10/22/2019 Lecture 17

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

• OH on Thursday are canceled.

• midterm hasn't been graded yet (Crowdmark).

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

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

$$U^\perp = \{ w \in W : w \perp u \ \forall u \in U \}.$$

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

$$\boxed{\begin{aligned} &(1). \quad \mathcal{N}(A) = (\mathcal{R}(A^T))^\perp \\ &(2). \quad \mathcal{N}(A^T) = (\mathcal{R}(A))^\perp. \end{aligned}}$$

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

Proof of (1): We will show that

(a). $[\mathcal{R}(A^T)]^\perp \subseteq \mathcal{N}(A)$, and

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

} Then it follows they are equal!.

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 $x = Ay$.

$$\Rightarrow \langle Ay, Ay \rangle = 0 \Leftrightarrow \|Ay\|_2^2 = 0 \Leftrightarrow Ay = 0$$

$$\Leftrightarrow y \in \mathcal{N}(A).$$

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

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

Then, $Ax = \vec{0}$

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

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

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

$\Leftrightarrow x \in [\mathcal{R}(A^T)]^\perp$. So, $\boxed{\mathcal{N}(A) \subseteq [\mathcal{R}(A^T)]^\perp}$

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

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 s.t. $Ax = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$?

Typical way of solving:

$$\left[\begin{array}{c:c} A & \begin{matrix} 2 \\ 1 \\ 3 \end{matrix} \end{array}\right] \rightsquigarrow \text{Gaussian elimination}$$

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

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

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

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

$$\text{rref}(A^T) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \begin{matrix} x_3 = s \\ x_1 = -s \\ x_2 = -s \end{matrix} \qquad \mathcal{N}(A^T) = \text{span}\left\{\begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix}\right\}.$$

So, we check if $\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \perp \mathcal{N}(A^T)$: $\left\langle \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}, \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} \right\rangle = 0$ ✓ 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 $b_1, b_2, \ldots, b_{10{,}000}$. Which of the systems $Ax = b_j$, $j = 1, 2, \ldots, 10{,}000$ [illegible] a solution?

Either: solve 10,000 linear systems and check each case $[A \mid b_j] \rightsquigarrow \dots$

or: compute $\left\langle b_j, \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} \right\rangle$, $j = 1, \dots, 10000$

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.,

CH_4, S_2, CS_2, H_2S

is a chemical system.

Components of a chemical system:

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

The "formula matrix" of a chemical system

$$\begin{array}{c} \\ C \\ H \\ S \end{array} \begin{array}{c} \begin{array}{cccc} CH_4 & S_2 & CS_2 & H_2S \end{array} \\ \begin{bmatrix} 1 & 0 & 1 & 0 \\ 4 & 0 & 0 & 2 \\ 0 & 1 & 2 & 1 \end{bmatrix} \end{array} =: A$$

Now, suppose we have a sample

n_1 moles of CH_4

n_2 moles of S_2 $\rightsquigarrow \vec{n} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{bmatrix}$.

n_3 moles of CS_2

n_4 moles of H_2S

C atoms: $n_1 \cdot 1 + n_2 \cdot 0 + n_3 \cdot 1 + n_4 \cdot 0 =: b_1$

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

S atoms: $n_1 \cdot 0 + n_2 \cdot 1 + n_3 \cdot 2 + n_4 \cdot 1 =: b_3$.

In matrix form:

$$A \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}.$$

"species abundance vector". "element abundance vector"

<u>Remark</u>: $b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \in \mathcal{R}(A)$.

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

<u>Chemical reactions</u>: For example,

$$CH_4 + 2S_2 = CS_2 + 2H_2S$$

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

$$LHS = A\underbrace{\begin{bmatrix} 1 \\ 2 \\ 0 \\ 0 \end{bmatrix}}_{x}; \quad RHS = A\underbrace{\begin{bmatrix} 0 \\ 0 \\ 1 \\ 2 \end{bmatrix}}_{y}$$

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

<u>Fact</u>: 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 $\mathcal{N}(A)$

<u>Example</u>: Consider our system above

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

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

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 $\mathcal{N}(A)$.

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

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

$$CH_4 + 2S_2 = CS_2 + 2H_2S.$$

<u>Example</u>: Consider a chemical system with CH_2, S_2, CS_2, H_2S and H_2.

Find all chemical reactions within this system.

<u>Sol</u>: Formula matrix

$$B = \begin{array}{c} \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 4 & 0 & 0 & 2 & 2 \\ 0 & 2 & 2 & 1 & 0 \end{bmatrix} \\ \begin{array}{ccccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ CH_4 & S_2 & CS_2 & H_2S & H_2 \end{array} \end{array}$$

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

Chemical reaction corresponding to v_1:

$$CH_4 + 2S_2 = CS_2 + 2H_2S \qquad (1)$$

v_2:

$$CH_4 + S_2 = CS_2 + 2H_2 \qquad (2)$$

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