

10/22/2019

Lecture 17

Announcements: • next 2 lectures will be given by Janiv Plan

- OH on Thursday are canceled.
- midterm homework has been graded yet (Goodman).

Recap: Orthogonality: $v \perp w \Leftrightarrow \langle v, w \rangle = 0$

Orthogonal complement of a subspace $U \subseteq W$ is

$$U^\perp = \{w \in W : w \perp u \text{ for all } u \in U\}.$$

Note: U^\perp is a subspace!

$$\boxed{(U^\perp)^\perp = U}.$$

e.g. $U = \text{span}\{e_1, e_2\} \subseteq \mathbb{R}^3$, then $U^\perp = \text{span}\{e_3\}$.

Orthogonality relations for $\mathcal{R}(A)$, $\mathcal{N}(A)$, $\mathcal{R}(A^T)$, $\mathcal{N}(A^T)$

$$(1). \quad \mathcal{N}(A) = (\mathcal{R}(A^T))^\perp$$

$$(2). \quad \mathcal{N}(A^T) = (\mathcal{R}(A))^\perp.$$

Note that (2) follows from (1) by replacing A with A^T .

Proof of (1): We will show that

$$\begin{aligned} \text{(a)} \quad & [\mathcal{R}(A^T)]^\perp \subseteq \mathcal{N}(A), \text{ and} \\ \text{(b)} \quad & \mathcal{N}(A) \subseteq [\mathcal{R}(A^T)]^\perp. \end{aligned} \quad \left. \vphantom{\begin{aligned} \text{(a)} \\ \text{(b)} \end{aligned}} \right\} \begin{array}{l} \text{Then it follows} \\ \text{they are} \\ \text{equal!} \end{array}$$

Let's show (a): let $y \in [\mathcal{R}(A^T)]^\perp$ be arbitrary.

Then, $y \perp \mathcal{R}(A^T)$. Recall $\mathcal{R}(A^T) = \{A^T x : x \in \mathbb{R}^m\}$.

$$\Leftrightarrow \langle y, A^T x \rangle = 0 \quad \forall x$$

$$\Leftrightarrow \underbrace{y^T A^T}_{(Ay)^T} x = 0 \quad \forall x$$

$$\Leftrightarrow \langle Ay, x \rangle = 0 \quad \forall x$$

Since this holds $\forall x$, it should also hold for $x = Ay$.

$$\Rightarrow \langle Ay, Ay \rangle = 0 \quad \Leftrightarrow \|Ay\|_2^2 = 0 \quad \Leftrightarrow Ay = 0 \\ \Leftrightarrow y \in \mathcal{N}(A).$$

$$\Rightarrow \boxed{[\mathcal{R}(A^T)]^\perp \subseteq \mathcal{N}(A)}$$

Let's show (b): let $x \in \mathcal{N}(A)$ be arbitrary.

$$\text{Then, } Ax = \vec{0}$$

$$\Rightarrow \langle y, Ax \rangle = 0 \quad \forall y$$

$$\Leftrightarrow \langle \underbrace{A^T y}_{\substack{\downarrow \\ \text{any vector in } \mathcal{R}(A^T)}}, x \rangle = 0 \quad \forall y$$

$$\Leftrightarrow x \perp \mathcal{R}(A^T)$$

$$\Leftrightarrow x \in [\mathcal{R}(A^T)]^\perp$$

$$\text{So, } \boxed{\mathcal{N}(A) \subseteq [\mathcal{R}(A^T)]^\perp}$$

$$\text{(a) + (b)} \Rightarrow \mathcal{N}(A) = [\mathcal{R}(A^T)]^\perp$$

An immediate use

Q: Let $A = \begin{bmatrix} 1 & 2 & 1 & 1 \\ 1 & 3 & 0 & 1 \\ 2 & 5 & 1 & 2 \end{bmatrix}$.

Does there exist x st. $Ax = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$?

Typical way of solving:

$$\left[A \mid \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \right] \rightsquigarrow \text{Gaussian elimination}$$

Rephrase question: Is $\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$ in $\mathcal{R}(A)$?

Equivalently, Is $\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$ in $\underbrace{\mathcal{N}(A^T)}_{=\mathcal{R}(A)}^\perp$?

Equivalently, Is $\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \perp \mathcal{N}(A^T)$?

Let's find a basis for $\mathcal{N}(A^T)$.

$$\text{rref}(A^T) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\begin{aligned} x_3 &= s \\ x_1 &= -s \\ x_2 &= -s \end{aligned}$$

$$\mathcal{N}(A^T) = \text{span} \left\{ \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} \right\}$$

So, we check if $\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \perp \mathcal{N}(A^T)$:

$$\left\langle \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}, \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} \right\rangle = 0 \quad \checkmark$$

yes.

$\Rightarrow \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \in \mathcal{R}(A) \Rightarrow Ax = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$ has a solution!

What's the point? Say we ask the same question for

10,000 different right-hand side vectors $b_1, b_2, \dots, b_{10,000}$.

Which of the systems $Ax = b_j$, $j=1, 2, \dots, 10,000$ has a solution?

Exercise: solve 10,000 linear systems and check each case $[A | b_j] \rightsquigarrow$ -

q: compute $\langle b_j, [-1] \rangle$, $j=1, \dots, 10000$ and check if it is 0!

The formula for a chemical reaction system (II.2.9).

Chemical system: a collection of molecules ("species"), e.g.,



is a chemical system.

Components of a chemical system:

Atoms. In our example: C, H, S.

The "formula matrix" of a chemical system

$$\begin{array}{c} \text{C} \\ \text{H} \\ \text{S} \end{array} \begin{bmatrix} \text{CH}_4 & \text{S}_2 & \text{CS}_2 & \text{H}_2\text{S} \\ 1 & 0 & 1 & 0 \\ 4 & 0 & 0 & 2 \\ 0 & 1 & 2 & 1 \end{bmatrix} =: A$$

Now, suppose we have a sample

n_1 moles of CH_4

n_2 moles of S_2

n_3 moles of CS_2

n_4 moles of H_2S

$$\vec{n} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{bmatrix}$$

$$\# \text{C atoms: } n_1 \cdot 1 + n_2 \cdot 0 + n_3 \cdot 1 + n_4 \cdot 0 =: b_1$$

$$\# \text{H atoms: } n_1 \cdot 4 + n_2 \cdot 0 + n_3 \cdot 0 + n_4 \cdot 2 =: b_2$$

$$\# \text{S atoms: } n_1 \cdot 0 + n_2 \cdot 1 + n_3 \cdot 2 + n_4 \cdot 1 =: b_3$$

In matrix form:

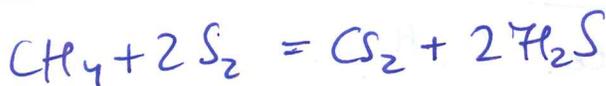
$$A \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

↑ "species abundance vector"
↑ "element abundance vector"

Remark: $b = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \in \mathcal{R}(A)$.

However, not all vectors in $\mathcal{R}(A)$ can be element abundance vectors = $\{Ax : x_j \geq 0\}$.

Chemical reactions: For example,



$$\underbrace{\begin{bmatrix} 1 \\ 4 \\ 0 \end{bmatrix}}_{\text{LHS}} + 2 \underbrace{\begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}}_{\text{RHS}} = \underbrace{\begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}}_{\text{RHS}} + 2 \underbrace{\begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}}_{\text{RHS}}$$

$$\text{LHS} = A \underbrace{\begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}}_x; \quad \text{RHS} = A \underbrace{\begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}}_y$$

That is, $Ax = Ay \Leftrightarrow A(x-y) = \vec{0} \Leftrightarrow x-y \in \mathcal{N}(A)$

Fact: Every chemical reaction in a system with formula matrix A corresponds to a vector in $\mathcal{N}(A)$. This gives a way of describing all possible chemical reactions in a system: find a basis for $\mathcal{N}(A)$.

Example: Consider our system above.

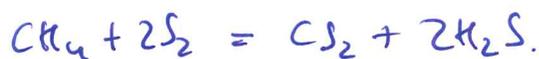
$$A = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 4 & 0 & 0 & 2 \\ 0 & 1 & 2 & 1 \end{bmatrix}, \quad \text{ref}(A) = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & -1/2 \\ 0 & 0 & 1 & -1/2 \end{bmatrix}$$

$$\Rightarrow \mathcal{N}(A) = \text{span} \left\{ \begin{bmatrix} -1/2 \\ -1 \\ 1/2 \\ 1 \end{bmatrix} \right\}.$$

Instead of $\begin{bmatrix} -1/2 \\ -1 \\ 1/2 \\ 1 \end{bmatrix}$, let's use $\begin{bmatrix} -1 \\ -2 \\ 1 \\ 2 \end{bmatrix}$ as the basis for $\mathcal{N}(A)$.

$$A \begin{bmatrix} -1 \\ -2 \\ 1 \\ 2 \end{bmatrix} = A \left(\begin{bmatrix} -1 \\ -2 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \\ 2 \end{bmatrix} \right) = \vec{0}$$

$$\Leftrightarrow A \begin{bmatrix} 1 \\ 2 \\ 0 \\ 0 \end{bmatrix} = A \begin{bmatrix} 0 \\ 0 \\ 1 \\ 2 \end{bmatrix}.$$



Example: Consider a chemical system with $\text{CH}_4, \text{S}_2, \text{CS}_2, \text{H}_2\text{S}$ and H_2 .

Find all chemical reactions within this system.

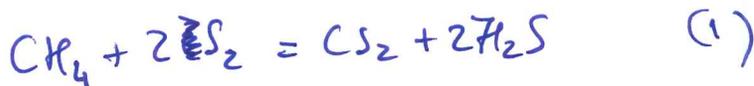
Sol: Formula matrix

$$B = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 4 & 0 & 0 & 2 & 2 \\ 0 & 2 & 2 & 1 & 0 \end{bmatrix}$$

$\uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow$
 $\text{CH}_4 \quad \text{S}_2 \quad \text{CS}_2 \quad \text{H}_2\text{S} \quad \text{H}_2$

$$\Rightarrow \mathcal{N}(B) = \text{span} \left\{ \underbrace{\begin{bmatrix} -1 \\ -2 \\ 1 \\ 2 \\ 0 \end{bmatrix}}_{v_1}, \underbrace{\begin{bmatrix} -1 \\ -1 \\ 1 \\ 0 \\ 2 \end{bmatrix}}_{v_2} \right\}.$$

Chemical reaction corresponding to v_1 :



Note: all other chemical reactions are linear combinations of (1) and (2).