Last time: The formula for chemical systems

1) A collection of molecules is a chemical system: \( \text{CH}_4, \text{S}_2, \text{CS}_2, \text{H}_2\text{S} \)

2) The components of a chemical systems are the atoms making up the molecules in the chemical system: C, H, S for the above chem. system

3) The formula matrix for the system above is

\[
\begin{bmatrix}
1 & 0 & 1 & 0 \\
4 & 0 & 0 & 2 \\
0 & 2 & 2 & 1
\end{bmatrix} = A
\]

\( \text{CH}_4, \text{S}_2, \text{CS}_2, \text{H}_2\text{S} \)

4) Let's assume in our system we have \( n_1 \) moles of CH\(_4\), \( n_2 \) moles of S\(_2\), \( n_3 \) moles of CS\(_2\), and \( n_4 \) moles of H\(_2\)S

\[
\mathbf{n} = \begin{bmatrix}
n_1 \\
n_2 \\
n_3 \\
n_4
\end{bmatrix}
\]

is the so called "species abundance vector".

5) The "elements abundance vector" is the vector \( \mathbf{b} = A\mathbf{n} \)

6) The set of all element abundances vectors is \( \{ A\mathbf{x} : x_j \geq 0 \} \)

7) If \( A \) is a formula matrix for a chem. system, then every possible chem. reaction in the system corresponds to a vector in \( \text{W}(A) \).

In order to get all possible reactions do the following steps:

1. Find a basis for \( \text{W}(A) \) and scale the basis vector such that they have integer-valued entries

2. Split the basis vector(s) into a sum of two vectors, where the first one has the positive entries of the basis vector in it and the second consists of the negative entries.

3. Read of the corresponding chem. reaction from the formula matrix.
Last time continued:

1) We get additional informations on the chemical system from the non-zero vectors of $W(\lambda)$.

2) Let $A$ be a formula matrix for a chem. system and $n$ a species abundance vector such that $An = b$. Then $bc_{\lambda}A = [W(\lambda)]^t$.

Thus any element abundance vector $b$ is orthogonal to the basis vectors of $W(\lambda)$.

In other words, the basis vectors of $W(\lambda)$ give us information on the molar amounts of the atoms present in our chem. systems. For chemical reactions to happen you need to have the right amount of atoms present. (preserved ratio)
Orthogonality (Projections onto lines and planes in $\mathbb{R}^3$)

Suppose $v \in \mathbb{R}^3$ and $L$ is the line spanned by $v$.

Def.: The projection of a vector $x$ onto $L = \text{span}(v)$ is the vector in $L$ that is closest to $x$. We denote this vector by $P_x v$ or just $P_x$ if it is clear from the context onto which vector we are projecting.

Q.: How to find $P_x v$?
Answer:

(i) \( \text{If } x \in \text{span}\{u\}, \text{ then } P_u x = s u \) for some \( s \in \mathbb{R} \).

(ii) Need to find the correct \( s \). From the definition we know that \( s \) minimizes the distance between \( x \) and \( P_u x \).

The square distance between \( x \) and \( P_u x \) is

\[
\|x - P_u x\|^2 = \|x - su\|^2 = f(s) \quad \text{(a function in the middle for the minimum)}
\]

Thus by minimizing \( f(s) \) we find \( P_u x \)

\[
f(s) = \|x - su\|^2 = \langle x - su, x - su \rangle
\]

\[
= \langle x, x \rangle - 2 \text{Re}(\langle x, su \rangle) + \|su\|^2
\]

\[
= \|x\|^2 - 2 s \text{Re}(\langle x, u \rangle) + s^2 \|u\|^2
\]

Gradient eq. in \( s \)

\[
\frac{\partial f(s)}{\partial s} = 2 s \|u\|^2 - 2 \text{Re}(\langle u, x \rangle) + 2 s \|u\|^2
\]

...
We differentiate in $s$ to find the minimum

$$f'(s) = 2s\|u\|^2 - 2\langle u, x \rangle = 0$$

$$\Rightarrow s^* = \frac{\langle u, x \rangle}{\|u\|^2} \text{ solves the equation.}$$

So we have

$$P_u x = s^* u = \frac{\langle u, x \rangle}{\|u\|^2} u$$

is the projection of the vector $x$ onto the line spanned by the vector $u$.

These are two ways to represent $P_u x$:

1. $$P_u x = \left\langle \frac{u}{\|u\|}, x \right\rangle \cdot \frac{u}{\|u\|}$$
   
   $\left\langle \text{unit vectors} \right\rangle$

2. $$P_u x = u \frac{\langle u, x \rangle}{\|u\|^2} = u \frac{u^T x}{\|u\|^2} = uu^T x \frac{1}{\|u\|^2} = \frac{uu^T}{\|u\|^2} x$$

$$\langle u, x \rangle = u^T x$$
What is $uu^T$:

$u : \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $u^T \begin{pmatrix} 1 & 1 & 0 \end{pmatrix}$

$\Rightarrow uu^T : \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$\Rightarrow P_u = \left( \frac{uu^T}{\|u\|^2} \right)$ is the orthogonal projector onto the span of $u$.

Example: $u = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$, what is $P_u$?

$\|u\|^2 = 1^2 + (-1)^2 = 2$; $uu^T = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$

$\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
\[ \Rightarrow \quad P_u = \frac{uu^T}{\|u\|^2} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

(i) \[ x = \begin{bmatrix} 2 \\ 4 \\ 3 \end{bmatrix} \quad \Rightarrow \quad P_u x = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 3 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \]

(ii) \[ y = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad \Rightarrow \quad P_u y = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \]

(iii) \[ z = \begin{bmatrix} -2 \\ 2 \\ 0 \end{bmatrix} \quad \Rightarrow \quad P_u z = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -2 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} = z \]
Important properties of \( P \)

1. \( P (P x) = P x \) for all \( x \) \( \iff \) \( P^2 = P \)

   **Proof:**
   \[
   P P u = \frac{u u^T}{\|u\|^2} \frac{u u^T}{\|u\|^2} = \frac{u (u^T u) u^T}{\|u\|^2 \|u\|^2} = \frac{u u^T}{\|u\|^2 \|u\|^2} = \frac{u u^T}{\|u\|^2} = u u^T
   \]

2. \( P^T = P \)

   **Proof:**
   \[
   (P u)^T = \left( \frac{u u^T}{\|u\|^2} \right)^T = \frac{1}{\|u\|^2} \left( u u^T \right)^T = \frac{1}{\|u\|^2} (u^T)^T u^T = \frac{u u^T}{\|u\|^2} = P u
   \]

Consequences of these properties

a) \( < y, P z > = < P y, z > \) for all \( y, z \)

   **Proof:**
   \[
   < y, P z > = y^T P z = y^T P^T z = (P y)^T z = < P y, z >
   \]

b) \( < y, P^2 z > = < y, P z > = < P y, z > \)

   (2) \( \iff \) (a)
(R(P_w)) = L = \text{span} S_{U^3}

\text{What is the projection on } L^\perp?

\mathbb{R}^2 \quad L^\perp

\mathbb{R}^3

\text{This would say that } q = x - P_x = (I - P)x

\text{Another way } Q = (I - P) \text{ is the matrix that projects onto } L^\perp
Example: Calculate the projection of \( \begin{bmatrix} 2 \\ 4 \\ 3 \end{bmatrix} \) onto the orthogonal complement of \( L = \text{span} \{ u \} \), where \( u = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \).

\[
Q = I - P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 1/2 & -1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

\[
Q \times \begin{bmatrix} 2 \\ 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ 3 \end{bmatrix}
\]
Orthogonal projection matrix

**Def.** An n x n matrix \( P \) is an **orthogonal projection matrix** iff

1) \( P^2 = P \)
2) \( P^T = P \)

**Remark.** \( P_0 = \frac{1}{\|u\|^2} uu^T \) is an example of an orthogonal projection matrix.

Let \( Q = I - P \) as before.

1. \( Q \) is an orthogonal projection matrix
2. \( P + Q = I \)
3. \( PQ = QP = 0 \)
4. \( P \) projects orthogonally onto \( \text{R}(P) \)
   (in other words: \( Px \) is the closest vector in \( \text{R}(P) \) to \( x \))
5. \( Q \) projects orthogonally onto \( \text{N}(P) = \text{R}(P)^\perp \)
Proof of the facts:

1. We need to check that \( Q = Q^2 \) and \( Q = QT \)
   i. \( Q^2 = (I - P)(I - P) \)
      \[
      = I - 2P + P^2 = I - 2P + P = I - P = Q
      \]
   ii. \( QT = (I - P)^T = I^T - PT = I - P = Q \)
      \[
      (A + B)^T = AT + BT
      \]

2. \( Q = I - P \iff P + Q = I \)
   \[
   PQ = P(I - P) = P - P^2 = P - P = 0
   \]
   \[
   QP = 0
   \]

Walls and問い
\[
IA = AI = A
\]