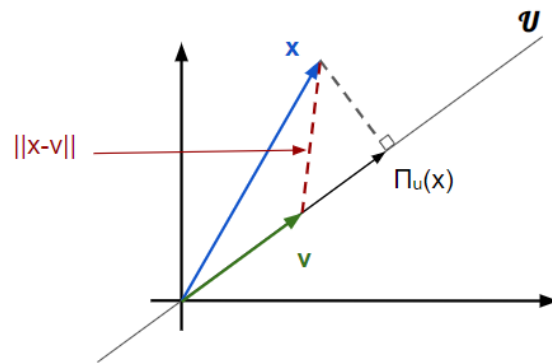


Figure 5: Illustration of the distance between x and v

4 Singular Value Decomposition

Theorem 38 (SVD). Any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $\text{rank}(\mathbf{A}) = r$ can be decomposed as:

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

where $\mathbf{U} \in \mathbb{R}^{m \times m}$ and $\mathbf{V} \in \mathbb{R}^{n \times n}$ are both orthogonal matrices (i.e. $\mathbf{U}^T\mathbf{U} = \mathbf{I}_m$ and $\mathbf{V}^T\mathbf{V} = \mathbf{I}_n$) and $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$ is a diagonal rectangular with positive entries matrix such that $\Sigma_{i,i} \neq 0$ if and only if $i \leq \text{rank}(\mathbf{A})$

The form $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ is called the full Singular-Value Decomposition (SVD) of \mathbf{A} .

Property 39. Let r be the rank of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$. Let \mathbf{U} and \mathbf{V} be the matrices from the SVD of \mathbf{A} with columns $\mathbf{u}_1, \dots, \mathbf{u}_m \in \mathbb{R}^m$ and $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^n$ respectively. Then the following hold:

- $\mathbf{u}_1, \dots, \mathbf{u}_r$ forms a basis a basis of $\mathcal{R}(\mathbf{A})$
- $\mathbf{u}_{r+1}, \dots, \mathbf{u}_m$ forms a basis of $\mathcal{N}(\mathbf{A}^T)$
- $\mathbf{v}_1, \dots, \mathbf{v}_r$ forms a basis a basis of $\mathcal{R}(\mathbf{A}^T)$
- $\mathbf{v}_{r+1}, \dots, \mathbf{v}_n$ forms a basis of $\mathcal{N}(\mathbf{A})$

In order to prove the above properties we can rewrite the SVD as follows:

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T = \begin{bmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{bmatrix} \begin{bmatrix} \mathbf{\Lambda} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V}_1^T \\ \mathbf{V}_2^T \end{bmatrix} \quad (1)$$

$(m \times n) \quad (m \times m)(m \times n)(n \times n) \quad \begin{matrix} (r \times r) & (r \times n-r) \\ (m-r \times r) & (m-r \times n-r) \end{matrix} \quad \begin{matrix} (r \times n) \\ (n-r \times n) \end{matrix}$

We can solve for $\mathbf{\Sigma}$ of the SVD as follows:

$$\mathbf{\Sigma} = \begin{bmatrix} \mathbf{\Lambda} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{U}_1^T \\ \mathbf{U}_2^T \end{bmatrix} \mathbf{A} \begin{bmatrix} \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{U}_1^T \mathbf{A} \mathbf{V}_1 & \mathbf{U}_1^T \mathbf{A} \mathbf{V}_2 \\ \mathbf{U}_2^T \mathbf{A} \mathbf{V}_1 & \mathbf{U}_2^T \mathbf{A} \mathbf{V}_2 \end{bmatrix} \quad (2)$$

$\begin{matrix} (r \times r) & (r \times n-r) \\ (m-r \times r) & (m-r \times n-r) \end{matrix} \quad \begin{matrix} (r \times m) \\ (m-r \times m) \end{matrix} \quad \begin{matrix} (n \times r) & (n \times n-r) \end{matrix}$

Here are the following proofs for the properties of the SVD¹

Proof.

(i) $\mathbf{u}_1, \dots, \mathbf{u}_r$ forms a basis a basis of $\mathcal{R}(\mathbf{A})$. We will prove $\mathcal{R}(\mathbf{A}) = \mathcal{R}(\mathbf{U}_1)$ where $\mathbf{u}_1, \dots, \mathbf{u}_r$ are the columns of \mathbf{U}_1 . We have $\mathbf{A} = \mathbf{U}_1 \mathbf{\Lambda} \mathbf{V}_1^T$. Since $\mathbf{\Lambda}$ is invertible and $\mathbf{V}_1^T \mathbf{V}_1 = \mathbf{I}_r$, we have $\mathbf{U}_1 = \mathbf{A} \mathbf{V}_1 \mathbf{\Lambda}^{-1}$. Suppose $\mathbf{v} \in \mathcal{R}(\mathbf{U}_1)$. Then, there exists \mathbf{a} such that $\mathbf{v} = \mathbf{U}_1 \mathbf{a} = \mathbf{A} \mathbf{V}_1 \mathbf{\Lambda}^{-1} \mathbf{a}$. Therefore, $\mathbf{v} \in \mathcal{R}(\mathbf{A})$. It follows that $\mathcal{R}(\mathbf{A}) \supset \mathcal{R}(\mathbf{U}_1)$. Conversely, if $\mathbf{v} \in \mathcal{R}(\mathbf{A})$, there exists \mathbf{x} such that $\mathbf{v} = \mathbf{A} \mathbf{x} = \mathbf{U}_1 \mathbf{\Lambda} \mathbf{V}_1 \mathbf{x} \in \mathcal{R}(\mathbf{U}_1)$, showing that $\mathcal{R}(\mathbf{A}) \subset \mathcal{R}(\mathbf{U}_1)$.

(ii) $\mathbf{u}_{r+1}, \dots, \mathbf{u}_m$ forms a basis of $\mathcal{N}(\mathbf{A}^T)$. We need to show that the vector columns of \mathbf{U}_2 form a basis of $\mathcal{N}(\mathbf{A}^T)$. From equation 2, we can extract the following:

$$[\mathbf{U}_2^T \mathbf{A} \mathbf{V}_1 \quad \mathbf{U}_2^T \mathbf{A} \mathbf{V}_2] = [\mathbf{0} \quad \mathbf{0}] \implies \mathbf{U}_2^T \mathbf{A} [\mathbf{V}_1^T \quad \mathbf{V}_2^T] = \mathbf{0} \implies \mathbf{U}_2^T \mathbf{A} \mathbf{V} = \mathbf{0} \implies \mathbf{U}_2^T \mathbf{A} = \mathbf{0} \implies \mathbf{A}^T \mathbf{U}_2 = \mathbf{0}$$

This implies $\mathcal{R}(\mathbf{U}_2) \subset \mathcal{N}(\mathbf{A}^T)$.

Conversely, if $\mathbf{x} \in \mathcal{N}(\mathbf{A}^T)$ we have $\mathbf{0} = \mathbf{A}^T \mathbf{x} = \mathbf{V}_1 \mathbf{\Lambda} \mathbf{U}_1^T \mathbf{x}$. Since \mathbf{V}_1 is orthogonal and $\mathbf{\Lambda}$ is invertible, this implies $\mathbf{U}_1^T \mathbf{x} = \mathbf{0}$ and therefore $\mathbf{x} \in \mathcal{R}(\mathbf{U}_1)^\perp = \mathcal{R}(\mathbf{U}_2)$. Hence $\mathcal{N}(\mathbf{A}^T) \subset \mathcal{R}(\mathbf{U}_2)$.

¹<https://jekyll.math.byuh.edu/courses/m343/handouts/svdbasis.pdf>

- (iii) $\mathbf{v}_1, \dots, \mathbf{v}_r$ forms a basis of $\mathcal{R}(\mathbf{A}^T)$. We will prove $\mathcal{R}(\mathbf{A}) = \mathcal{R}(\mathbf{V}_1)$ where $\mathbf{v}_1, \dots, \mathbf{v}_r \in \mathbf{V}_1$.
From equation 1, We can extract $\mathbf{A} = \mathbf{U}_1 \mathbf{\Lambda} \mathbf{V}_1^T$.

Because $\mathbf{\Lambda}$ is invertible and $\mathbf{U}_1^T \mathbf{U}_1 = \mathbf{I}_r$ because \mathbf{U}_1 is orthogonal. Then,
 $\mathbf{A}^T = \mathbf{V}_1 \mathbf{\Lambda} \mathbf{U}_1^T \implies \mathbf{V}_1 = \mathbf{A}^T \mathbf{\Lambda}^{-1} \mathbf{U}_1$.

Suppose there exists $\mathbf{v} \in \mathcal{R}(\mathbf{V}_1)$. Then, $\mathbf{v} = \mathbf{V}_1 \mathbf{a} = \mathbf{A}^T \mathbf{\Lambda}^{-1} \mathbf{U}_1 \mathbf{a} = \mathbf{A}^T \mathbf{a}^*$

Therefore, $\mathbf{v} \in \mathcal{R}(\mathbf{A}^T)$

It follows that $\mathcal{R}(\mathbf{A}^T) = \mathcal{R}(\mathbf{V}_1)$. Therefore $\mathbf{v}_1, \dots, \mathbf{v}_r$ is a basis of $\mathcal{R}(\mathbf{A}^T)$.

- (iv) $\mathbf{v}_{r+1}, \dots, \mathbf{v}_m$ forms a basis of $\mathcal{N}(\mathbf{A})$ we need to show that the vector columns of \mathbf{V}_2 form the $\mathcal{N}(\mathbf{A})$.
From equation 2, we can extract the following:

$$\begin{bmatrix} \mathbf{U}_1^T \mathbf{A} \mathbf{V}_2 \\ \mathbf{U}_2^T \mathbf{A} \mathbf{V}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \implies \begin{bmatrix} \mathbf{U}_1^T \\ \mathbf{U}_2^T \end{bmatrix} \mathbf{A} \mathbf{V}_2 = \mathbf{0} \implies \mathbf{U}^T \mathbf{A} \mathbf{V}_2 = \mathbf{0} \implies \mathbf{A} \mathbf{V}_2 = \mathbf{0}$$

This implies $\mathbf{V}_2 \in \mathcal{N}(\mathbf{A})$. Because the vector columns of \mathbf{V}_2 are orthonormal they are linearly independent and therefore form a basis of the $\mathcal{N}(\mathbf{A})$.

□

Reduced SVD

Given $\mathbf{A} \in \mathbb{R}^{m \times n}$, with the rank $\mathcal{R}(\mathbf{A}) = r$ and $m \geq n$, the Singular Value Decomposition of \mathbf{A} can be written in the following reduced forms. The idea behind these reduced forms is that, as the size of the matrix decreases, so does the memory footprint. Therefore, the cost of storing the matrix in memory reduces substantially compared to full SVD. This will also increase the speed of computation to some extent.

In **Thin SVD**, only the n column vectors of \mathbf{U} corresponding to the n row vectors of \mathbf{V}^T are kept. Equivalently, we keep only the top square sub-matrix from the diagonal matrix $\mathbf{\Sigma}$. The remaining column vectors of \mathbf{U} are not used and therefore are discarded. This has a positive effect on the memory footprint as there are less parameters to store, especially when $n \ll m$.

In **Compact SVD**, only the r column vectors of \mathbf{U} and r row vectors of \mathbf{V}^T corresponding to the r non-zero singular values $\mathbf{\Sigma}_r$ are kept. Equivalently, the top-left square sub-matrix with non-zero diagonal element is kept from the original $\mathbf{\Sigma}$ and the storage saving is increased. Up to this point, the *Thin* and *Compact* SVD were "free" in the sense that it didn't change the resulting matrix \mathbf{A} .

Finally, **Truncated SVD** is available to the user ready to forsake some accuracy in computations by discarding some information from $\mathbf{\Sigma}$. The Truncated SVD is an approximation to the full SVD, where the t column vectors of \mathbf{U} and t row vectors of \mathbf{V}^T corresponding to the t largest singular values $\mathbf{\Sigma}_t$ are kept. This again reduces the memory footprint in proportion of the singular values of $\mathbf{\Sigma}$ that are discarded. When a lot of these singular values are "close enough" to 0 to be deemed useless by the user chosen heuristic, we can eventually reach $t \ll r$.

$$\begin{aligned} \mathbf{A}_{m \times n} &= \mathbf{U}_{m \times m} \mathbf{\Sigma}_{m \times n} \mathbf{V}_{n \times n}^T & \text{(Full)} & \quad \mathbf{\Sigma}_{m \times n} = \begin{pmatrix} \mathbf{\Sigma}_{n \times n} \\ \mathbf{0} \end{pmatrix}, \\ &= \mathbf{U}_{m \times n} \mathbf{\Sigma}_{n \times n} \mathbf{V}_{n \times n}^T & \text{(Thin)} & \quad \mathbf{\Sigma}_{n \times n} = \begin{pmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{\Sigma}_{r \times r} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}_{n \times n} \end{aligned}$$

where, $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$.

$$\begin{aligned} &= \mathbf{U}_{m \times r} \mathbf{\Sigma}_{r \times r} \mathbf{V}_{r \times n}^T & \text{(Compact)} \\ &\approx \mathbf{U}_{m \times t} \mathbf{\Sigma}_{t \times t} \mathbf{V}_{t \times n}^T & \text{(Truncated)} \quad \text{for } t \ll r \end{aligned}$$

Definition 40 (Thin SVD). If $m \geq n$, Theorem 38 can be rewritten as:

$$\mathbf{A}_{(m \times n)} = \mathbf{U}_{(m \times m)} \mathbf{\Sigma}_{(m \times n)(n \times n)} \mathbf{V}^T_{(n \times n)} = \mathbf{U}_{(m \times m)} \begin{bmatrix} \mathbf{\Sigma}_{(n \times n)} \\ \mathbf{0} \end{bmatrix}_{(n \times n)} \mathbf{V}^T_{(n \times n)} = \mathbf{U}_n_{(m \times n)} \mathbf{\Sigma}_{(n \times n)(n \times n)} \mathbf{V}^T_{(n \times n)}$$

where:

- $\mathbf{\Lambda} \in \mathbb{R}^{r \times r}$ is diagonal with $\Lambda_{i,i} \neq 0$
- \mathbf{U}_n only keep the first n columns of \mathbf{U}
- $\mathbf{U}^T \mathbf{U} = \mathbf{V}^T \mathbf{V} = \mathbf{I}_r$ (\mathbf{U} and \mathbf{V} are both orthogonal matrices)

The form $\mathbf{A} = \mathbf{U}_n \mathbf{\Sigma} \mathbf{V}^T$ is called the thin Singular-Value Decomposition (thin SVD) of \mathbf{A} . If $m \leq n$ then rows of \mathbf{V}^T or omitted instead of columns of \mathbf{U} .

Definition 41 (Compact SVD). Given that $\text{rank}(\mathbf{A}) = r$, Theorem 38 can be rewritten as:

$$\mathbf{A}_{(m \times n)} = \mathbf{U}_{(m \times m)} \mathbf{\Sigma}_{(m \times n)(n \times n)} \mathbf{V}^T_{(n \times n)} = \begin{bmatrix} \tilde{\mathbf{U}}_{(m \times r)} & \tilde{\mathbf{U}}_{\perp} \end{bmatrix}_{(m \times m-r)} \begin{bmatrix} \mathbf{\Lambda}_{(r \times r)} & \mathbf{0}_{(r \times n-r)} \\ \mathbf{0}_{(m-r \times r)} & \mathbf{0}_{(m-r \times n-r)} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{V}}^T_{(r \times n)} \\ \tilde{\mathbf{V}}^T_{\perp} \end{bmatrix}_{(n-r \times n)} = \tilde{\mathbf{U}}_{(m \times r)} \mathbf{\Lambda}_{(r \times r)} \tilde{\mathbf{V}}^T_{(r \times n)}$$

where:

- $\mathbf{\Lambda} \in \mathbb{R}^{r \times r}$ is diagonal with $\Lambda_{i,i} \neq 0$, $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$
- $\tilde{\mathbf{U}}^T \tilde{\mathbf{U}} = \tilde{\mathbf{V}}^T \tilde{\mathbf{V}} = \mathbf{I}_r$ ($\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ are both orthogonal matrices)

The form $\mathbf{A} = \tilde{\mathbf{U}} \mathbf{\Lambda} \tilde{\mathbf{V}}^T$ is called the Compact Singular-Value Decomposition (Compact SVD) of \mathbf{A} .

Definition 42 (Truncated SVD). Given that $\text{rank}(\mathbf{A}) = r$, if $t < r$, we can approximate the SVD as:

$$\mathbf{A}_{(m \times n)} = \mathbf{U}_{(m \times m)} \mathbf{\Sigma}_{(m \times n)(n \times n)} \mathbf{V}^T_{(n \times n)} = \tilde{\mathbf{U}}_{(m \times t)} \mathbf{\Lambda}_{(t \times t)} \tilde{\mathbf{V}}^T_{(t \times n)}$$

for some $t \leq r$ Where:

- $\mathbf{\Lambda} \in \mathbb{R}^{r \times r}$ is diagonal with $\Lambda_{i,i} \neq 0$, $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$
- $\tilde{\mathbf{U}}^T \tilde{\mathbf{U}} = \tilde{\mathbf{V}}^T \tilde{\mathbf{V}} = \mathbf{I}_r$ ($\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ are both orthogonal matrices)

The form $\mathbf{A} = \tilde{\mathbf{U}} \mathbf{\Lambda} \tilde{\mathbf{V}}^T$ is called the Truncated Singular-Value Decomposition (Truncated SVD) of \mathbf{A} .

* if all the values of σ decay as they go to r , then we loose a lot less data when using the truncated version, because the σ values closes to r have less importance.

Remark : In truncated SVD, $\tilde{\mathbf{U}}$ is such that $\tilde{\mathbf{U}}^T \tilde{\mathbf{U}} = \mathbf{I}_r$. However, it is not true in general that $\tilde{\mathbf{U}} \tilde{\mathbf{U}}^T = \mathbf{I}_m$. If $r < m$, we actually know that $\tilde{\mathbf{U}} \tilde{\mathbf{U}}^T \neq \mathbf{I}_m$ because \mathbf{I}_m is of rank m , and cannot be linearly generated by $\tilde{\mathbf{U}}$ of rank $r < m$.

\mathbf{U} is orthogonal, so we have:

$$\mathbf{U}^T \mathbf{U}_{(m \times m)} = \begin{bmatrix} \tilde{\mathbf{U}}^T_{(R \times m)} \\ \tilde{\mathbf{U}}^T_{\perp} \end{bmatrix}_{(m-R \times m)} \begin{bmatrix} \tilde{\mathbf{U}}_{(m \times R)} & \tilde{\mathbf{U}}_{\perp} \end{bmatrix}_{(m \times m-R)} = \begin{bmatrix} \tilde{\mathbf{U}}^T \tilde{\mathbf{U}}_{(r \times r)} & \tilde{\mathbf{U}}^T \tilde{\mathbf{U}}_{\perp} \\ \tilde{\mathbf{U}}^T_{\perp} \tilde{\mathbf{U}} & \tilde{\mathbf{U}}^T_{\perp} \tilde{\mathbf{U}}_{\perp} \end{bmatrix}_{(m-r \times m-r)} = \begin{bmatrix} \mathbf{I}_r_{(r \times r)} & \mathbf{0}_{(r \times m-r)} \\ \mathbf{0}_{(m-r \times r)} & \mathbf{I}_{m-r} \end{bmatrix}_{(m-r \times m-r)}$$

The same holds for $\mathbf{V}^T \mathbf{V}$ with n instead of m .

5 The QR decomposition

In this section, we briefly present the QR decomposition which can be used to solve the linear least squares problem for example.

Theorem 43. Any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ can be written as $\mathbf{A} = \mathbf{Q}\mathbf{R}$ where $\mathbf{Q} \in \mathbb{R}^{m \times m}$ is orthogonal and $\mathbf{R} \in \mathbb{R}^{m \times n}$ is upper triangular. This decomposition of \mathbf{A} is called the QR decomposition.

If $m > n$ then the reduced (thin) QR decomposition of \mathbf{A} is defined as:

$$\mathbf{A} = [\mathbf{Q}_1 \quad \mathbf{Q}_2] \begin{bmatrix} \mathbf{R}_1 \\ 0 \end{bmatrix} = \mathbf{Q}_1 \mathbf{R}_1$$

where $\mathbf{Q}_1 \in \mathbb{R}^{m \times n}$ is orthogonal and $\mathbf{R}_1 \in \mathbb{R}^{n \times n}$ is upper triangular.

Remark 44. If $\mathbf{U} \in \mathbb{R}^{n \times k}$ and $\text{rank}(\mathbf{U}) = k$ (i.e full rank) then its thin QR decomposition $\mathbf{U} = \mathbf{Q}\mathbf{R}$ is such that:

- $\mathcal{R}(\mathbf{Q}) = \mathcal{R}(\mathbf{U})$
- \mathbf{R} is invertible

where $\mathbf{Q} \in \mathbb{R}^{n \times k}$ and $\mathbf{R} \in \mathbb{R}^{k \times k}$

If $\mathbf{u}_1, \dots, \mathbf{u}_k \in \mathbb{R}^n$ is a basis of \mathcal{U} , which is **not necessarily orthonormal**, and $\mathbf{U} \in \mathbb{R}^{n \times k}$ such that

$$\mathbf{U} = \begin{bmatrix} | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_k \\ | & & | \end{bmatrix}$$

then we have the following property: $\Pi_u(\mathbf{x}) = \mathbf{U}(\mathbf{U}^T \mathbf{U})^{-1} \mathbf{U}^T \mathbf{x}$

Proof. In order to show the previous property, let us consider the thin QR decomposition of \mathbf{U} , i.e, $\mathbf{U} = \mathbf{Q}\mathbf{R}$ where $\mathbf{Q} \in \mathbb{R}^{n \times k}$ is orthogonal and $\mathbf{R} \in \mathbb{R}^{k \times k}$ is upper triangular and invertible. The invertability follows from the previous remark since \mathbf{U} is full rank. We have

$$\begin{aligned} \mathbf{U}(\mathbf{U}^T \mathbf{U})^{-1} \mathbf{U}^T \mathbf{x} &= \mathbf{Q} \underbrace{\mathbf{R}(\mathbf{R}^T \mathbf{Q}^T \mathbf{Q} \mathbf{R})^{-1} \mathbf{R}^T}_{\mathbf{I}} \mathbf{Q}^T \mathbf{x} \\ &= \mathbf{Q} \mathbf{Q}^T \mathbf{x} \\ &= \Pi_u(\mathbf{x}) \end{aligned} \tag{3}$$

□

6 Linear regression

In the context of statistical learning theory, we are often interested in fitting the best model to a training set (i.e. perform regression).

Formally, we aim to learn a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ from a training set of examples which has the following form:

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\} \subseteq \mathbb{R}^d \times \mathbb{R} \quad (4)$$

where $y_i \approx f(\mathbf{x}_i)$ for each $i = 1, 2, \dots, N$.

Suppose the function f is linear, meaning $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$, for all $\mathbf{x} \in \mathbb{R}^d$, and some weight vector $\mathbf{w} \in \mathbb{R}^d$. One plausible approach to learning this function is by minimizing the Squared Error (SE) loss on an observed dataset \mathcal{D} :

$$\mathbf{w}^* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \sum_{i=1}^N (\mathbf{w}^T \mathbf{x}_i - y_i)^2 \quad (5)$$

If we take

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_N^T \end{pmatrix} \in \mathbb{R}^{N \times d}, \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} \in \mathbb{R}^N, \quad (6)$$

then (5) can be written in matrix form as

$$\mathbf{w}^* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2, \quad (7)$$

in which case $\mathbf{X}\mathbf{w} \in \mathcal{R}(\mathbf{X})$.

To solve for the Eq. 7, which is convex, we can take the gradient and solve it for 0 :

$$\begin{aligned} \nabla_{\mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 &= 2(\mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y}) = 0 \\ &\Rightarrow \mathbf{X}^T \mathbf{X} \mathbf{w} = \mathbf{X}^T \mathbf{y} \\ \mathbf{w}^* &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \end{aligned} \quad (8)$$

In fact, finding a solution to the linear regression problem can be seen as projecting the dataset onto the hyperplane spanned by \mathbf{X} . For instance, assuming the rank of \mathbf{X} is d (i.e. full-rank), the predictions $\hat{\mathbf{y}}$ follows

$$\begin{aligned} \hat{\mathbf{y}} &= \arg \min_{\mathbf{v} \in \mathcal{R}(\mathbf{X})} \|\mathbf{v} - \mathbf{y}\|^2 \\ &= \Pi_{\mathcal{R}(\mathbf{X})}(\mathbf{y}) \\ &= \mathbf{X} \underbrace{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}}_{\mathbf{w}^*}, \end{aligned} \quad (9)$$

7 Matrix inverses and pseudo-inverses

Definition 45 (Matrix inversion). A matrix $\mathbf{A} \in \mathbb{R}^{m \times m}$ is invertible if $\exists \mathbf{A}^{-1} \in \mathbb{R}^{m \times m}$ such that $\mathbf{A}^{-1} \mathbf{A} = \mathbf{I}$.

The matrix inverse has the following properties:

- $\mathbf{A} \mathbf{A}^{-1} = \mathbf{I} \Leftrightarrow \mathbf{A}^{-1} \mathbf{A} = \mathbf{I}$
- $(\mathbf{A} \mathbf{B})^{-1} = \mathbf{B}^{-1} \mathbf{A}^{-1}$

The following statements regarding the matrix inverse are equivalent:

- $\det(\mathbf{A}) \neq 0$
- \mathbf{A}^{-1} exists, i.e. \mathbf{A} is invertible
- \mathbf{A} has full rank
- $\mathcal{N}(\mathbf{A}) = \{\mathbf{0}\}$

Definition 46 (Moore-Penrose pseudo-inverse). Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ and let $\mathbf{A} = \underbrace{\mathbf{U}}_{m \times R} \mathbf{D} \underbrace{\mathbf{V}^T}_{R \times m}$ be a compact SVD where $R = \text{rank}(\mathbf{A})$. Then, the Moore-Penrose pseudo-inverse of \mathbf{A} is defined as $\mathbf{A}^\dagger = \mathbf{V} \mathbf{D}^{-1} \mathbf{U}^T \in \mathbb{R}^{n \times m}$.

We note that \mathbf{D} is a diagonal matrix with strictly positive entries. The Moore-Penrose pseudo-inverse has the following properties:

- $\mathbf{A} \mathbf{A}^\dagger \mathbf{A} = \mathbf{A}$
- $\mathbf{A}^\dagger \mathbf{A} \mathbf{A}^\dagger = \mathbf{A}^\dagger$
- $(\mathbf{A} \mathbf{A}^\dagger)^T = \mathbf{A} \mathbf{A}^\dagger$
- $(\mathbf{A}^\dagger \mathbf{A})^T = \mathbf{A}^\dagger \mathbf{A}$

Suppose (as a special case) that $\text{rank}(\mathbf{A}) = m \leq n$ (i.e. \mathbf{A} is full-rank). Then,

$$\begin{aligned} \mathbf{A} \mathbf{A}^\dagger &= (\mathbf{U} \underbrace{\mathbf{D} \mathbf{V}^T}_{\text{identity}}) (\mathbf{V} \mathbf{D}^{-1} \mathbf{U}^T) \\ &= \mathbf{U} \mathbf{U}^T \\ &= \underbrace{\mathbf{I}}_{m \times m}, \end{aligned} \tag{10}$$

where the last equality holds since $\text{rank}(\mathbf{A}) = m$ hence \mathbf{U} is square and $\mathbf{U} \mathbf{U}^T = \mathbf{U}^T \mathbf{U}$. However, this simplification does not hold for $\mathbf{A}^\dagger \mathbf{A}$. For instance, if $m < n$, then

$$\begin{aligned} \mathbf{A}^\dagger \mathbf{A} &= (\mathbf{V} \mathbf{D}^{-1} \mathbf{U}^T) (\mathbf{U} \mathbf{D} \mathbf{V}^T) \\ &= \mathbf{V} \mathbf{V}^T \neq \mathbf{I} \\ &= \Pi_{\mathcal{R}(\mathbf{A})} \end{aligned} \tag{11}$$

For this last equation, we can also note that since $\mathcal{R}(\mathbf{V}) = \mathcal{R}(\mathbf{A})$ and \mathbf{V} is orthogonal the following $\Pi_{\mathcal{R}(\mathbf{A})} = \mathbf{V} \mathbf{V}^T = \Pi_{\mathcal{R}(\mathbf{V})}$ is true.

In other words, we have shown that $\mathbf{A}^\dagger \mathbf{A} = \Pi_{\mathcal{R}(\mathbf{A})}$, i.e. the orthogonal projection onto the range; and $\mathbf{A} \mathbf{A}^\dagger = \Pi_{\mathcal{R}(\mathbf{A}^T)}$, i.e. the orthogonal projection onto the row space.

Example: We consider the problem of solving under-determined system of equations, and will show how the smallest solution of such a system (in terms of the 2-norm) is related to the pseudo-inverse of the matrix of the system.

We consider an under-determined system of equations:

$$\text{Solve } \underbrace{\mathbf{A}}_{m \times n} \mathbf{x} = \mathbf{y}, \text{ for } \mathbf{x} \in \mathbb{R}^n, \text{ where } m < n.$$

Since $m < n$, this system has an infinite number of solutions. Assuming that \mathbf{A} is full-rank, we want to show that $\mathbf{A}^\dagger \mathbf{y}$ is the least norm solution. For this, we make the following claims:

Claim 1 $\mathbf{x}_{LN} = \mathbf{A}^\dagger \mathbf{y}$ is a solution, i.e. $\mathbf{A}\mathbf{x}_{LN} = \mathbf{y}$

Proof. We can easily show that $\mathbf{A}\mathbf{x}_{LN} = \underbrace{\mathbf{A}\mathbf{A}^\dagger}_{\mathbf{I}} \mathbf{y} = \mathbf{y}$, because \mathbf{A} is full rank. But there are infinite number of solutions to this equation! \mathbf{x}_{LN} is just one of them. \square

Now we make the following interesting claim:

Claim 2 \mathbf{x}_{LN} is the solution with the smallest 2-norm.

Proof. To prove that, let \mathbf{x} be another solution, i.e., $\mathbf{A}\mathbf{x} = \mathbf{y}$. We want to show that this second solution has larger norm than the first one, i.e., $\|\mathbf{x}\| \geq \|\mathbf{x}_{LN}\|$.

The idea of the proof is to first show that \mathbf{x} and $(\mathbf{x} - \mathbf{x}_{LN})$ are orthogonal, and then use the Pythagorean theorem (on the triangle with vertices $\mathbf{0}$, \mathbf{x} and \mathbf{x}_{LN}) to show that $\|\mathbf{x}\| \geq \|\mathbf{x}_{LN}\|$.

Let $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$ be the compact SVD of \mathbf{A} . The inner product of \mathbf{x}_{LN} and the difference between \mathbf{x}_{LN} and \mathbf{x} is

$$\begin{aligned} \langle \mathbf{x}_{LN}, \mathbf{x} - \mathbf{x}_{LN} \rangle &= \mathbf{x}_{LN}^T (\mathbf{x} - \mathbf{x}_{LN}) \\ &= \mathbf{y}^T \mathbf{A}^{\dagger T} (\mathbf{x} - \mathbf{x}_{LN}) \\ &= \mathbf{y}^T \mathbf{U} \mathbf{D}^{-1} \mathbf{V}^T (\mathbf{x} - \mathbf{x}_{LN}) \end{aligned} \quad (12)$$

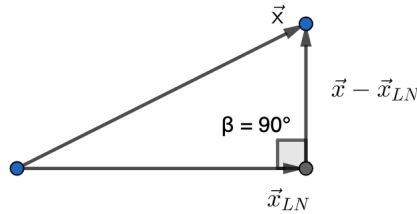
Now observe that

$$\mathbf{A}(\mathbf{x} - \mathbf{x}_{LN}) = \mathbf{y} - \mathbf{y} = \mathbf{0}. \quad (13)$$

Using the fact that \mathbf{U} and \mathbf{D} are both invertible (since $m < n$) this implies that $\mathbf{V}^\top (\mathbf{x} - \mathbf{x}_{LN}) = \mathbf{0}$ (multiply Eq. (13) to the left by $\mathbf{D}^{-1} \mathbf{U}^\top$).

It follows that $\langle \mathbf{x}_{LN}, \mathbf{x} - \mathbf{x}_{LN} \rangle = 0$ and we can use the Pythagorean theorem to obtain

$$\begin{aligned} \|\mathbf{x}\|^2 &= \|\mathbf{x}_{LN}\|^2 + \|\mathbf{x} - \mathbf{x}_{LN}\|^2 \\ &\geq \|\mathbf{x}_{LN}\|^2. \end{aligned} \quad (14)$$



\square

8 Eigenvalues and eigenvectors

Definition 47 (Eigenvalue, eigenvector and eigenspace). Let $\mathbf{A} \in \mathbb{R}^{m \times m}$. Any $\mathbf{v} \in \mathbb{R}^m$ such that $\mathbf{v} \neq 0$ and satisfying

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

for $\lambda \in \mathbb{C}$ is called an eigenvector of \mathbf{A} corresponding to the eigenvalue λ . The space $E_\lambda = \{\mathbf{v} \in \mathbb{R}^m | \mathbf{A}\mathbf{v} = \lambda\mathbf{v}\}$ is called the eigenspace of \mathbf{A} corresponding to λ .

For example, if $\mathbf{A} = \mathbf{I}$ then $\mathbf{A}\mathbf{v} = \mathbf{I}\mathbf{v} = \mathbf{v}$ for all \mathbf{v} and 1 is an eigenvalue with corresponding eigenspace $E_1 = \mathbb{R}^m$. Eigenvalues can be found by finding the roots of the characteristic polynomial:

$$\begin{aligned} \mathbf{A}\mathbf{v} = \lambda\mathbf{v} &\iff (\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0 \\ &\iff \mathbf{v} \in \mathcal{N}(\mathbf{A} - \lambda\mathbf{I}) \\ &\iff \det(\mathbf{A} - \lambda\mathbf{I}) = 0 \end{aligned} \tag{15}$$

As an example, let's find the eigenvalues for a given matrix \mathbf{A} .

$$\mathbf{A} = \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix}$$

Its characteristic polynomial is

$$\det \left(\begin{pmatrix} 1-\lambda & 1 \\ 0 & 2-\lambda \end{pmatrix} \right) = (1-\lambda)(2-\lambda)$$

which implies that the eigenvalues are $\lambda \in \{1, 2\}$.

As a special case, if \mathbf{A} is triangular, then its determinant is the product of its eigenvalues and the eigenvalues are the diagonal entries of \mathbf{A} .

Definition 48 (Diagonalization). A matrix $\mathbf{A} \in \mathbb{R}^{n \times m}$ is diagonalizable iff there exists a basis $\mathbf{v}_1, \dots, \mathbf{v}_n$ of \mathbb{R}^n consisting of eigenvectors of \mathbf{A} . In this case, $\mathbf{V}^{-1}\mathbf{A}\mathbf{V} = \mathbf{D}$ is diagonal.

An example of a matrix diagonalizable over \mathbb{C} but not over \mathbb{R} is

$$\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

For instance, consider the problem of finding the eigenvectors of \mathbf{A} . Simplifying the characteristic polynomial equation implies that we have to solve $\lambda^2 + 1 = 0$. The equation has no real roots but has two complex roots, $\lambda \in \{i, -i\}$, which allows for \mathbf{A} to be diagonalizable over \mathbb{C} .

An example of a non-diagonalizable matrix is

$$\mathbf{A} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

Definition 49 (Eigenvalues multiplicities). Let λ be an eigenvalue of \mathbf{A} then :

- The geometric multiplicity, $m_g(\lambda)$ is the dimension of E_λ where $E_\lambda = \{\mathbf{v} | \mathbf{A}\mathbf{v} = \lambda\mathbf{v}\}$
 - The algebraic multiplicity $m_a(\lambda)$, is the multiplicity of λ as root of $\det(\mathbf{A} - \lambda\mathbf{I})$ (the characteristic polynomial of \mathbf{A}). Equivalently, $m_a(\lambda)$ is the dimension of the generalized eigenspace $\bigcup_{k \geq 0} \mathcal{N}((\mathbf{A} - \lambda\mathbf{I})^k)$
- where $\bigcup_{k \geq 0} \mathcal{N}((\mathbf{A} - \lambda\mathbf{I})^k) = \mathcal{N}(\mathbf{I}) \cup \mathcal{N}(\mathbf{A} - \lambda\mathbf{I}) \cup \mathcal{N}((\mathbf{A} - \lambda\mathbf{I})^2) \cup \dots \cup \mathcal{N}((\mathbf{A} - \lambda\mathbf{I})^k)$

Observe that :

- $\mathcal{N}(\mathbf{A} - \lambda\mathbf{I}) = E_\lambda$.

Proof. By definition, $\mathcal{N}(\mathbf{A} - \lambda\mathbf{I}) = \{\mathbf{v} \mid (\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}\} = \{\mathbf{v} \mid \mathbf{A}\mathbf{v} = \lambda\mathbf{v}\} = E_\lambda$ \square

- $m_g(\lambda) \leq m_a(\lambda)$.

Proof. As seen above, $m_a(\lambda)$ is the dimension of the generalized eigenspace $\bigcup_{k \geq 0} \mathcal{N}((\mathbf{A} - \lambda\mathbf{I})^k)$ which includes $\mathcal{N}(\mathbf{A} - \lambda\mathbf{I}) = E_\lambda$ (the dimension of $m_g(\lambda)$). Thus, we have $m_g(\lambda) \leq m_a(\lambda)$. \square

- If the geometric multiplicity is strictly smaller than the algebraic multiplicity of an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$, $m_g(\lambda) < m_a(\lambda)$, then \mathbf{A} is not diagonalizable.

Proof. Let $\lambda_1, \dots, \lambda_k$ be the eigenvalues of \mathbf{A} . Suppose $m_g(\lambda_1) < m_a(\lambda_1)$. Then, it follows that the eigenspace E_1 has dimension strictly less than $m_a(\lambda_1)$, and consequently the dimension of $\bigcup_{i=1}^k E_k$ is strictly less than n and there cannot exist a basis of \mathbb{R}^n consisting of eigenvectors of \mathbf{A} . \square

Example 50. Let $\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 0 & 2 \end{bmatrix}$, the corresponding characteristic polynomial is $(2 - \lambda)^2$. The eigenvalue of \mathbf{A} is 2 with multiplicity $m_a(\lambda) = 2$.

$$\begin{aligned} E_\lambda &= \mathcal{N}(\mathbf{A} - 2\mathbf{I}) \\ &= \mathcal{N}\left(\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\right) \\ &= \text{span}\left(\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) \end{aligned} \tag{16}$$

We have $m_g(\lambda) = \dim(E_\lambda) = 1$ which is different from its eigenvalue multiplicity $m_a(\lambda) = 2$ hence the matrix \mathbf{A} is not diagonalizable.

Property 51. The eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_n$ associated with distinct eigenvalues of \mathbf{A} are linearly independent.

Proof. Let \mathbf{v}_1 and \mathbf{v}_2 two eigenvectors of \mathbf{A} associated with the distinct eigenvalues λ_1 and λ_2 and let a and b such that $a\mathbf{v}_1 + b\mathbf{v}_2 = \mathbf{0}$. It follows that :

$$\begin{aligned} \mathbf{A}(a\mathbf{v}_1 + b\mathbf{v}_2) &= \mathbf{0} \\ a\mathbf{A}\mathbf{v}_1 + b\mathbf{A}\mathbf{v}_2 &= \mathbf{0} \\ a\lambda_1\mathbf{v}_1 + b\lambda_2\mathbf{v}_2 &= \mathbf{0} \end{aligned} \tag{17}$$

But by multiplying $a\mathbf{v}_1 + b\mathbf{v}_2 = \mathbf{0}$ by λ_2 , we also have :

$$a\lambda_2\mathbf{v}_1 + b\lambda_2\mathbf{v}_2 = \mathbf{0} \tag{18}$$

Hence by subtracting (3) and (4) we have :

$$\begin{aligned} (a\lambda_1\mathbf{v}_1 + b\lambda_2\mathbf{v}_2) - (a\lambda_2\mathbf{v}_1 + b\lambda_2\mathbf{v}_2) &= \mathbf{0} \\ a(\lambda_1 - \lambda_2)\mathbf{v}_1 &= \mathbf{0} \end{aligned} \tag{19}$$

If the eigenvalues λ_1 and λ_2 are distinct, i.e. $\lambda_1 \neq \lambda_2$, we can conclude $a = 0$. Similar conclusion can be drawn for $b = 0$. Therefore the eigenvectors \mathbf{v}_1 and \mathbf{v}_2 are linearly independent.

We can then repeat the process for each pair of eigenvectors of \mathbf{A} and we would conclude that the eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_n$ associated with *distinct* eigenvalues of \mathbf{A} are linearly independent. \square

9 Spectral Theorem

Definition 52 (Positive definite and semi-definite matrices). A symmetric matrix $\mathbf{A} \in \mathbb{R}^{m \times m}$ is :

- positive definite if and only if all of its eigenvalues are strictly positive.
- positive semi-definite or non-negative definite if all of its eigenvalues are non-negative.

Property 53. For any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{A}^\top \mathbf{A}$ is positive semi-definite

Proof. Suppose $\mathbf{A} \in \mathbb{R}^{m \times n}$. Let \mathbf{v} be an eigenvector of $\mathbf{A}^\top \mathbf{A}$, and λ the corresponding eigenvalue. Therefore, we have

$$\begin{aligned}\mathbf{A}^\top \mathbf{A} \mathbf{v} &= \lambda \mathbf{v} \\ \mathbf{v}^\top \mathbf{A}^\top \mathbf{A} \mathbf{v} &= \mathbf{v}^\top \lambda \mathbf{v} \\ \mathbf{v}^\top \mathbf{A}^\top \mathbf{A} \mathbf{v} &= \lambda \|\mathbf{v}\|^2\end{aligned}\tag{20}$$

Since $(\mathbf{A}\mathbf{v})^\top = \mathbf{v}^\top \mathbf{A}^\top$

$$\begin{aligned}(\mathbf{A}\mathbf{v})^\top \mathbf{A} \mathbf{v} &= \lambda \|\mathbf{v}\|^2 \\ \|\mathbf{A}\mathbf{v}\|^2 &= \lambda \|\mathbf{v}\|^2\end{aligned}\tag{21}$$

We also have

$$\|\mathbf{A}\mathbf{v}\|^2 \geq 0 \text{ and } \|\mathbf{v}\|^2 \geq 0\tag{22}$$

Therefore, $\lambda \geq 0$ □

Theorem 54 (Spectral theorem). If $\mathbf{A} \in \mathbb{R}^{m \times m}$ is symmetric then:

- (2) *[label=()]All of its eigenvalues are real \mathbf{A} is diagonalizable by an orthogonal matrix meaning that there exists an orthogonal matrix $\mathbf{U} \in \mathbb{R}^{m \times m}$ such that $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^\top$ with $\mathbf{D} \in \mathbb{R}^{m \times m}$ being diagonal*

Proof.

[label=()]Let $\lambda \in \mathbb{C}$ be an eigenvalue and $\mathbf{v} \neq 0$, a corresponding eigenvector of \mathbf{A} . we denote $\bar{\mathbf{v}}$ by the complex conjugate of \mathbf{v} .

$$\mathbf{v}^\top \mathbf{A} \bar{\mathbf{v}} = \mathbf{v}^\top \mathbf{A}^\top \bar{\mathbf{v}} = (\mathbf{A}\mathbf{v})^\top \bar{\mathbf{v}} = \lambda \mathbf{v}^\top \bar{\mathbf{v}}\tag{23}$$

Since \mathbf{A} is real and symmetric, hence we have $\mathbf{A} = \bar{\mathbf{A}}$ and $\mathbf{A}^\top = \mathbf{A}$. We also have :

$$\mathbf{v}^\top \mathbf{A} \bar{\mathbf{v}} = \mathbf{v}^\top \cdot \bar{\mathbf{A}} \cdot \bar{\mathbf{v}} = \mathbf{v}^\top \overline{\mathbf{A}\mathbf{v}} = \mathbf{v}^\top \overline{\lambda \mathbf{v}} = \bar{\lambda} \mathbf{v}^\top \bar{\mathbf{v}}\tag{24}$$

Now we have $\lambda \mathbf{v}^\top \bar{\mathbf{v}} = \bar{\lambda} \mathbf{v}^\top \bar{\mathbf{v}}$ and since $\mathbf{v}^\top \bar{\mathbf{v}} \neq 0$, then $\lambda = \bar{\lambda}$ hence $\lambda \in \mathbb{R}$. Let $\mathbf{v} \neq 0$ a unit eigenvector for λ , i.e. $\mathbf{A}\mathbf{v} = \lambda \mathbf{v}$, and $\mathbf{v}^\top \mathbf{v} = 1$. Let $\mathcal{U} = \text{span}(\mathbf{v})^\perp = \{\mathbf{u} \in \mathbb{R}^m | \langle \mathbf{u}, \mathbf{v} \rangle = 0\}$. We observe that \mathcal{U} is \mathbf{A} invariant, i.e. if $\mathbf{u} \in \mathcal{U}$, then $\mathbf{A}\mathbf{u} \in \mathcal{U}$. $\langle \mathbf{A}\mathbf{u}, \mathbf{v} \rangle = (\mathbf{A}\mathbf{u})^\top \mathbf{v} = \mathbf{u}^\top \mathbf{A}^\top \mathbf{v} = \mathbf{u}^\top \mathbf{A} \mathbf{v} = \lambda \mathbf{u}^\top \mathbf{v} = 0$ which implies that we have $\mathbf{A}\mathbf{u} \in \mathcal{U}$.

Let $\mathbf{u}_1, \dots, \mathbf{u}_{m-1} \in \mathbb{R}^m$ be an orthonormal basis of \mathcal{U} , and let $\mathbf{U} = \begin{pmatrix} | & | & & | \\ \mathbf{v} & \mathbf{u}_1 & \dots & \mathbf{u}_{m-1} \\ | & | & & | \end{pmatrix} \in \mathbb{R}^{m \times m}$.

We claim that \mathbf{U} is orthogonal and $\mathbb{R}^m = \mathcal{U} \oplus \mathcal{U}^\perp = \mathcal{U} \oplus \text{span}(\mathbf{v})$, with $\dim(\text{span}(\mathbf{v})) = 1$. We first prove that \mathbf{U} is orthogonal since $\mathcal{U} = \text{span}(\mathbf{v})^\perp$. Let's look at the first column of $\mathbf{U}^\top \mathbf{A} \mathbf{U}$. $(\mathbf{A}\mathbf{U})_{:1} =$

$$\mathbf{A}\mathbf{U}_{:1} = \mathbf{A}\mathbf{v} = \lambda \mathbf{v}. \text{ Thus, we have } (\mathbf{U}^\top \mathbf{A} \mathbf{U})_{:1} = \lambda \mathbf{U}^\top \mathbf{v} = \lambda \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \text{ Since } \mathbf{U} \text{ is } \mathbf{A}\text{-invariant, for each } i,$$

we have $\mathbf{A}\mathbf{u}_i \in \mathcal{U}$, which means that $\mathbf{A}\mathbf{u}_i = \mathbf{U} \begin{pmatrix} 0 \\ \mathbf{b}_i \end{pmatrix}$ for some $\mathbf{b}_i \in \mathbb{R}^{m-1}$ (indeed, $\mathbf{A}\mathbf{u}_i$ is orthogonal

to \mathbf{v}). We also have $\mathbf{A}\mathbf{v} = \lambda\mathbf{v} = \mathbf{U} \begin{pmatrix} \lambda \\ 0 \\ \vdots \\ 0 \end{pmatrix}$, from which $\mathbf{A}\mathbf{U} = \mathbf{U} \begin{pmatrix} \lambda & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & \mathbf{B} & \\ 0 & & & \end{pmatrix}$ follows. Now, we want to prove that \mathbf{B} is symmetric or $\mathbf{B} = \mathbf{B}^\top$. Since \mathbf{U} is square and $\mathbf{U} \in \mathbb{R}^{m \times m}$, $\mathbf{U}\mathbf{U}^\top = \mathbf{I}$. We have $\mathbf{A} = \mathbf{U} \begin{pmatrix} \lambda & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & \mathbf{B} & \\ 0 & & & \end{pmatrix} \mathbf{U}^\top$. Then, $\mathbf{A}^\top = (\mathbf{U} \begin{pmatrix} \lambda & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & \mathbf{B} & \\ 0 & & & \end{pmatrix} \mathbf{U}^\top)^\top$. Because we know \mathbf{A} is symmetric, $\mathbf{A}^\top = \mathbf{A} = \mathbf{U} \begin{pmatrix} \lambda & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & \mathbf{B}^\top & \\ 0 & & & \end{pmatrix} \mathbf{U}^\top = \mathbf{U} \begin{pmatrix} \lambda & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & \mathbf{B} & \\ 0 & & & \end{pmatrix} \mathbf{U}^\top$. Therefore, $\mathbf{B} = \mathbf{B}^\top$. Since \mathbf{B} is symmetric, we can reiterate the process $m - 1$ times to diagonalize \mathbf{B} and end up with $\mathbf{A} = \begin{pmatrix} | & & | \\ \mathbf{v}_1 & \dots & \mathbf{v}_m \\ | & & | \end{pmatrix} \begin{pmatrix} \lambda_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \lambda_m \end{pmatrix} \begin{pmatrix} - & \mathbf{v}_1 & - \\ & \vdots & \\ - & \mathbf{v}_m & - \end{pmatrix}$ where \mathbf{v}_i is the eigenvector associated with an eigenvalue λ_i for each $i \in \{1, \dots, m\}$.

□

10 Schur decomposition and the Jordan canonical form

Definition 55 (Conjugate transpose and unitary matrices). Let $\mathbf{U} \in \mathbb{C}^{m \times m}$:

- The conjugate transpose of \mathbf{U} , denoted \mathbf{U}^* , is the transpose of the conjugate matrix $\overline{\mathbf{U}}$. Therefore, $\mathbf{U}^* = \overline{\mathbf{U}}^T$
- \mathbf{U} is a unitary matrix if $\mathbf{U}^* \mathbf{U} = \mathbf{I}$

Theorem 56 (Schur decomposition). For any matrix $\mathbf{A} \in \mathbb{R}^{m \times m}$:

- There exists a unitary matrix $\mathbf{U} \in \mathbb{C}^{m \times m}$ such that $\mathbf{U}^* \mathbf{A} \mathbf{U}$ is upper triangular.
- There exists an orthogonal matrix $\mathbf{Q} \in \mathbb{R}^{m \times m}$ such that:

$$\mathbf{Q}^T \mathbf{A} \mathbf{Q} = \begin{bmatrix} \mathbf{R}_{1,1} & \dots & \dots & \mathbf{R}_{1,k} \\ 0 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \mathbf{R}_{k,k} \end{bmatrix} \quad (25)$$

where for all $i \in \{1, 2, \dots, k\}$, $\mathbf{R}_{i,i}$ is either a 1×1 matrix (corresponding to a real eigenvalue of \mathbf{A}) or a 2×2 matrix (corresponding to a pair of conjugate complex eigenvalues, with the block having the form $\begin{pmatrix} \alpha & -\beta \\ \beta & -\alpha \end{pmatrix}$).

Theorem 57 (Jordan canonical form). For any matrix $\mathbf{A} \in \mathbb{C}^{m \times m}$:

- There is an invertible matrix $\mathbf{P} \in \mathbb{C}^{m \times m}$ such that:

$$\mathbf{P}^{-1} \mathbf{A} \mathbf{P} = \begin{bmatrix} \mathbf{J}_1 & 0 & \dots & 0 \\ 0 & \mathbf{J}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \mathbf{J}_p \end{bmatrix} \quad (26)$$

where \mathbf{J}_i for all $i \in \{1, 2, \dots, p\}$ are called Jordan blocks.

- A Jordan block, \mathbf{J}_i , corresponding to eigenvalue λ_i contains repeated values of λ_i in its diagonal, and 1s above this diagonal. All other elements of the block are 0s. Visually, the Jordan blocks are of the form

$$\mathbf{J}_i = \begin{bmatrix} \lambda_i & 1 & 0 & 0 \\ 0 & \lambda_i & 1 & 0 \\ \vdots & \ddots & \ddots & 1 \\ 0 & \dots & 0 & \lambda_i \end{bmatrix} \in \mathbb{C}^{m_i \times m_i} \quad (27)$$

where λ_i corresponds to an eigenvalue of \mathbf{A} .

- The eigenvalues λ_i associated with each \mathbf{J}_i do not need to be distinct
- The number of Jordan blocks associated with an eigenvalue λ is the geometric multiplicity of λ in \mathbf{A} .
- The above decomposition is unique up to the ordering of the Jordan blocks
- The sum of the sizes of each Jordan block sums to the size of \mathbf{P} and \mathbf{A} , i.e., $m_1 + m_2 + \dots + m_p = m$

11 The Singular Value Decomposition

In a previous section we defined the Singular Value Decomposition (SVD), now that we have defined the spectral theorem we can prove the SVD decomposition.

Theorem 58 (SVD). Any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ can be written as:

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

where $\mathbf{U} \in \mathbb{R}^{m \times m}$ and $\mathbf{V} \in \mathbb{R}^{n \times n}$ are both orthogonal matrices (i.e. $\mathbf{U}^\top \mathbf{U} = \mathbf{I}_m$ and $\mathbf{V}^\top \mathbf{V} = \mathbf{I}_n$) and $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$ is a diagonal rectangular matrix such that $\Sigma_{i,i} \neq 0$ if and only if $i \leq \text{rank}(\mathbf{A})$

The form $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$ is called the Singular-Value Decomposition (SVD) of \mathbf{A} .

Proof. Recall that $\mathbf{A}^\top \mathbf{A}$ is positive semi-definite and symmetric. Using the spectral theorem we can write $\mathbf{A}^\top \mathbf{A} = \mathbf{V}\mathbf{\tilde{\Sigma}}^2\mathbf{V}^\top$ with \mathbf{V} orthogonal and $\mathbf{\tilde{\Sigma}}$ diagonal. Let $\mathbf{A}^\top \mathbf{A} = [\mathbf{V}_1 \mathbf{V}_2] \begin{pmatrix} \mathbf{\tilde{\Sigma}}^2 & \\ & \mathbf{0} \end{pmatrix} \begin{bmatrix} \mathbf{V}_1^\top \\ \mathbf{V}_2^\top \end{bmatrix}$ with $\mathbf{\tilde{\Sigma}} \in \mathbb{R}^{r \times r}$ with strictly positive entries, where r is the rank of $\mathbf{A}^\top \mathbf{A}$. It follows that $\mathbf{A}^\top \mathbf{A} = \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^2 \mathbf{V}_1^\top$. Let $\mathbf{U}_1 = \mathbf{A} \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^{-1}$. We have to prove:

$$(i) \quad \mathbf{U}_1^\top \mathbf{U}_1 = \mathbf{I}$$

$$(ii) \quad \mathbf{U}_1^\top \mathbf{A} \mathbf{V}_1 = \mathbf{\tilde{\Sigma}}$$

For (i), we have:

$$\begin{aligned} \mathbf{U}_1^\top \mathbf{U}_1 &= \mathbf{\tilde{\Sigma}}^{-1} \mathbf{V}_1^\top \mathbf{A}^\top \mathbf{A} \mathbf{V}_1 \mathbf{\tilde{\Sigma}} \\ &= \mathbf{\tilde{\Sigma}}^{-1} \mathbf{V}_1^\top \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^2 \mathbf{V}_1^\top \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^{-1} \\ &= \mathbf{I} \end{aligned}$$

(ii) simply follows from the equality $\mathbf{U}_1^\top \mathbf{A} \mathbf{V}_1 = \mathbf{\tilde{\Sigma}}^{-1} \mathbf{V}_1^\top \mathbf{A}^\top \mathbf{A} \mathbf{V}_1 = \mathbf{\tilde{\Sigma}}^{-1} \mathbf{V}_1^\top \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^2 \mathbf{V}_1^\top \mathbf{V}_1 = \mathbf{\tilde{\Sigma}}$.

Now we define $\mathbf{U}_2 \in \mathbb{R}^{m \times (m-r)}$ orthogonal such that $\mathcal{R}(\mathbf{U}_2) = \mathcal{R}(\mathbf{U}_1)^\perp$ and let $\mathbf{U} = [\mathbf{U}_1 \mathbf{U}_2] \in \mathbb{R}^{m \times m}$. Observe that \mathbf{U} is orthogonal by construction. We have

$$\begin{aligned} \mathbf{U}^\top \mathbf{A} \mathbf{V} &= \begin{bmatrix} \mathbf{U}_1^\top \\ \mathbf{U}_2^\top \end{bmatrix} \mathbf{A} [\mathbf{V}_1 \mathbf{V}_2] \\ &= \begin{bmatrix} \mathbf{U}_1^\top \mathbf{A} \mathbf{V}_1 & \mathbf{U}_1^\top \mathbf{A} \mathbf{V}_2 \\ \mathbf{U}_2^\top \mathbf{A} \mathbf{V}_1 & \mathbf{U}_2^\top \mathbf{A} \mathbf{V}_2 \end{bmatrix} \end{aligned}$$

By (ii), we already know that the top left block is equal to $\mathbf{\tilde{\Sigma}}$. Since \mathbf{V} is orthogonal, for any column \mathbf{v}_2 of \mathbf{V}_2 , $\mathbf{V}_1^\top \mathbf{v}_2 = \mathbf{0}$ and

$$\mathbf{A}^\top \mathbf{A} \mathbf{v}_2 = \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^2 \mathbf{V}_1^\top \mathbf{v}_2 = \mathbf{0}$$

Hence, $\mathbf{v}_2^\top \mathbf{A}^\top \mathbf{A} \mathbf{v}_2 = \|\mathbf{A} \mathbf{v}_2\|_2^2 = 0$, which is equivalent to $\mathbf{A} \mathbf{v}_2 = \mathbf{0}$. Therefore, the two blocks in the second column are both zeros. It remains to show that $\mathbf{U}_2^\top \mathbf{A} \mathbf{V}_1 = \mathbf{0}$, which follows from the fact that $\mathbf{U}_2^\top \mathbf{U}_1 = \mathbf{0} = \mathbf{U}_2^\top \mathbf{A} \mathbf{V}_1 \mathbf{\tilde{\Sigma}}^{-1}$ and since $\mathbf{\tilde{\Sigma}}^{-1}$ is an invertible matrix.

In conclusion, we have

$$\mathbf{U}^\top \mathbf{A} \mathbf{V} = \begin{bmatrix} \mathbf{\tilde{\Sigma}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \mathbf{\Sigma}$$

□

The columns of \mathbf{V} (respectively \mathbf{U}) contain the eigenvectors of $\mathbf{A}^\top \mathbf{A}$ (respectively $\mathbf{A} \mathbf{A}^\top$), also called the left (respectively right) singular vectors.

In the case where \mathbf{A} is symmetric, its SVD can be retrieved from its spectral decomposition : $\mathbf{A} = \mathbf{U} \mathbf{D} \mathbf{U}^\top$. Since we want a diagonal matrix $\mathbf{\Sigma}$ with non negative elements (the singular values), we can define $\mathbf{\Sigma} = |\mathbf{D}|$, where the absolute value is taken element-wise and we construct $\mathbf{V}^\top = \text{sign}(\mathbf{\Sigma}) \mathbf{U}^\top$, where the **sign** function is taken element-wise.

12 Matrix Norms

12.1 Matrix p-norm

We start by defining the basic building block of the matrix p -norm:

Definition 59 (Vector p -norm). *The vector p -norm, where $p \in \mathbb{R}$ is greater than 1, is defined as:*

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |\mathbf{x}_i|^p \right)^{1/p}.$$

See [1] for more information on vector norms.

Now, any norm on vectors induces a norm on matrices. The matrix p -norm of an arbitrary matrix \mathbf{A} , denoted $\|\mathbf{A}\|_p$, is defined as:

$$\|\mathbf{A}\|_p = \sup_{\mathbf{x} \neq 0} \frac{\|\mathbf{A}\mathbf{x}\|_p}{\|\mathbf{x}\|_p}.$$

Remember that the difference between the supremum and the maximum is that the maximum must be an element of the set while the supremum need not to be. More specifically, if \mathcal{X} is an ordered set, and \mathcal{S} is a subset, then s_0 is the *supremum* of \mathcal{S} iff:

- (1) $s \leq s_0, \forall s \in \mathcal{S}$
- (2) if $x \in \mathcal{X}$ and $s \leq x, \forall s \in \mathcal{S}$, then $s_0 \leq x$

On the other hand, an element m is the *maximum* of \mathcal{S} iff:

- (1) $s \leq m, \forall s \in \mathcal{S}$
- (2) $m \in \mathcal{S}$

Considering that a property of a vector norm is $\|c\mathbf{x}\|_p = |c|\|\mathbf{x}\|_p$, for any scalar c , we choose c such that $\|\mathbf{x}\|_p = 1$. Therefore, the following equivalent² statement defines the matrix p -norm.

Definition 60 (Matrix p -norm). *The matrix p -norm, where $p \in \mathbb{R}$, is defined as:*

$$\|\mathbf{A}\|_p = \max_{\|\mathbf{x}\|=1} \|\mathbf{A}\mathbf{x}\|_p$$

Some geometric intuition about the matrix p -norm can be seen in [3].

As a side note, the main difference between a norm and a distance is that one can consider the norm of only one element, while a distance needs at least two elements.

12.2 Matrix Frobenius Norm

Definition 61 (Frobenius Norm). *The Frobenius norm is the 2-norm of the vector obtained by concatenating the rows (or equivalently the columns) of the matrix \mathbf{A} :*

$$\|\mathbf{A}\|_F = \left(\sum_{i=1}^n \sum_{j=1}^m |a_{ij}|^2 \right)^{1/2}$$

²Since we restrict the optimization to unit vectors, the subset \mathcal{S} is closed and bounded. It implies that the supremum is a maximum.

From the previous definition, the Frobenius norm can also be obtained by rearranging the square of the norm in the following way:

$$\|\mathbf{A}\|_F^2 = \sum_{i=1}^n \sum_{j=1}^m |a_{ij}|^2 = (\mathbf{A}^T \mathbf{A}) = (\mathbf{A} \mathbf{A}^T)$$

Where we used the following property of traces: $(\mathbf{ABC}) = (\mathbf{CAB}) = (\mathbf{BCA})$

Property 62. Let $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{x} \in \mathbb{R}^n$ and let $\mathbf{P} \in \mathbb{R}^{m \times m}$, $\mathbf{Q} \in \mathbb{R}^{n \times n}$ be two orthogonal matrices. Then, the following holds:

- Matrix norms induced by vector norms: $\|\mathbf{Ax}\|_p \leq \|\mathbf{A}\|_p \|\mathbf{x}\|_p$
- Orthogonal matrices preserve the Frobenius norm: $\|\mathbf{PAQ}\|_F = \|\mathbf{A}\|_F$
- Orthogonal matrices preserve the 2-norm: $\|\mathbf{PAQ}\|_2 = \|\mathbf{A}\|_2$

In particular, the last two points implies that any matrix has the same 2-norm and Frobenius norm as the diagonal rectangular matrix Σ from its SVD.

Proof. (1)

$$\begin{aligned} \|\mathbf{A}\|_p &= \sup_{\mathbf{x}} \frac{\|\mathbf{Ax}\|_p}{\|\mathbf{x}\|_p} \\ &\geq \frac{\|\mathbf{Ay}\|_p}{\|\mathbf{y}\|_p} \\ &\Rightarrow \|\mathbf{A}\|_p \|\mathbf{y}\|_p \geq \|\mathbf{Ay}\|_p \forall \mathbf{y} \end{aligned}$$

(2) $\|\mathbf{PAQ}\|_F = (\mathbf{Q}^T \mathbf{A}^T \mathbf{P}^T \mathbf{PAQ}) = (\mathbf{Q}^T \mathbf{A}^T \mathbf{AQ}) = (\mathbf{QQ}^T \mathbf{A}^T \mathbf{A}) = (\mathbf{A}^T \mathbf{A}) = \|\mathbf{A}\|_F$, where we used the fact that $\mathbf{QQ}^T = \mathbf{I}_n$ since \mathbf{Q} is a square orthogonal matrix.

(3)

$$\begin{aligned} \|\mathbf{PAQ}\|_2 &= \sup_{\mathbf{x}, \|\mathbf{x}\|_2=1} \|\mathbf{PAQx}\|_2 \\ &= \sup_{\mathbf{x}, \|\mathbf{x}\|_2=1} (\mathbf{x}^T \mathbf{Q}^T \mathbf{A}^T \mathbf{P}^T \mathbf{PAQx})^{\frac{1}{2}} \\ &= \|\mathbf{AQ}\|_2 & (\mathbf{P}^T \mathbf{P} = \mathbf{I}_m) \\ &= \sup_{\mathbf{x}: \|\mathbf{x}\|_2=1} \|\mathbf{AQx}\|_2 \\ &= \sup_{\mathbf{y}: \|\mathbf{y}\|_2=1} \|\mathbf{Ay}\|_2 & (\|\mathbf{Qx}\|_2 = (\mathbf{x}^T \mathbf{Q}^T \mathbf{Qx})^{1/2} = (\mathbf{x}^T \mathbf{x})^{1/2} = \|\mathbf{x}\|_2) \\ &= \|\mathbf{A}\|_2 \end{aligned}$$

□

Property 63. For any $\mathbf{A} \in \mathbb{R}^{m \times n}$, we have $\|\mathbf{A}\|_2 = \sigma_1$, where σ_1 is the largest singular value of \mathbf{A} .

Proof. Let $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ be the SVD of \mathbf{A} with the singular values in decreasing order.

$$\begin{aligned} \|\mathbf{A}\|_2 &= \|\Sigma\|_2 & (\text{by the last point of Property 62}) \\ &= \max_{\|\mathbf{x}\|=1} \|\Sigma\mathbf{x}\|_2 & (\text{definition of the 2-norm}) \end{aligned}$$

Since for any real unit vector $\mathbf{x} = [x_1, \dots, x_n]^\top$ we have,

$$\begin{aligned}
 \|\Sigma \mathbf{x}\|_2 &= \left\| \begin{bmatrix} \sigma_1 x_1 & \cdots & \sigma_r x_r & 0 & \cdots & 0 \end{bmatrix}^\top \right\|_2 && \text{(with } r \text{ the rank of } \mathbf{A}) \\
 &= \left(\sum_{i=1}^r (\sigma_i x_i)^2 \right)^{\frac{1}{2}} \\
 &\leq \left(\sum_{i=1}^r (\sigma_1 x_i)^2 \right)^{\frac{1}{2}} && \text{(since } \sigma_1 \text{ is the largest singular value)} \\
 &= \sigma_1 \left(\sum_{i=1}^r x_i^2 \right)^{\frac{1}{2}} \\
 &\leq \sigma_1 \left(\sum_{i=1}^n x_i^2 \right)^{\frac{1}{2}} \\
 &= \sigma_1 && \text{(since } \mathbf{x} \text{ has norm 1)}
 \end{aligned}$$

Taking $\mathbf{x} = [1 \ 0 \ \cdots \ 0]$ gives exactly σ_1 , therefore it is the maximum.

□

13 Low Rank Approximation

Low rank approximation is a minimization problem with a cost function that measures the difference between a given matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and an approximating matrix with reduced rank. This minimization problem has an analytical solution in terms of the singular value decomposition.

Theorem 64 (Eckart-Young-Mirsky). *Let $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ be the SVD of \mathbf{A} , where*

- $\sigma_i \in \mathbb{R}, \mathbf{u}_i \in \mathbb{R}^m, \mathbf{v}_i \in \mathbb{R}^n$
- $r = \text{rank}(\mathbf{A})$ and $\sigma_1 > \sigma_2 > \dots > \sigma_r > 0$ are the singular values of \mathbf{A}
- $\mathbf{U} \in \mathbb{R}^{m \times m}, \mathbf{V} \in \mathbb{R}^{n \times n}$ are orthogonal matrices.

Now, let $\mathbf{A}_k = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, where only the first k terms are kept from the sum defining \mathbf{A} . Then

$$\min_{\mathbf{X} \text{ s.t. } \text{rank}(\mathbf{X}) \leq k} \|\mathbf{A} - \mathbf{X}\|_F = \|\mathbf{A} - \mathbf{A}_k\|_F$$

Note that this is a convex optimization problem over a non convex set. Also, the same result holds for the 2-norm:

$$\min_{\mathbf{X} \text{ s.t. } \text{rank}(\mathbf{X}) \leq k} \|\mathbf{A} - \mathbf{X}\|_2 = \|\mathbf{A} - \mathbf{A}_k\|_2$$

Proof. We show the result for the 2-norm. We start by showing that $\|\mathbf{A}\|_2 = \sigma_{k+1}$. Let $\mathbf{\Sigma}_k$ be the diagonal matrix with diagonal entries $0, \dots, 0, \sigma_{k+1}, \dots, \sigma_r, 0, \dots, 0$.

$$\mathbf{\Sigma}_k = \begin{bmatrix} 0 & & & & & & & \\ & \ddots & & & & & & \\ & & 0 & & & & & \\ & & & \sigma_{k+1} & & & & \\ & & & & \ddots & & & \\ & & & & & \sigma_r & & \\ & & & & & & 0 & \\ & & & & & & & \ddots \\ & & & & & & & & 0 \end{bmatrix}$$

We have

$$\begin{aligned} \|\mathbf{A} - \mathbf{A}_k\|_2 &= \left\| \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T - \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right\|_2 && \text{(Definition of } \mathbf{A}_k) \\ &= \left\| \sum_{i=k+1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right\|_2 \\ &= \|\mathbf{U} \mathbf{\Sigma}_k \mathbf{V}^T\|_2 && \text{(Definition of } \mathbf{\Sigma}_k) \\ &= \|\mathbf{\Sigma}_k\|_2 && \text{(By Property 4, since } \mathbf{U} \text{ and } \mathbf{V} \text{ are orthogonal)} \\ &= \sigma_{k+1} && \text{(By Property 5)} \end{aligned}$$

We want to show that for any matrix $\mathbf{B} = \mathbf{X}\mathbf{Y}$, where $r = \text{rank}(\mathbf{B})$, $\mathbf{X} \in \mathbb{R}^{m \times r}$, $\mathbf{Y} \in \mathbb{R}^{r \times n}$, \mathbf{A}_k will always be closer to \mathbf{A} than \mathbf{B} with respect to the matrix 2-norm.

$$\|\mathbf{A} - \mathbf{B}\|_2 \geq \|\mathbf{A} - \mathbf{A}_k\|_2 \quad \text{(Statement to prove)}$$

Let $\mathbf{V}_{k+1} = \begin{bmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_{k+1} \\ | & & | \end{bmatrix}$, Where $\mathbf{v}_1, \dots, \mathbf{v}_{k+1}$ are the eigenvectors associated with the top $k+1$ singular values.

By the Rank-Nullity Theorem:

$$\dim \mathcal{N}(\mathbf{B}) = n - \text{rank}(\mathbf{B})$$

hence,

$$\dim \mathcal{N}(\mathbf{B}) + \dim \mathcal{R}(\mathbf{V}_{k+1}) > n$$

Which implies that $\mathcal{N}(\mathbf{B}) \cap \mathcal{R}(\mathbf{V}_{k+1}) \neq \{\mathbf{0}\}$. Then, by taking a unit vector $\mathbf{x} \in \mathcal{N}(\mathbf{B}) \cap \mathcal{R}(\mathbf{V}_{k+1})$, we have:

$$\begin{aligned}
\|\mathbf{A} - \mathbf{B}\|_2^2 &\geq \|(\mathbf{A} - \mathbf{B})\mathbf{x}\|_2^2 \\
&= \|\mathbf{A}\mathbf{x}\|_2^2 && \text{(Since } \mathbf{x} \text{ is in } \mathcal{N}(\mathbf{B}), \text{ then } \mathbf{B}\mathbf{x} = \mathbf{0}) \\
&= \|\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T\mathbf{x}\|_2^2 && \text{(SVD of } \mathbf{A}.) \\
&= \|\mathbf{\Sigma}\mathbf{V}^T\mathbf{x}\|_2^2 && \text{(By Property 4, since } \mathbf{U} \text{ is orthogonal)} \\
&= \sum_{i=1}^r \sigma_i^2 \langle \mathbf{v}_i, \mathbf{x} \rangle^2 \\
&= \sum_{i=k+1}^r \sigma_i^2 \langle \mathbf{v}_i, \mathbf{x} \rangle^2 && (\langle \mathbf{v}_i, \mathbf{x} \rangle = 0 \text{ for } i \leq k \text{ since } \mathbf{x} \in \mathcal{R}(\mathbf{V}_{k+1})) \\
&\geq \sigma_{k+1}^2 \sum_{i=k+1}^r \langle \mathbf{v}_i, \mathbf{x} \rangle^2 && (\sigma_{k+1} \text{ is the largest singular value of } \mathbf{\Sigma}_k) \\
&= \sigma_{k+1}^2 \|\mathbf{V}_{k+1}^T \mathbf{x}\|_2^2 && \text{(Definition of 2-norm)} \\
&= \sigma_{k+1}^2 \|\mathbf{V}^T \mathbf{x}\|_2^2 && (\mathbf{V}_{k+1}^T \mathbf{x} = \mathbf{V}^T \mathbf{x} \text{ because } \mathbf{x} \in \mathcal{R}(\mathbf{V}_{k+1})) \\
&= \sigma_{k+1}^2 \|\mathbf{x}\|_2^2 && \text{(By Property 4, since } \mathbf{V} \text{ is orthogonal)} \\
&= \sigma_{k+1}^2 && (\mathbf{x} \text{ is of unit length)} \\
&= \|\mathbf{A} - \mathbf{A}_k\|_2^2 && \text{(As shown in the first part of the proof)}
\end{aligned}$$

By taking the square root on each side of the inequality, we obtain that for any matrix $\mathbf{B} = \mathbf{X}\mathbf{Y}$:

$$\|\mathbf{A} - \mathbf{B}\|_2 \geq \|\mathbf{A} - \mathbf{A}_k\|_2$$

We now show the result for Frobenius norm. The proof relies on the following inequality, known as Weyl's inequality!(we let the proof of this inequality as an exercise):

$$\sigma_{i+j-1}(\mathbf{X} + \mathbf{Y}) \leq \sigma_i(\mathbf{X}) + \sigma_j(\mathbf{Y}).$$

Let $\mathbf{A}_k = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ be the matrix obtained from the truncated SVD of the matrix \mathbf{A} . We want to show that \mathbf{A}_k is the rank k matrix which is the closest to \mathbf{A} in Frobenius norm. Let \mathbf{B} be any rank k matrix, we want to show that

$$\|\mathbf{A} - \mathbf{A}_k\|_F \leq \|\mathbf{A} - \mathbf{B}\|_F.$$

Applying Weyl's inequality to $\mathbf{X} = \mathbf{A} - \mathbf{B}$ and $\mathbf{Y} = \mathbf{B}$ we get

$$\sigma_{i+k}(\mathbf{A}) \leq \sigma_i(\mathbf{A} - \mathbf{B}) + \sigma_{k+1}(\mathbf{B})$$

and since \mathbf{B} is of rank k we have $\sigma_{k+1}(\mathbf{B}) = 0$, hence

$$\sigma_{i+k}(\mathbf{A}) \leq \sigma_i(\mathbf{A} - \mathbf{B}).$$

Using this inequality we obtain

$$\begin{aligned}
 \|\mathbf{A} - \mathbf{A}_k\|_F &= \sum_{i=k+1}^r \sigma_i(\mathbf{A})^2 \\
 &= \sum_{i=1}^{r-k} \sigma_{i+k}(\mathbf{A})^2 \\
 &\leq \sum_{i=1}^{r-k} \sigma_i(\mathbf{A} - \mathbf{B})^2 \\
 &\leq \sum_{i=1}^{\min(m,n)} \sigma_i(\mathbf{A} - \mathbf{B})^2 \\
 &= \|\mathbf{A} - \mathbf{B}\|_F.
 \end{aligned}$$

□

14 Variational Characterization of Eigenvalues of Symmetric Matrices

Definition 65 (Rayleigh Quotient). Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be symmetric, then the Rayleigh Quotient is the ratio

$$\frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

The quotient is independent of the scale of \mathbf{x} since the denominator is the squared norm of \mathbf{x} .

Theorem 66 (Rayleigh-Ritz). Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be symmetric. The solution to maximizing (resp. minimizing) the Rayleigh-Ritz Quotient for $\mathbf{x} \neq \mathbf{0}$ is given by the largest (resp. smallest) eigenvalue of \mathbf{A} :

$$\max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \max_{\|\mathbf{x}\|_2=1} \mathbf{x}^T \mathbf{A} \mathbf{x} = \lambda_{\max}(\mathbf{A}) \quad (28)$$

$$\min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\|\mathbf{x}\|_2=1} \mathbf{x}^T \mathbf{A} \mathbf{x} = \lambda_{\min}(\mathbf{A}) \quad (29)$$

Moreover, if $\mathbf{v}_1, \dots, \mathbf{v}_k$ are the eigenvectors corresponding to the top k eigenvalues $\lambda_1, \dots, \lambda_k$ of \mathbf{A} , then

$$\max_{\substack{\|\mathbf{x}\|_2=1 \\ \mathbf{x} \in \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)^\perp}} \mathbf{x}^T \mathbf{A} \mathbf{x} = \lambda_{k+1}(\mathbf{A}) \quad (30)$$

where the maximum is obtained by letting $\mathbf{x} = \mathbf{v}_{k+1}$. The constraint $\mathbf{x} \in \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)^\perp$ means that \mathbf{x} must be orthogonal to the first k eigenvectors of \mathbf{A} . Since \mathbf{A} is assumed to be symmetric, all its eigenvectors are orthogonal.

Proof. (1) Let $\mathbf{A} = \mathbf{V} \mathbf{D} \mathbf{V}^T$ be the eigendecomposition of \mathbf{A} , where $\mathbf{v}_1, \dots, \mathbf{v}_n$ are the eigenvectors of \mathbf{A} and \mathbf{V} is an orthogonal matrix constructed as:

$$\mathbf{V} = \begin{bmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_n \\ | & & | \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Let $\mathbf{x} \in \mathbb{R}^n$ be of unit norm ($\|\mathbf{x}\|_2 = 1$) and let \mathbf{y} be a linear combination of the eigenbasis of \mathbf{A} , such that $\mathbf{y} = \mathbf{V}^T \mathbf{x} \in \mathbb{R}^n$. By **Property 5**, since \mathbf{V} is orthogonal, $\|\mathbf{y}\|_2 = \|\mathbf{x}\|_2 = 1$. Then we can derive the following inequality:

$$\begin{aligned} \mathbf{x}^T \mathbf{A} \mathbf{x} &= \mathbf{x}^T \mathbf{V} \mathbf{D} \mathbf{V}^T \mathbf{x} && \text{(Eigendecomposition of } \mathbf{A} \text{)} \\ &= \mathbf{y}^T \mathbf{D} \mathbf{y} && \text{(Definition of } \mathbf{y} \text{)} \\ &= \sum_{i=1}^n \lambda_i \mathbf{y}_i^2 && \text{(Where } \lambda_i \text{ are the diagonal elements of } \mathbf{D} \text{)} \\ &\leq \lambda_{\max}(\mathbf{A}) \sum_{i=1}^n \mathbf{y}_i^2 && (\lambda_{\max}(\mathbf{A}) \geq \lambda_i \forall i) \\ &= \lambda_{\max}(\mathbf{A}) \|\mathbf{y}\|_2^2 \\ &= \lambda_{\max}(\mathbf{A}) \end{aligned}$$

□

Proof. (2) We are using the same matrices \mathbf{A} and \mathbf{V} , vector \mathbf{x} and \mathbf{y} as in (1). Then, we can derive the following inequality:

$$\begin{aligned}
 \mathbf{x}^T \mathbf{A} \mathbf{x} &= \mathbf{x}^T \mathbf{V} \mathbf{D} \mathbf{V}^T \mathbf{x} && \text{(Eigendecomposition of } \mathbf{A} \text{)} \\
 &= \mathbf{y}^T \mathbf{D} \mathbf{y} && \text{(Definition of } \mathbf{y} \text{)} \\
 &= \sum_{i=1}^n \lambda_i \mathbf{y}_i^2 && \text{(Where } \lambda_i \text{ are the diagonal elements of } \mathbf{D} \text{)} \\
 &\geq \lambda_{\min}(\mathbf{A}) \sum_{i=1}^n \mathbf{y}_i^2 && (\lambda_{\min}(\mathbf{A}) \leq \lambda_i \forall i) \\
 &= \lambda_{\min}(\mathbf{A}) \|\mathbf{y}\|_2^2 \\
 &= \lambda_{\min}(\mathbf{A})
 \end{aligned}$$

□

Proof. (3) We will split the matrix \mathbf{V} in two partitions such that $\mathbf{V} = [\mathbf{V}_1 \quad \mathbf{V}_2]$, where $\mathbf{V}_1 \in \mathbb{R}^{n \times k}$ represents the top k eigenvectors of \mathbf{A} and $\mathbf{V}_2 \in \mathbb{R}^{n \times n-k}$ represents the last $n - k$ eigenvectors of \mathbf{A} . If $\mathbf{x} \in \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)^\perp$, then \mathbf{x} is orthogonal to all vectors in \mathbf{V}_1 and, most importantly, \mathbf{x} is in the range of \mathbf{V}_2 ($\mathbf{x} \in \mathcal{R}(\mathbf{V}_2)$). Then, we can write

$$\begin{aligned}
 \mathbf{x}^T \mathbf{A} \mathbf{x} &= \mathbf{x}^T \mathbf{V}_2 \mathbf{V}_2^T \mathbf{A} \mathbf{V}_2 \mathbf{V}_2^T \mathbf{x} && \text{(Replace each } \mathbf{x} \text{ by its projection onto } \mathcal{R}(\mathbf{V}_2), \text{ which} \\
 &&& \text{does not change } \mathbf{x} \text{ since it is initially assumed that } \mathbf{x} \in \mathcal{R}(\mathbf{V}_2) \text{)} \\
 &= \mathbf{x}^T \mathbf{V}_2 \mathbf{V}_2^T \mathbf{V} \mathbf{D} \mathbf{V}^T \mathbf{V}_2 \mathbf{V}_2^T \mathbf{x} && \text{(Eigendecomposition of } \mathbf{A} \text{)}
 \end{aligned} \tag{31}$$

Now, using the fact that

$$\mathbf{V}_2^T \mathbf{V} = \mathbf{V}_2^T [\mathbf{V}_1 \quad \mathbf{V}_2] = [\mathbf{V}_2^T \mathbf{V}_1 \quad \mathbf{V}_2^T \mathbf{V}_2] = [\mathbf{0} \quad \mathbf{I}]$$

it follows that

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{V} \underbrace{\begin{bmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \lambda_{k+1} & & \\ & & & & \ddots & \\ & & & & & \lambda_n \end{bmatrix}}_{\tilde{\mathbf{A}}} \mathbf{V}^T \mathbf{x}$$

Hence,

$$\max_{\substack{\|\mathbf{x}\|_2=1 \\ \mathbf{x} \in \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)^\perp}} \mathbf{x}^T \mathbf{A} \mathbf{x} = \max_{\|\mathbf{x}\|_2=1} \mathbf{x}^T \tilde{\mathbf{A}} \mathbf{x} \quad \text{(The constraint } \mathbf{x} \in \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)^\perp \text{ is now incorporated into the } \tilde{\mathbf{A}} \text{).}$$

We now have the same maximization problem as in (1),

except that $\tilde{\mathbf{A}}$ replaces \mathbf{A}

$$= \lambda_{k+1}(\mathbf{A}) \quad \text{(By (1), since the largest eigenvalue of } \tilde{\mathbf{A}} \text{ is } \lambda_{k+1})$$

□

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