Perron-Frobenius Theory

- **Definition** An $n \times n$ real matrix is positive if all it's entries are positive *i. e.* $T_{i,j} > 0$.
for all $1 \leq i, j \leq n$
- **Perron's theorem**

Theorem

Given a positive square matrix T , there is a positive real number r, called the **Perron–Frobenius eigenvalue** *of T , such that r is an eigenvalue of T and any other eigenvalue λ of T has $|\lambda| < r$. Moreover, there is a positive vector ψ with $T\psi = r\psi$. Any other vector with this property is a scalar multiple of ψ.*

J. C. Baez and J. D. Biamonte, arXiv:1209.3632 [quant-ph].

Perron-Frobenius Theory

- **Perron-Frobenius theorem**

Theorem

Given an irreducible non-negative square matrix T, there is a positive real number r, called the **Perron–Frobenius eigenvalue** *of T, such that r is an eigenvalue of T and any other eigenvalue λ of T has $|\lambda| \leq r$. Moreover, there is a positive vector ψ with $T\psi = r\psi$. Any other vector with this property is a scalar multiple of ψ.*

- $T = A + cI$
- Perron-Frobenius eigenvalue satisfies the inequality

$$\min_i \sum_j T_{ij} \leq r \leq \max_i \sum_j T_{ij}$$

- Which implies that as long as A is irreducible it has a unique positive eigenvector corresponding to the 0-eigenvalue.

J. C. Baez and J. D. Biamonte, arXiv:1209.3632 [quant-ph].

$\delta = \dim(\operatorname{Im} A \cap \ker Y)$

$\delta = 0 \Rightarrow \dim(\operatorname{Im} A \cap \ker Y) = 0$

or

$\operatorname{Im} A \cap \ker Y = \{0\}$

$\Rightarrow (\operatorname{Im} A \cap \ker Y)^{\perp} = \mathbb{R}^c$

we will now use the relations

$$(\operatorname{Im} A)^{\perp} = \ker A^T$$

$$\& \quad (\ker A)^{\perp} = \operatorname{Im} A^T$$

To motivate this:

(1) consider a case where $\ker A = 0$ such as identity matrix or $\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \rightarrow$ upper or lower triangular

The orthogonal subspace will clearly consist of all 3 ind. vectors in $\mathbb{R}^3$ which are the columns of A^T (& rows of A). The rows of A are important for the kernel since they are the ones which multiply a column vector.

(2) $\begin{pmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \rightarrow$ # of ind column vectors = # of ind row vectors = rank = 2

The orthogonal subspace of the image of this matrix is the vector $\perp$ to the 2-ind column vectors. This is the same as $\ker A^T$ since in the transpose these columns become the rows & act on a column vector to annihilate it

So we have $\underline{\mathrm{Im}\, Y^T} + \ker A^T = \mathbb{R}^c$

This implies that any vector in $\mathbb{R}^c$ should be describable by ~~any~~ a linear combination of a vector in $\mathrm{Im}\, Y^T$ & $\ker A^T$.

Let's check for our enzyme-kinetics example

$$\mathrm{Im}\, Y^T = \mathrm{Im} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$ → all 4 column vectors

$$\ker A^T \Rightarrow \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \text{ \& } \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

which are independent of the 4 vectors in $\mathrm{Im}\, Y^T$

So the 6 together span $\mathbb{R}^6$ ⇒ any vector should be expressable as a linear combination of them.

In particular if we consider a $\hat{\Psi}$ in the kernel of A

$$\ln \hat{\Psi} = \alpha + Y^T \ln x$$

In our example $\alpha \to \begin{pmatrix} a \\ a \\ a \\ b \\ b \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

$$\Rightarrow \boxed{e^{-\alpha} * \hat{\Psi} = x^Y}$$

component-wise product

In our example

$$\alpha \to \begin{pmatrix} a \\ a \\ a \\ b \\ b \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

(most general linear combination of the basis of A^T)

$$\Rightarrow \quad \hat{\Psi} = e^{\alpha} x^{Y}$$

or

$$e^{-\alpha} \hat{\Psi} = x^{Y}$$

$\downarrow$

component-wise product

We can see that $A(e^{-\alpha}\hat{\Psi}) = 0$ since all we are doing is multiplying the components of $\hat{\Psi}$ in one linkage class by a constant (& the components in the second linkage class by another constant). This is always allowed $\Leftrightarrow$ a symmetry.

- In the enzyme kinetics network if we just solve the rate eqn. by brute force we get

$$\Psi \to \begin{array}{c} \\ \left[\begin{array}{c} 1 \\ a \\ b \\ c \\ d \\ e \end{array} \right] \end{array} \begin{array}{l} \phi \\ x_E \\ x_S \\ x_E x_S \\ x_{ES} \\ x_E x_P \end{array}$$

$a = \bar{k}_3 / k_3$

$b = \bar{k}_4 / k_4$

$c = \bar{k}_3 / k_3 \; \bar{k}_4 / k_4$

$d = k_1 / \bar{k}_1 \; \bar{k}_3 / k_3 \; \bar{k}_4 / k_4$

$$e = \frac{\bar{k}_3}{k_3} \frac{k_1}{\bar{k}_1} \frac{\bar{k}_4}{k_4} \frac{\bar{k}_2}{k_2}$$

Let's see if we get the same solution from the kernel of A

$$A\hat{\psi} = 0$$

$$\Rightarrow e^{-\alpha\hat{\psi}} \rightarrow \begin{bmatrix} a \\ a\bar{k}_3/k_3 \\ a\bar{k}_4/k_4 \\ b \\ b\,k_1/\bar{k}_1 \\ b\,k_1/\bar{k}_1\;\bar{k}_2/k_2 \end{bmatrix}$$

we should be able to write this as

$$\begin{bmatrix} 1 \\ x_E \\ x_S \\ x_E x_S \\ x_{ES} \\ x_E x_P \end{bmatrix}$$

set $a = 1$ & $b = \dfrac{\bar{k}_3}{k_3}\dfrac{\bar{k}_4}{k_4}$ & we get $\hat{\psi}$!

- The solution is "complex-balanced". In fact, here it is even detailed-balanced.

- Lets consider another example

$$\begin{tikzcd} A \arrow[r, shift left, "k_1"] & 2A \arrow[l, shift left, "\bar{k}_1"] \arrow[dl, "k_2"] \\ B \arrow[u, "k_3"] & \end{tikzcd}$$

$c = 3$
$\ell = 1$
$s = 2$
$\Rightarrow \delta = 0$

Now we know that the A matrix null eigenvector is the soln.

$$\begin{array}{c} \begin{array}{ccc} A & 2A & B \end{array} \\ \begin{bmatrix} -k_1 & \bar{k}_1 & k_3 \\ k_1 & -\bar{k}_1 - \bar{k}_2 & 0 \\ 0 & k_2 & -k_3 \end{bmatrix} \end{array} \begin{bmatrix} x_A \\ x_A^2 \\ x_B \end{bmatrix} = 0$$

complex-balance
$$\begin{cases} k_1 x_A = \bar{k}_1 x_A^2 + k_3 x_B \\ k_1 x_A = (\bar{k}_1 + k_2)\, x_A^2 \\ k_2 x_A^2 = k_3 x_B \end{cases}$$

For each complex, we equate those reactions for which it is the source & it is the product. This can be solved to give

$$x_A = \left(\frac{k_1}{\bar{k}_1 + k_2}\right) \; ; \; x_B = \frac{k_2}{k_3}\left(\frac{k_1}{\bar{k}_1 + k_2}\right)^2$$