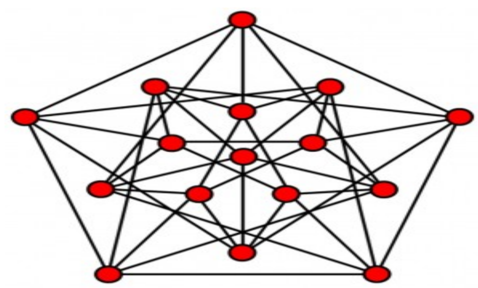
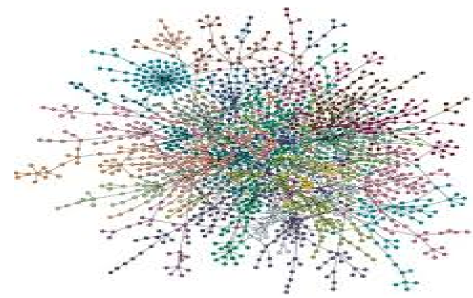
Portland-Corvallis, Febr 2023





Chemical Reaction Networks

Based on various sources, among which:

J. J. P. Veerman, T. Whalen-Wagner, E. Kummel *Chemical Reaction Networks in a Laplacian Framework*, **Chaos, Solitons, and Fractals** 136, Article 112859, 2023.

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SUMMARY:

* We start by describing boundary operators and how they can be used to build Laplacians.

* Since the eigenvalues of a Laplacian L have non-negative real part, and so the long term behavior of the differential equations $\dot{x} = -Lx$ and $\dot{x} = -xL$ is dominated by the zero eigenvalues and their eigenvectors: the left and right kernels of L.

* The differential equations governing the behavior of chemical reaction networks can be built up using the boundary operators. This gives rise, very naturally, to a Laplacian formulation of the dynamics.

* These differential equations are *nonlinear*. In spite of that, in many cases, the Laplacian approach can be used to describe the global dynamics of the network.

OUTLINE:

The headings of this talk are color-coded as follows:

Boundary Operators

Kernels of Laplacians

Chemical Reaction Networks

Difference with Earlier Work

The Zero Deficiency Theorem

Further 0 Deficiency Results

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BOUNDARY OPERATORS

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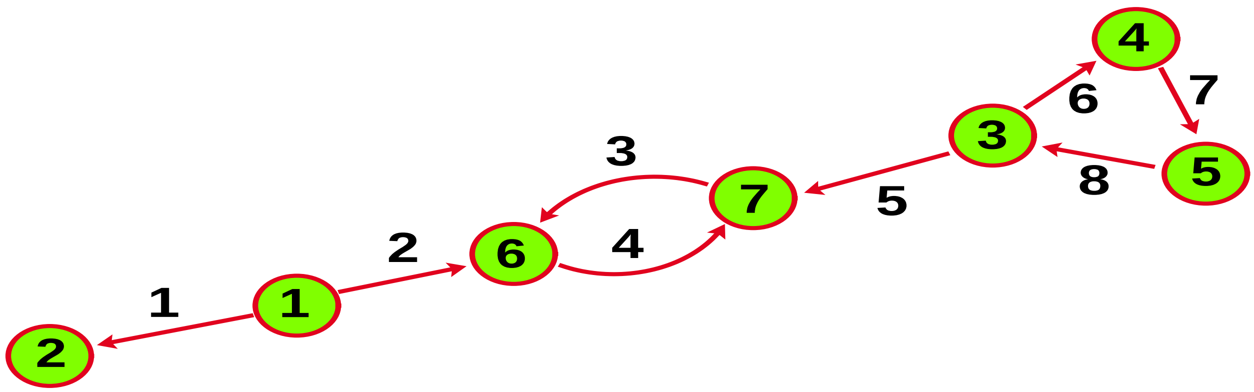
The Boundary Matrices



Definition: Given a digraph G, define matrices B (for Begin) and E (for End), as maps Edges $\rightarrow$ Vertices.

$$E_{ij} = \begin{cases} 1 & \text{if vertex } i \textbf{ ends} \text{ edge } j \\ 0 & \text{else} \end{cases}$$

$$B_{ij} = \begin{cases} 1 & \text{if vertex } i \textbf{ starts} \text{ edge } j \\ 0 & \text{else} \end{cases}$$

$$E = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Edges are columns. Vertices are rows.

Consistent with **definition** of boundary operator in topology:

$$\partial := E - B$$

From Boundary to Adjacency

Let v number of vertices. Want an operator mapping $\mathbb{C}^v$ to itself. Thus EE^T, EB^T, BE^T, and BB^T are natural candidates. We investigate these operators.

FACT 1:

$$(\mathbf{EE^T})_{ij} = \sum_k E_{ik} E_{jk}$$

is the # edges that end in i and in j.
Thus it is the **diagonal in-degree matrix**.
Similarly, $\mathbf{BB^T}$ is the **diagonal out-degree matrix**.

FACT 2:

$$(\mathbf{EB^T})_{ij} = \sum_k E_{ik} B_{jk}$$

is the # edges that start in j and end in i.
It is the **comb. in-degree adj. matrix** Q (as in [8]).
And $\mathbf{BE^T}$ is the **comb. out-degree adj. matrix** or Q^T.

Lemma: In the notation of [8], we have:

$$D = EE^T \quad \text{and } Q = EB^T$$

Exercise: Check the facts as well as the ones mentioned for BB^T and BE^T.

Exercise: Interpret as operators $\mathbb{C}^e \to \mathbb{C}^e$ (e number of edges).

... and on to Laplacians

The Lemma immediately implies:

Theorem 1: In the notation of [8], we have:

$$L = E(E^T - B^T) \quad \textbf{and} \quad L_{\textbf{out}} = -B(E^T - B^T)$$

where $L_{\textbf{out}}$ is the Laplacian of the graph G with all orientations reversed.

The example in the next pages illustrate the following two remarks.

Remark1: Be careful to note that $L_{\textbf{out}} \neq L^T$!!

Remark 2: Note that the sum of L and L_{out} is the Lapl. of the **underlying graph** $\underline{G}$. Thus:

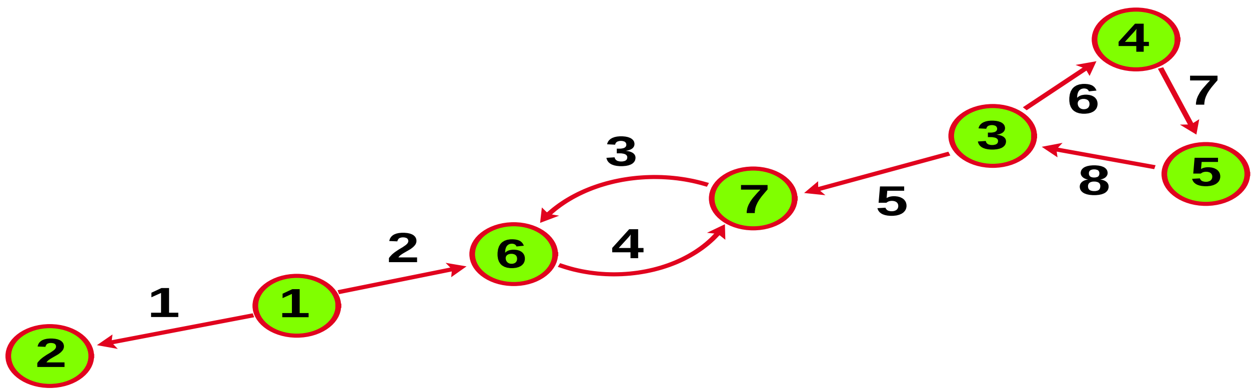
Corollary: We have:

$$\underline{L} = L + L_{\text{out}} = (E - B)(E^T - B^T) = \partial\partial^T$$

Remark: This is the traditional definition of the Laplacian in topology.

Re-Definition: L is the standard comb. Lapl. of [8, 9, 10, 11]. Better notation in this context: From now on, replace L by $L_{\textbf{in}}$,

Example



$$L_{\text{in}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 2 & -1 \\ 0 & 0 & -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

$$L_{\text{out}} = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & -1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

And $\underline{L} = L_{\text{in}} + L_{\text{out}}$ is symmetric. (Note that the edge between vertices 6 and 7 doubles or acquires weight 2 in this process.)

Exercise: Find these Laplacians from Theorem 1.

Weighted Laplacians

Definition: We can “weight" the edges. Let W be a diagonal weight matrix.

$$L_{\text{in},W} = (EW)(E^T - B^T)$$

We drop the subscript “W". In particular

$$\mathcal{L}_{\text{in}} = (ED^{-1})(E^T - B^T)$$

where $D_{ii} = 1$ if the in-degree in 0. (see [8])

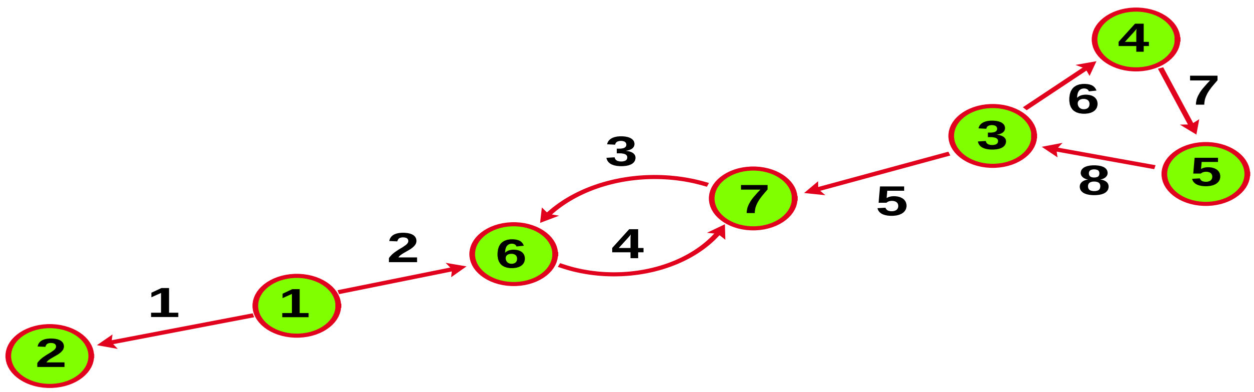
Remark: Note that

$$\left[(EW)B^T\right]_{ij} = \sum_k E_{ik} W_{kk} B_{jk}$$

which means the weights go to the edges (not the vertices).

Be careful: The symbol $\mathcal{L}_{\textbf{out}}$ is reserved for the out-degree rw Laplacian. The edges have a weight different from that of $\mathcal{L}_{\text{in}}$. See example.

Example with Weights



$$\mathcal{L}_{\text{in}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ -1/2 & 0 & 0 & 0 & 0 & 1 & -1/2 \\ 0 & 0 & -1/2 & 0 & 0 & -1/2 & 1 \end{pmatrix}$$

$$\mathcal{L}_{\text{out}} = \begin{pmatrix} 1 & -1/2 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1/2 & 0 & 0 & -1/2 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

Notice that the sum of these two is NOT symmetric. Edge 6 ($\mathcal{L}_{in,4,3}$ and $\mathcal{L}_{out,3,4}$) received two different weights in each case.

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LEFT AND RIGHT KERNELS OF LAPLACIANS

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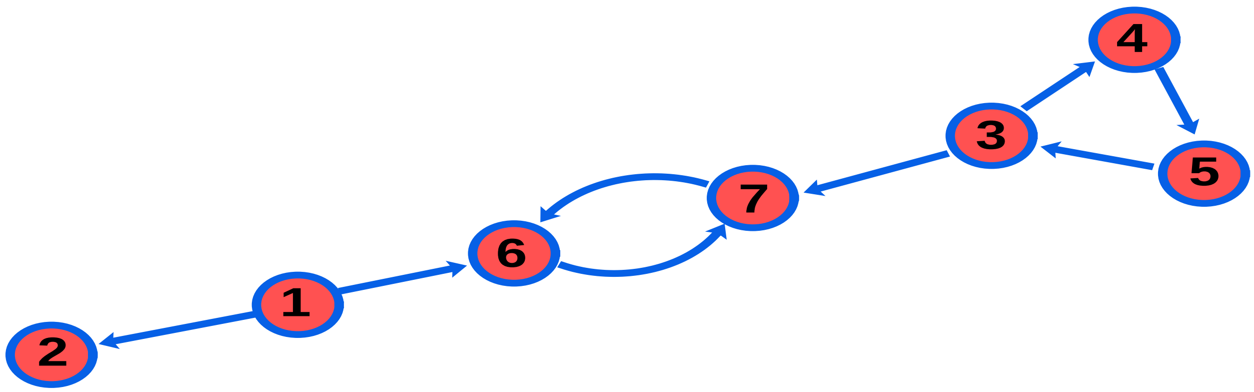
Connectedness of Digraphs

Undirected graphs are connected or not. But...



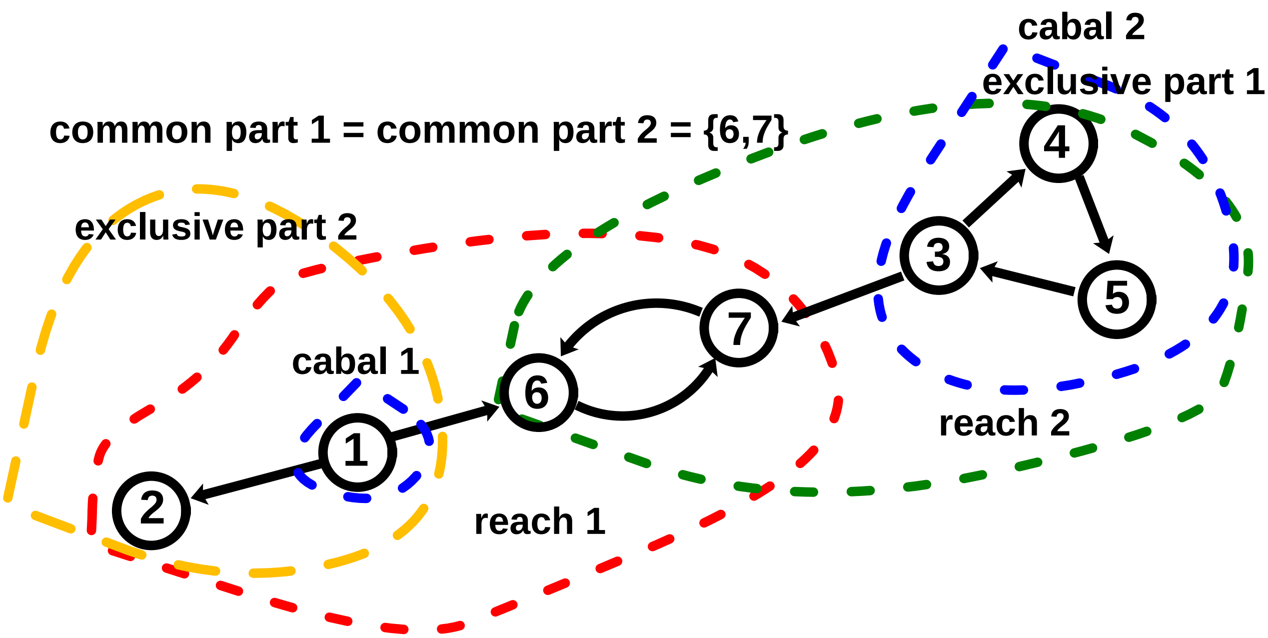
Definition:

* A directed edge from i to j is indicated as $i \to j$ or ij.
* A digraph G is **strongly connected** if for every ordered pair of vertices (i, j), there is a directed path $i \rightsquigarrow j$.
* A digraph G is **unilaterally connected** if for every ordered pair of vertices (i, j), there is a path $i \rightsquigarrow j$ or a path $j \rightsquigarrow i$.
* A digraph G is **weakly connected** if the **underlying UNdirected graph** is connected.
* A digraph G is **not connected:** if it is not weakly connected.

Definition: Multilaterally connected: **weakly connected** but not **unilaterally connected**.

Note: Maximal Strongly Connected Component: **SC** component, or **SCC**.

Graph Structure



leadership = SCC w. no incoming edges: {1} and {3,4,5}

following = SCC w. no outgoing edges: {2} and {6,7}

Think of arrows as indicating flow of information!!!

Definition: Only the blue definitions are used downstream.

* **Reachable Set** $R(i) \subseteq V$**:** $j \in R(i)$ if $i \rightsquigarrow j$.

* **Reach** $R \subseteq V$**:** A maximal reachable set. Or: a maximal unilaterally connected set.

* **Exclusive part** $H \subseteq R$**:** vertices in R that do not “see" vertices from other reaches. If not in cabal, called **minions**.

* **Common part** $C \subseteq R$**:** vertices in R that also “see" vertices from other reaches.

* **Leadership or Cabal** $B \subseteq H$**:** set of vertices from which the entire reach R is reachable. If single, called **leader**.

The Right Kernel of L

Theorem 2 [1]: Spectrum of L has non-negative real part.

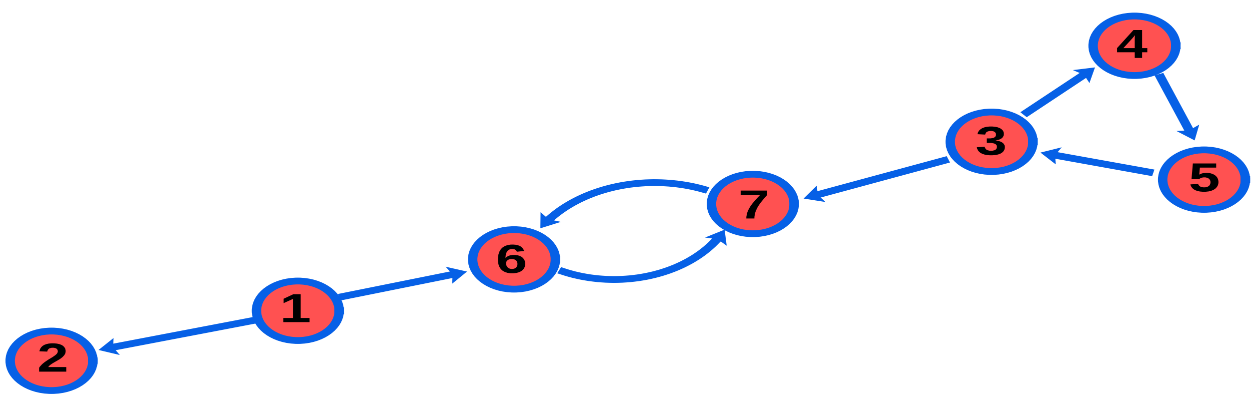
From Now On: (i) There are exactly k **reaches** $\{R_i\}_{i=1}^k$.
ii) L is a general Laplacian of the form $L = D - DS$ [1].

Theorem 3 [1]: The algebraic and geometric multiplicity of the eigenvalue 0 of L equals k.

Thus: **no non-trivial Jordan blocks in kernel!**

Theorem 4 [1]: The *right* kernel of L consists of the *column* vectors $\{\gamma_1, \cdots, \gamma_k\}$, where:

$$\begin{array}{lll} \gamma_m(j) = 1 & \text{if} & j \in H_m \quad \textbf{(excl.)} \\ \gamma_m(j) \in (0,1) & \text{if} & j \in C_m \quad \textbf{(common)} \\ \gamma_m(j) = 0 & \text{if} & j \notin R_m \quad \textbf{(reach)} \\ \sum_{m=1}^k \gamma_m = \mathbf{1} & \textbf{(all ones vector)} & \end{array}$$



$$\gamma_1^T = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & \frac{2}{3} & \frac{1}{3} \end{pmatrix} \quad \text{and} \quad \gamma_2^T = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & \frac{1}{3} & \frac{2}{3} \end{pmatrix}$$

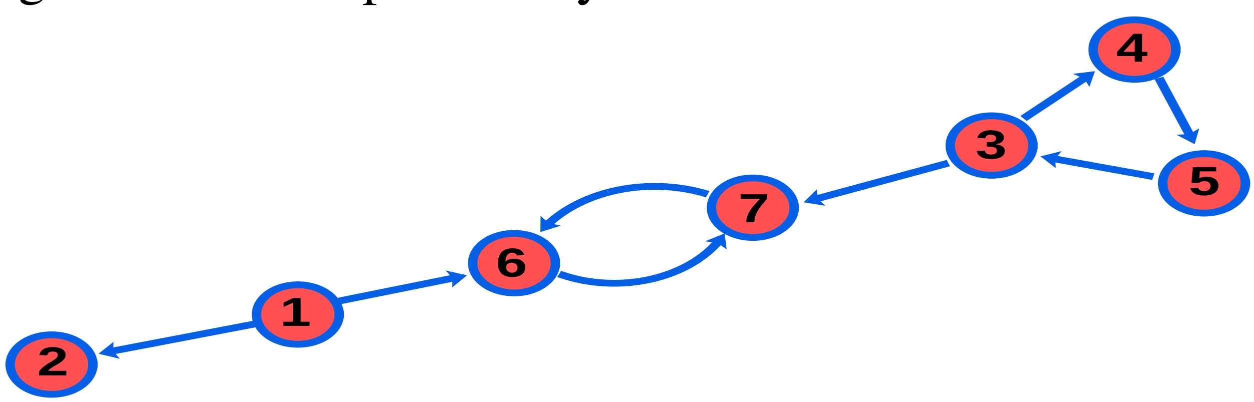
The Left Kernel of L

Theorem 5 [5]: The *left* kernel of L consists of the *row* vectors $\{\bar{\gamma}_1, \cdots, \bar{\gamma}_k\}$, where:

$$\begin{array}{ll} \bar{\gamma}_m(j) > 0 & \text{if} \quad j \in B_m \ \textbf{(cabal)} \\ \bar{\gamma}_m(j) = 0 & \text{if} \quad j \notin B_m \\ \sum_{j=1}^{k} \bar{\gamma}_m(j) = 1 & \\ \{\bar{\gamma}_m\}_{m=1}^{k} \ \textbf{are orthogonal} & \end{array}$$

Mnemonic: the horizontal "bar" on $\bar{\gamma}$ indicates a (horizontal) row vector.

Thus in this case the row vectors $\{\bar{\gamma}_1, \cdots, \bar{\gamma}_k\}$ are a set of orthogonal invariant probability measures.



$$\bar{\gamma}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \bar{\gamma}_2 = \begin{pmatrix} 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \end{pmatrix}$$

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C H E M I C A L
R E A C T I O N
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"C R N" s

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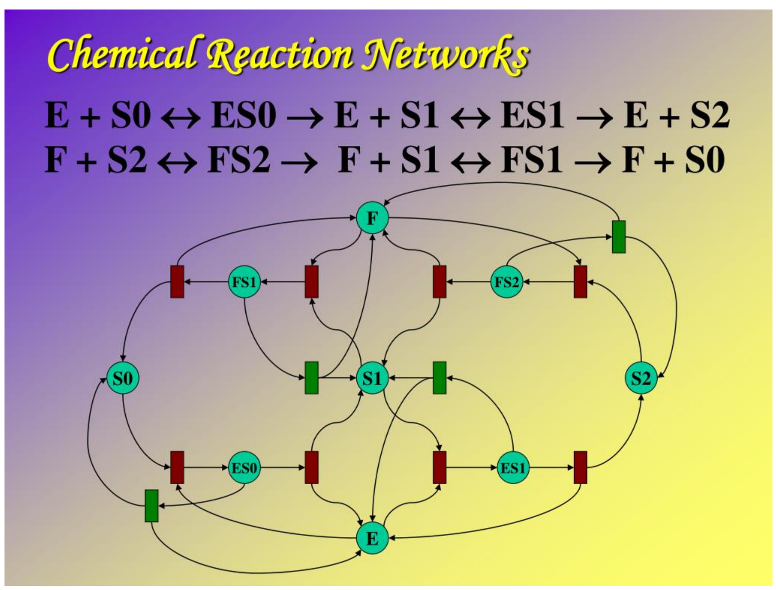


From a presentation by David Angeli, Univ of Firenze, Italy. Chemical networks can have thousands of vertices.

A Simple Example

$$\text{Reaction 1:} \qquad 2\,H_2 + O_2 \;\rightarrow\; 2\,H_2O$$
$$\text{Reaction 2:} \qquad C + O_2 \;\rightarrow\; CO_2$$

Concentration of $C + O_2$ is an ambiguous concept.
Can measure only concentrations of molecules: H_2O, H_2.
But *rate of change* of conc. of O_2 due to (eg) reaction 1 is fine!

Set x_i equal to concentration of following molecules:

$$x_1 \leftrightarrow H_2\,,\;\; x_2 \leftrightarrow O_2\,,\;\; x_3 \leftrightarrow H_2O\,,\;\; x_4 \leftrightarrow C\,,\;\; x_5 \leftrightarrow CO_2$$

Assume all molecules are unif. distr. in the mix.

Observation 1. Reaction 1 says: for every 2 molecules H_2 and 1 molecule O_2 that disappear we get 2 molecules H_2O back.
Observation 2. Reaction rate is proportional to the chance that that the reacting molecules “meet". For reaction 1 that is $x_1^2 x_2$. The constant of the proportionality is called k_1.

The same for reaction 2. So:

$$\begin{aligned}
\dot{x}_1 &= -2k_1 x_1^2 x_2 \\
\dot{x}_2 &= -k_1 x_1^2 x_2 - k_2 x_2 x_4 \\
\dot{x}_3 &= 2k_1 x_1^2 x_2 \\
\dot{x}_4 &= -k_2 x_2 x_4 \\
\dot{x}_5 &= k_2 x_2 x_4
\end{aligned}$$

Observation 2 is called the **mass action principle.**

Two More Definitions

$$\begin{array}{ccc} v_1 & \stackrel{e_1}{\rightarrow} & v_2 \\ v_3 & \stackrel{e_2}{\rightarrow} & v_4 \end{array} \quad \text{where} \quad \begin{array}{l} e_1 : \; 2\,H_2 + O_2 \;\rightarrow\; 2\,H_2O \\ e_2 : \; C + O_2 \;\rightarrow\; CO_2 \end{array} \quad \text{with}$$

$$x_1 \leftrightarrow H_2 \,,\; x_2 \leftrightarrow O_2 \,,\; x_3 \leftrightarrow H_2O \,,\; x_4 \leftrightarrow C \,,\; x_5 \leftrightarrow CO_2$$

Definition: # i-molecules (belonging to x_i) at jth vertex v_j equals S_{ij}. S has no zero rows. Rate $\dot{x}_i$ equals the sum of rates of change of those mixtures in which that molecule occurs.

$$\dot{x} = S\dot{v} \qquad \text{or} \qquad \dot{x}_j = \sum_i S_{ji}\dot{v}_i \,.$$

Exercise: Show that for this example

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

(*Hint: vertex v_1 contains 2 x_1-molecules and 1 x_2-molecule.*)

Mass Action Principle. The probability ψ_i that all molecules of v_i "meet" is proportional to

$$\psi_i(x) := \prod_j x_j^{S_{ji}}$$

Exercise: Show that for this example

$$\psi_1 = x_1^2 x_2 \,,\quad \psi_2 = x_3^2 \,,\quad \psi_3 = x_2 x_4 \,,\quad \psi_4 = x_5$$

The Basic Idea ...

Definition: (conc. means concentration)

$\mathbb{R}^c$	"conc.s of molecules"	variables x_i
$\mathbb{R}^v$	"conc.s of reacting mixtures"	variables v_i
$\mathbb{R}^e$	"reaction rates"	

ith reaction denoted by e_i.

Relevant Operators:

$$\psi \text{ (non-linear)} \ : \ \mathbb{R}^c \to \mathbb{R}^v$$

$$E, B \text{ (linear)} \ : \ \mathbb{R}^e \to \mathbb{R}^v \quad \text{and} \quad E^T, B^T \ : \ \mathbb{R}^v \to \mathbb{R}^e$$

$$S \text{ (linear)} \ : \ \mathbb{R}^v \to \mathbb{R}^c$$

Key Idea 1. Use mass action to give ode for conc.s of $\{x_i\}_1^c$.

$$\mathbb{R}^c \xleftarrow{S} \mathbb{R}^v \xleftarrow{\partial = E - B} \mathbb{R}^e \xleftarrow{W} \mathbb{R}^e \xleftarrow{B^T} \mathbb{R}^v \xleftarrow{\psi} \mathbb{R}^c$$

Key Idea 2. Form a **network** by putting together the reactions $v_i \xrightarrow{e_\ell} v_j$ with the v_i as its vertices. Our example:

$$v_1 \xrightarrow{e_1} v_2$$

$$v_3 \xrightarrow{e_2} v_4$$

v_1 is "conc." of the reacting mixture, i.e. $2H_2 + O_2$, etc. **Look at the associated Laplacian !!!**

...and Putting Things Together

Prescription 1: Form the diff eqns step by step:

$\mathbb{R}^c \to \mathbb{R}^v$;	convert conc.s to mass action terms;	ψ
$\mathbb{R}^v \to \mathbb{R}^e$;	assign initial m.a. term to each edge;	B^T
$\mathbb{R}^e \to \mathbb{R}^e$;	weight each e_i by its reaction rate;	W
$\mathbb{R}^e \to \mathbb{R}^v$;	add @endvertex, subtr. @beginvertex;	$E - B$
$\mathbb{R}^v \to \mathbb{R}^c$;	convert to conc. of molecules;	S

$$\mathbb{R}^c \xleftarrow{S} \mathbb{R}^v \underbrace{\xleftarrow{\partial = E - B} \mathbb{R}^e \xleftarrow{W} \mathbb{R}^e \xleftarrow{B^T}}_{-L_{\text{out}}^T} \mathbb{R}^v \xleftarrow{\psi} \mathbb{R}^c$$

Prescription 2: Recall out-degree Lapl. (Thm 1), so that

$$\dot{x} = -S L_{\text{out}}^T \psi(x)$$

Exercise: Compute B, E, and W for this example.

Exercise: Use B, E, and W to compute L_{out} and L_{out}^T.

Exercise: Use S, ψ, and L_{out}^T to show that for the example:

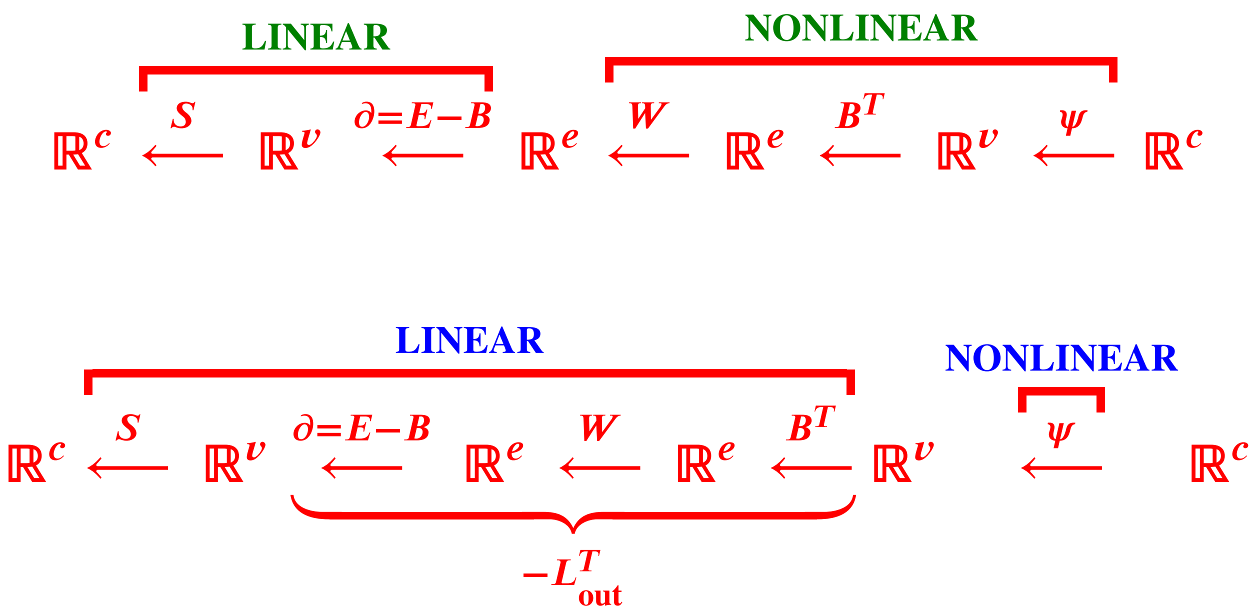
$$\begin{aligned}
\dot{x}_1 &= -2k_1 x_1^2 x_2 \\
\dot{x}_2 &= -k_1 x_1^2 x_2 - k_2 x_2 x_4 \\
\dot{x}_3 &= 2k_1 x_1^2 x_2 \\
\dot{x}_4 &= -k_2 x_2 x_4 \\
\dot{x}_5 &= k_2 x_2 x_4
\end{aligned}$$

DIFFERENCE WITH EARLIER WORK

"The wheel was great, but what have you done for me lately?"

Blue Beats Green?

Since pioneering work by Horn, Jackson, and Feinberg in the 1970's [2, 3, 4], the split into nonlinear and linear parts has been different from what we propose.
Below the classical split (green) and the proposed split (blue).



The matrix W contains the reaction rates which are (a) difficult to measure, and (b) may strongly influence the result (zero deficiency).

	advantage	disadvantage
Green	no dependence on W	weaker results
Blue	stronger results	results may depend on W

To get stronger results, need kernels of directed Laplacians, not (well-)known in the 70's.

THE ZERO DEFICIENCY THEOREM

"I'm sorry, there's no such thing as a chocolate deficiency."

The Theorem

Recall: $\dot{x} = -SL_{\text{out}}^{T}\psi(x)$

Definition. The Laplacian deficiency is given by

$$\delta := \dim \operatorname{Ker} SL_{\text{o}}^{T} - \dim \operatorname{Ker} L_{\text{o}}^{T}$$

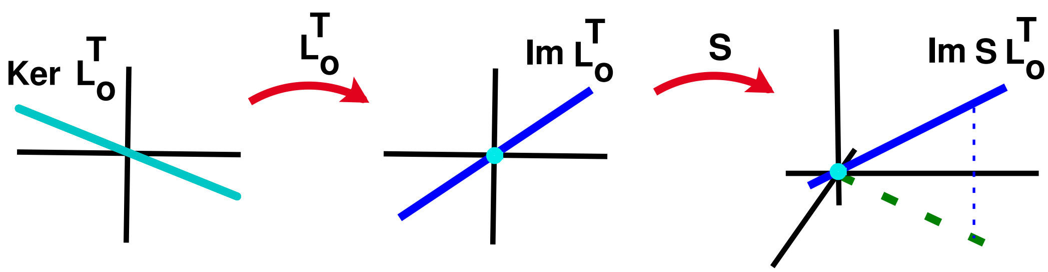


Figure: dim of Im L_{o}^{T} equals that of Im SL_{o}^{T}. So $\delta = 0$ and
None of the dynamics is hidden by S !

Lemma. The condition $\delta = 0$ is equivalent to

$$\operatorname{Im} S^{T} + \operatorname{Ker} L_{o} = \mathbb{R}^{v}$$

The theorem that initiated the mathematical study of CRNs was proved in 1972 [2]. We give a modern version due to [7].

Theorem. (Zero Laplacian Deficiency) Suppose a CRN has $\delta = 0$. Then

$$\dot{x} = -SL_{\text{out}}^{T}\psi(x)$$

has a (strictly) pos. equil. $\Longleftrightarrow$ its graph is CSC.

Proof of $\Longrightarrow$

In what follows, x denotes a vector in $\mathbb{R}^{\upsilon}$, a a real number, and $\mathbf{1_S}$ a vector in $\mathbb{R}^{\upsilon}$ that is 1 on S and 0 else. $x > 0$ means componentwise, Ln is a componentwise function etc.

Proof of $\Longrightarrow$. Assume

$$\dot{x} = -SL_{\text{out}}^{T}\psi(x)$$

has pos. equil. x^*, then prove CSC.

Existence of pos. equil. ($x^* > 0$ and $SL^T\psi(x^*) = 0$) shows

$$\psi(x^*) > 0 \quad \text{such that} \quad SL_{\text{out}}^{T}\psi(x^*) = 0$$

No hidden dynamics (or zero defciciency) then gives

$$L_{\text{out}}^{T}\psi(x^*) = 0 \quad \text{or} \quad \psi(x^*)^T L_{\text{out}} = 0$$

By theorems on left kernels (see [9]), we may therefore write

$$\psi(x^*)^T = \sum_{i=m}^{k} a_m \bar{\gamma}_m \quad \text{and} \quad \forall\, a_m > 0$$

But $\psi(x^*) > 0$ and γ_m are positive on cabals only. So every vertex is in a cabal. Therefore the graph is CSC. **Done.**

Proof of $\Longleftarrow$

Exercise: Show that if $x > 0$, then $\mathrm{Ln}\,\psi(x) = S^T \mathrm{Ln}\,x$.

Exercise: Show that if $a > 0$ and $x > 0$, then

$$\mathrm{Ln}\,ax = \ln a \cdot \mathbf{1} + \mathrm{Ln}\,x$$

Proof of $\Longleftarrow$. Assume CSC, then establish pos. equil. or

$$\exists\ x^* > 0 \ \text{ such that } \ \psi(x^*) = \sum_{i=m}^{k} a_m \bar{\gamma}_m^T \ \text{ and } \ \forall\ a_m > 0$$

Exercise: Use above exercises to rewrite **blue** equation as

$$S^T \mathrm{Ln}\,x^* = \sum_{m=1}^{k} (\ln a_m)\,\mathbf{1}_{\mathbf{R_m}} + \mathrm{Ln}\,\sum_{m=1}^{k} \bar{\gamma}_m^T.$$

where $\mathbf{1}_{\mathbf{R_m}}$ is the characteristic vector of the mth reach (component in this case).

Proof continued: Then re-arrange this as

$$\mathrm{Ln}\,\sum_{m=1}^{k} \bar{\gamma}_m^T = S^T \mathrm{Ln}\,x^* - \sum_{m=1}^{k} (\ln a_m)\,\mathbf{1}_{\mathbf{R_m}}$$

1st term of RHS ranges over Im S^T and 2nd over Ker L.

This has a solution if

$$\mathrm{Im}\,S^T + \mathrm{Ker}\,L = \mathbb{R}^{\upsilon}.$$

Guaranteed by zero deficiency condition (use the Lemma). **Done.**

Returning to the Example:

$$\begin{array}{ccc} v_1 & \overset{e_1}{\rightarrow} & v_2 \\ v_3 & \overset{e_2}{\rightarrow} & v_4 \end{array}$$

This graph has two weak components, neither of which is SC.

$$S = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad L_o^T = \begin{pmatrix} k_1 & 0 & 0 & 0 \\ -k_1 & 0 & 0 & 0 \\ 0 & 0 & k_2 & 0 \\ 0 & 0 & -k_2 & 0 \end{pmatrix}$$

Exercise: Find the span of Im L_o^T and of Ker S.

Conclude from the exercise that $\delta = 0$.

Conclude from 0-def thm that there is no strictly pos equil.

Confirm that conclusion from the equations:

$$\begin{aligned} \dot{x}_1 &= -2k_1x_1^2x_2 \\ \dot{x}_2 &= -k_1x_1^2x_2 - k_2x_2x_4 \\ \dot{x}_3 &= 2k_1x_1^2x_2 \\ \dot{x}_4 &= -k_2x_2x_4 \\ \dot{x}_5 &= k_2x_2x_4 \end{aligned}$$

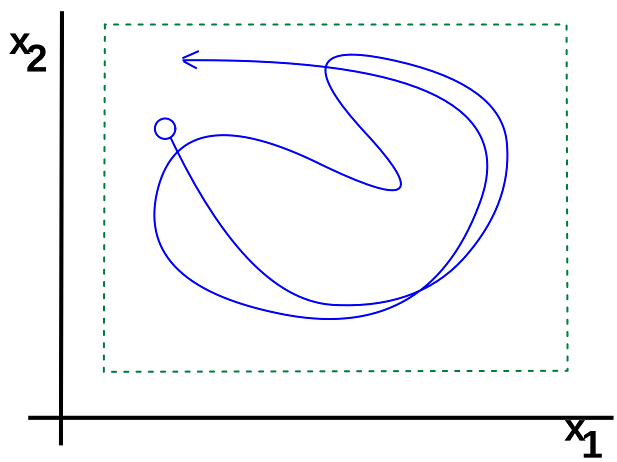
We Can Do A Little Better

Theorem [7]. Suppose $\delta = 0$. Then

$$\dot{x} = -SL_{\text{out}}^{T}\psi(x)$$

has pos. orbit $x(t)$ with Ln $x(t)$ bdd $\Longleftrightarrow$ graph is CSC.

Note: $\Longleftarrow$ follows from 0-def. But $\Longrightarrow$ strengthens it.

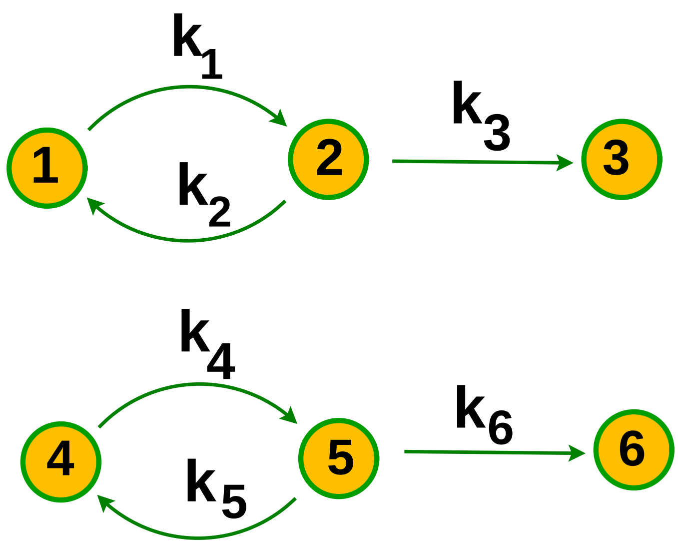


The 0-def thm says: CSC implies existence of equilibrium. So:

Corollary. A 0-def system with an orbit $x(t)$ whose Log is bounded (see figure) must have a fixed point.

New Beats Old

Consider the following network CRN, based on work by [12],



$$S = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Exercise: Show that $\delta = 0$ (for $k_i > 0$).

Definition. The older definition of the deficiency is

$$\delta_{old} := \dim \operatorname{Ker} S\partial - \dim \operatorname{Ker} \partial$$

Exercise: Show that $\delta_{old} = 1$. (*Thus old thm has no implications, while new thm predicts absence of pos. bdd. orbits.*)

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FURTHER 0 DEFICIENCY RESULTS

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Sorry Professor, you're right:
I DID skip a line of the instructions...

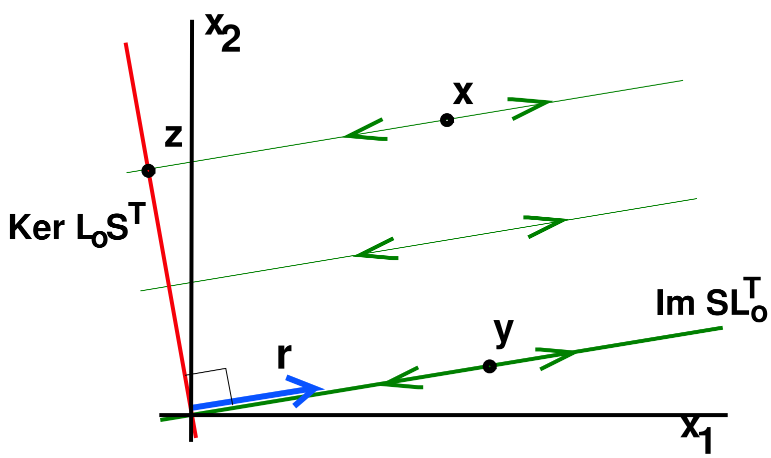
Explicit Equations for Equilibrium

Exercise: Show that for any matrix $(\mathrm{Im}\, A)^{\perp} = \mathrm{Ker}\, A^T$.

Thus the orbit $x(t)$ of

$$\dot{x} = -S L_{\mathrm{out}}^T \psi(x)$$

$\dot{x}$ is parallel to Im $S L_o^T$ and orthogonal to Ker $L_o^T S$.



Given a system with υ vertices, k reaches, and c concentrations. Denote by z_0 the orth. proj. $x(0)$ to Ker $L_o S^T$.

Theorem [7]. If $\delta = 0$, equilibria determined by υ polynomial equations in υ unknowns $\{u_i\}_{i=1}^{\upsilon-k}$ and $\{a_m\}_{m=1}^{k}$:

$$\psi\left(z_0 + \sum_{i=1}^{\upsilon-k} u_i r_i\right) = \sum_{m=1}^{k} a_m \bar{\gamma}_m^T ,$$

the $\{r_i\}_{i=1}^{\upsilon-k}$ are a basis for Im $S L^T$ and $\{\bar{\gamma}_m\}_{m=1}^{k}$ for Ker L^T.

The Example Again:

Reaction 1: $2\,H_2 + O_2 \;\rightarrow\; 2\,H_2O$

Reaction 2: $C + O_2 \;\rightarrow\; CO_2$

$$\psi_1 = x_1^2 x_2\,, \quad \psi_2 = x_3^2\,, \quad \psi_3 = x_2 x_4\,, \quad \psi_4 = x_5$$

$$S = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad L_o^T = \begin{pmatrix} k_1 & 0 & 0 & 0 \\ -k_1 & 0 & 0 & 0 \\ 0 & 0 & k_2 & 0 \\ 0 & 0 & -k_2 & 0 \end{pmatrix}$$

Exercise: Show that Ker $S L_o^T$ is spanned by

$$(1,0,1,0,0)^T,\; (1/2,-1,0,1,0)^T,\; (-1/2,1/2,0,0,1)^T\,.$$

Exercise: Show that c_3, c_4, and c_5 are preserved by the flow:

$$c_3 = x_1 + x_3, \qquad c_4 = \tfrac{1}{2}x_1 - x_2 + x_4 \quad \text{and} \quad c_5 = -\tfrac{1}{2}x_1 + x_2 + x_5$$

Exercise: Show that Im $S L_o^T$ has dimension 2.

Exercise: Set x_1 and x_2 as independent variables. Eliminate x_3, x_4, x_5 in favor of the c_i to get equilibrium eqns:

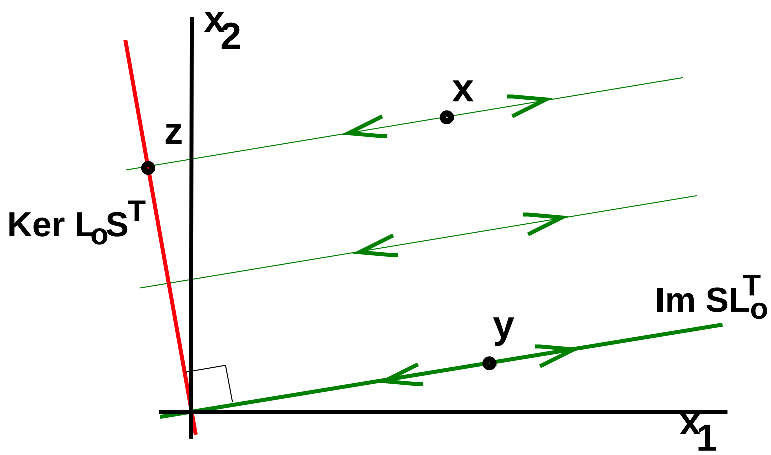
$$\begin{aligned} \psi_1 &= x_1^2 x_2 &&= 0 \\ \psi_2 &= (c_3 - x_1)^2 &&= a_1 \\ \psi_3 &= x_2(c_4 - \tfrac{1}{2}x_1 + x_2) &&= 0 \\ \psi_4 &= c_5 + \tfrac{1}{2}x_1 - x_2 &&= a_2 \end{aligned}$$

Given the constants c_i, we can solve for x_1, x_2, a_1, and a_2.

Existence and Uniqueness of Equilibria

$$\dot{x} = -SL_{\text{out}}^{T}\psi(x)$$

Flow is parallel to Im SL_o^T and orthogonal to Ker L_oS^T.

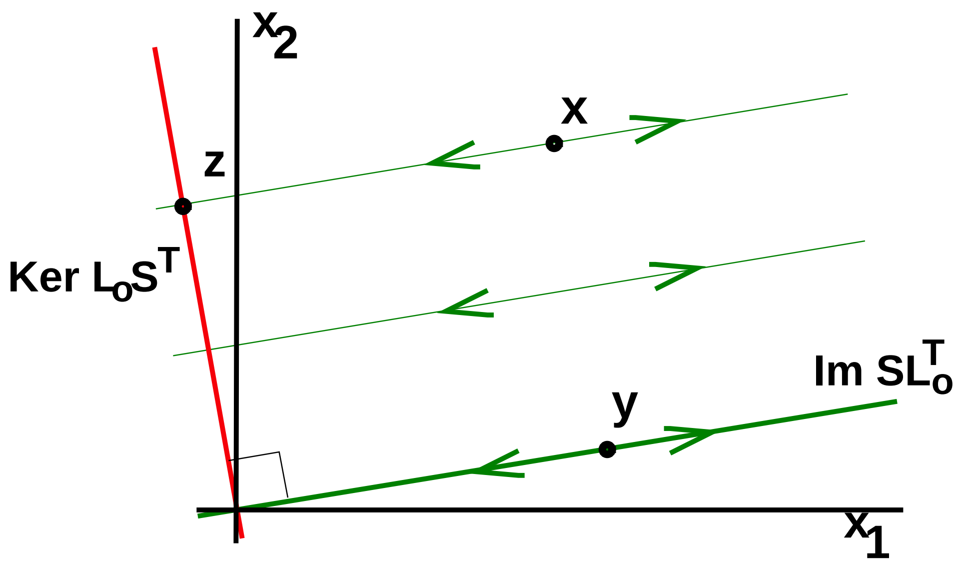


Theorem [7]. Suppose $\delta = 0$ and CSC.
Then for every $z \in$ Ker LS^T, there **exists** a **unique** $y \in$ Im SL^T such that $y + z$ is a positive equilibrium.

The proof of this result is indirect and we refer to [7].

Local Stability of Equilibria

$$\dot{x} = -S L_{out}^{T} \psi(x)$$



Theorem [7]. Suppose $\delta = 0$ and CSC.
The ω-limit set of any positive initial condition either equals that equilibrium or is a bounded set contained in the boundary of the positive orthant.

The proof of this result is indirect and we refer to [7].

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