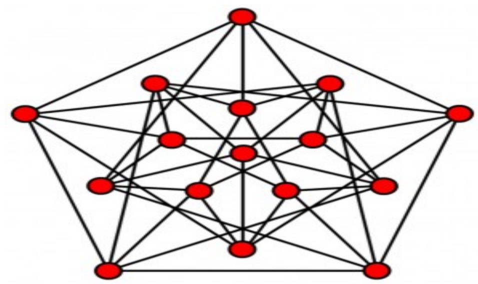
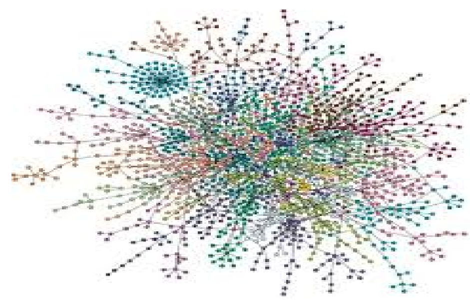
Como, Italy, October 2022

DIGRAPHS IV
Chemical Networks
The Matrix Tree Theorem

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**, accepted, 2022.

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SUMMARY:

* We 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.

* Matrix tree theorems connect different branches of mathematics (combinatorics, linear algebra, probability) in unexpected ways. For this reason, they play an important role in the graph theory literature.

* We give a detailed description of various matrix tree theorems. These theorems relate the determinant of certain submatrices of the usual Laplacian to the number of spanning trees rooted at each vertex.

* We give a simple, short, combinatorial proof loosely inspired by [1].

* We include a discussion that relates the number of spanning trees at each vertex to the stable probability measure of random walk on a strongly connected graph.

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

Boundary Operators

Chemical Reaction Networks

The Zero Deficiency Theorem

Example and Further Develeopments

Matrix Tree Theorems

Proof of Matrix Tree Theorems

Trees and Unicycles

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BOUNDARY OPERATORS

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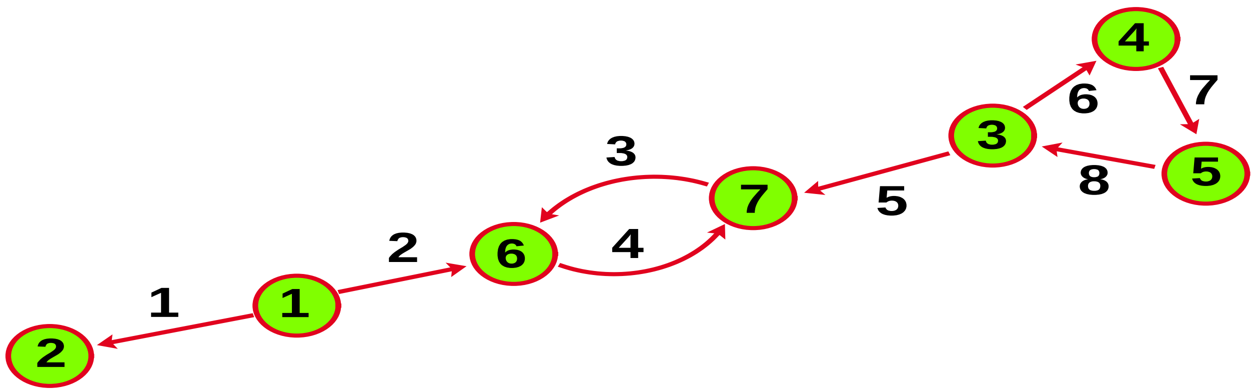
The Boundary Matrices



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

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

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

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

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 DI).
And $\mathbf{BE^T}$ is the **comb. out-degree adj. matrix** or Q^T.

Lemma: In the notation of DI, 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 DI, we have:

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

where L_{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 $L_{\text{out}} \neq L^T$!!

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

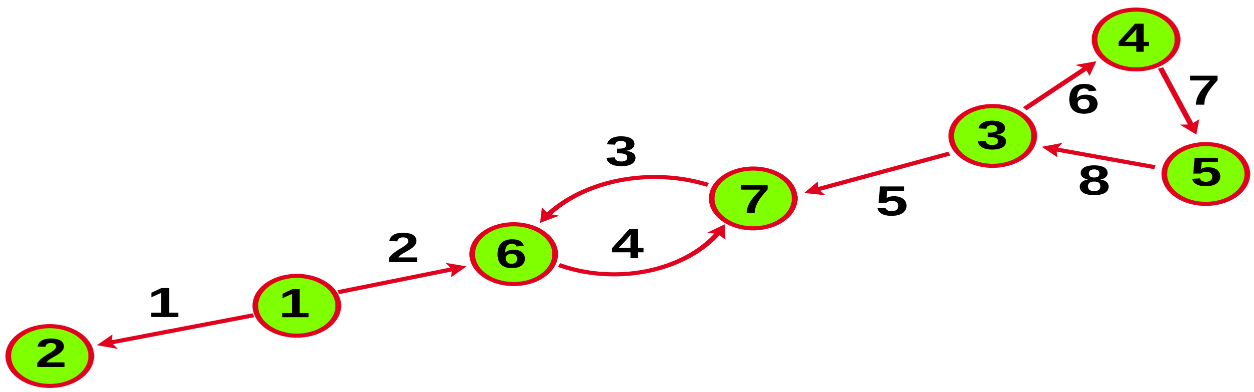
Corollary: We have:

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

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

Re-Definition: L is the standard comb. Lapl. of the previous lectures. Better notation in this context: From now on, replace L by L_{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.

Linegraphs

$E^T B - 2I$ and $B^T E - 2I$ give versions of the adjacency matrix of the linegraph of G. This needs working out. See the Graph Theory handbook page 679.

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 DI)

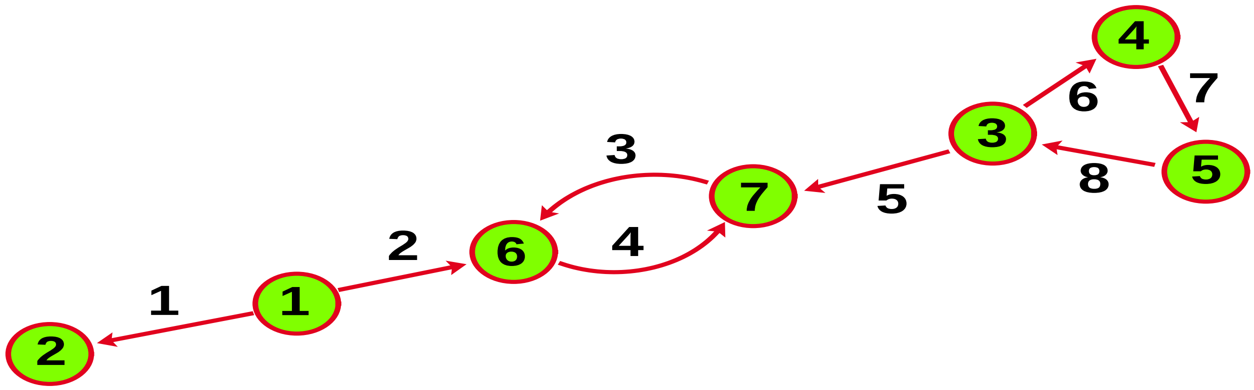
Remark: Note that

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

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

Be careful: The symbol $\mathcal{L}_{\text{out}}$ 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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CHEMICAL REACTION NETWORKS OR CRN

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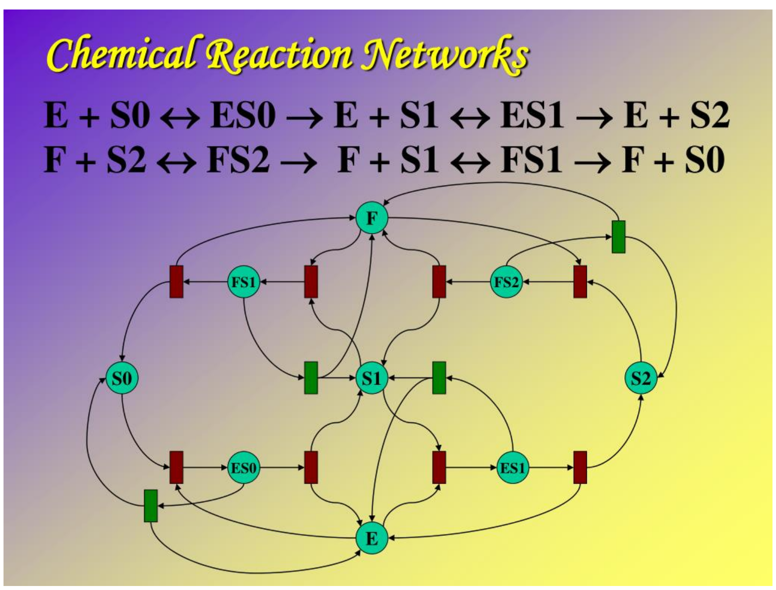

From a presentation by David Angeli, Univ of Firenze, Italy. Chemical networks can have thousands of vertices.

A Simple Example

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

Concentrations of $C + O_2$ is an ambiguous concept.
Can measure only concentrations of molecules: H_2O, H_2 etc.

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 react 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:

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

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

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
$\mathbb{R}^e$	"reactions"	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 $\{x_i\}_1^c$.

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

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

$$v_1 \overset{e_1}{\to} v_2$$
$$v_3 \overset{e_2}{\to} v_4$$

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

... and Some Details

$$v_1 \stackrel{e_1}{\rightarrow} v_2$$
$$v_3 \stackrel{e_2}{\rightarrow} v_4 \qquad \text{where}$$

$$e_1 : \qquad 2\,H_2 + O_2 \rightarrow 2\,H_2O$$
$$e_2 : \qquad C + O_2 \rightarrow CO_2 \qquad \text{with}$$

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

Definition: The count of i-molecules (belonging x_i) in the jth vertex v_j equals S_{ij}. S has no zero rows. Rate of change $\dot{x}_i$ 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 our example

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

and Apply Mass Action

Mass Action Lemma. The probability ψ_i that all molecules in v_i “meet" is

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

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

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

Putting the Equations Together

Prescription 1: Form the diff eqns as follows:

$\mathbb{R}^c \to \mathbb{R}^v$;	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. @startvertex;	$E - B$
$\mathbb{R}^v \to \mathbb{R}^c$;	convert to conc. of molecules;	S

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

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:

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

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DIFFERENCE WITH EARLIER WORK

Later is Better?

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 proposed split (blue) and the classical split (green).

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

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

The matrix W contains the reaction rates which are (a) difficult to measure, and (b) may strongly influence the result (zero deficiency). If you want conclusions independent from reaction rates, then put W in “nonlinear".

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

Some Definitions ...

Definition. The Laplacian deficiency is given by

$$\delta := \dim \operatorname{Ker} S L_o^T - \dim \operatorname{Ker} L_o^T$$

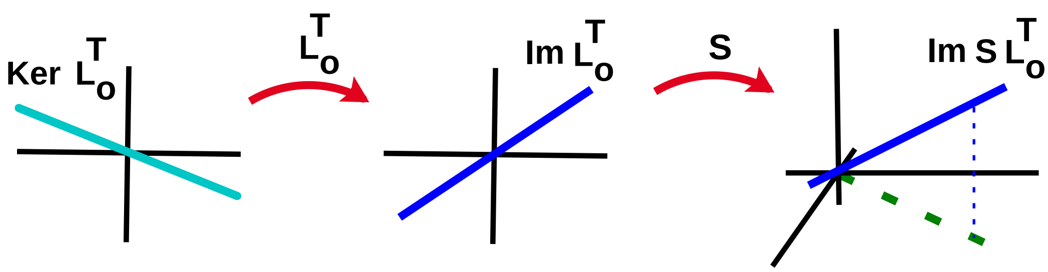

Figure: dim of Im L_o^T equals that of Im SL_o^T. So $\delta = 0$ and **None of the dynamics is hidden by S !**

Recall:

(i) Graph G is componentwise strongly connected (CSC) if each weak component is strongly connected (see DI).

(ii) The algebraic and geometric multiplicity of the eigenvalue 0 of L equals k, the number of reaches (see DII).

(iii) *Left* kernel of L is spanned by *row* vectors $\bar{\gamma}_i$ (see DII):

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

Definition. **(i)** For x, y in $\mathbb{R}^n$: $x > y$ if true componentwise.
(ii) For $x > 0$ in $\mathbb{R}^n$, define $\operatorname{Ln} x$ as $(\ln x_1, \cdots, \ln x_n)$.

... and the Theorem

The theorem that inititated the mathematical study of CRNs was proved in 1972 [2]. We give a modern version due to [5].

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

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

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

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

In what follows, x denotes a vector in $\mathbb{R}^v$, a a real number, and $\mathbf{1}_S$ a vector in $\mathbb{R}^v$ that is 1 on S and 0 else.

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

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

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

$$\mathrm{Im}\, S^T + \mathrm{Ker}\, L_o = \mathbb{R}^v$$

Proof. $\delta = 0$ is equivalent to $\mathrm{Ker}\, S \cap \mathrm{Im}\, L_o^T = \{0\}$.
Take orthogonal complement of both sides to get

$$(\mathrm{Ker}\, S)^T + \mathrm{Im}\,(L_o^T)^T = \mathbb{R}^v$$

The LHS equals $\mathrm{Im}\, S^T + \mathrm{Ker}\, L_o$ by linear algebra. **Done.**

Proof of $\Longrightarrow$

Assume

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

has pos. equil. x^* and prove CSC.

Existence of pos. equil. $x^* > 0$ shows that, since there is $x^* > 0$ with $\dot{x}^* = 0$,

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

No hidden dynamics (or $\delta = 0$) 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 DII), 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 $\Leftarrow$

Assume CSC, then show that

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

Exercise: Use the two exercises on pg 22 to deduce that the **blue** equation can be rewritten 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 $\mathrm{Im}\, S^T$ and 2nd over $\mathrm{Ker}\, L$.

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:

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

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:

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

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FURTHER DEVELOPMENTS

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

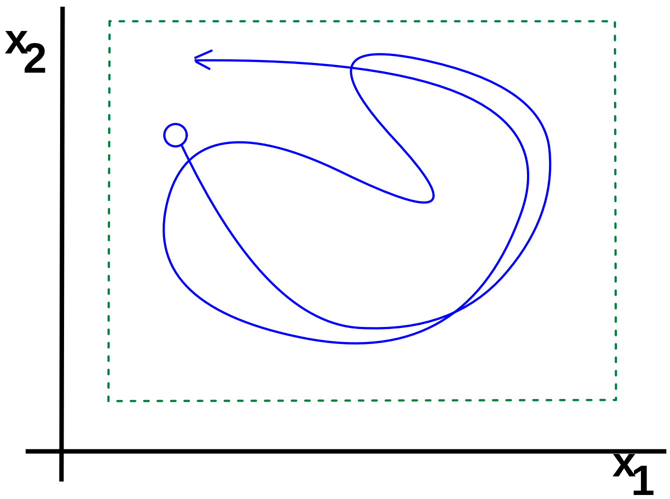
Bounded Orbits

Theorem [5]. Suppose $\boldsymbol{\delta} = \mathbf{0}$. Then

$$\dot{\boldsymbol{x}} = -\boldsymbol{S}\boldsymbol{L}_{\mathbf{out}}^{T}\boldsymbol{\psi}(\boldsymbol{x})$$

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

Note: $\Leftarrow$ follows from 0-def. But $\Rightarrow$ 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.

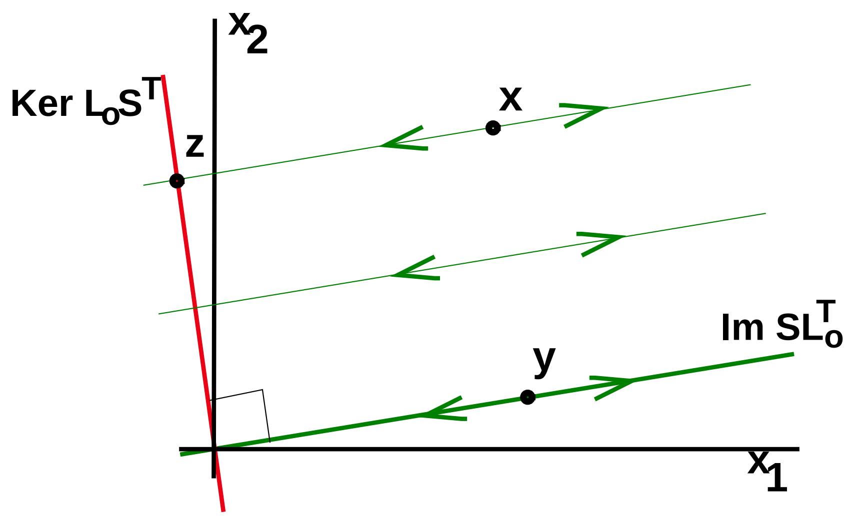
Constants of the Motion and Stability

Exercise: Show that $(\text{Im } A)^{\perp} = \text{Ker } A^T$.

Thus the orbit $x(t)$ of

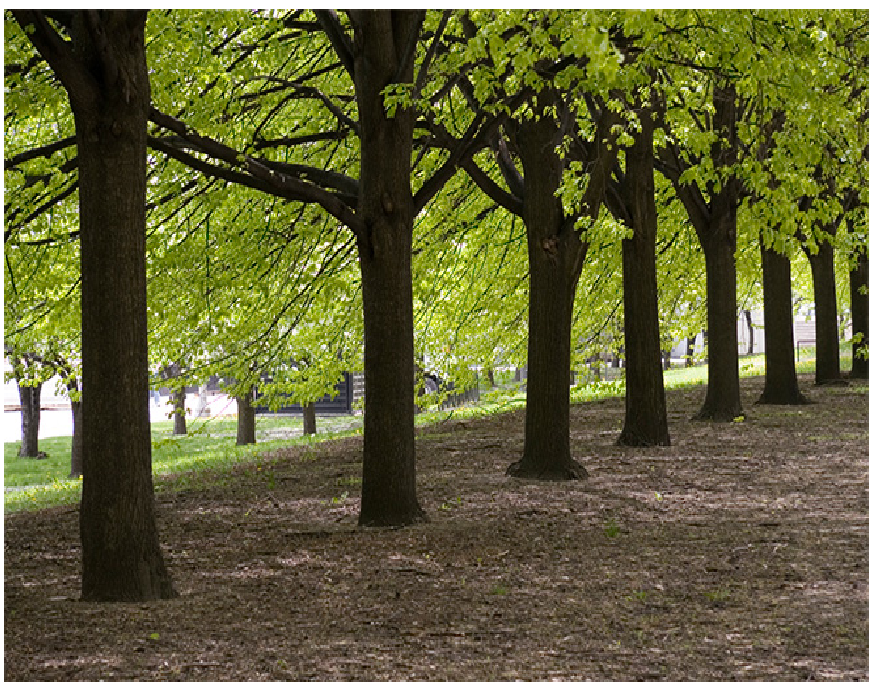
$$\dot{x} = -SL_{\text{out}}^T \psi(x)$$

$\dot{x}$ is parallel to Im SL_o^T and $x(t) = z + y(t)$, z constant.
z is the orthogonal proj onto Ker $L_o S^T$.



Theorem [5]. Suppose $\delta = 0$ and CSC. Then:
(i) For every $z \in \text{Ker } LS^T$, there is a unique $y \in \text{Im } SL^T$ such that $y + z$ is a positive equilibrium.
(ii) 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.

FORMULATION OF THE MATRIX TREE THEOREM



Lots of Trees

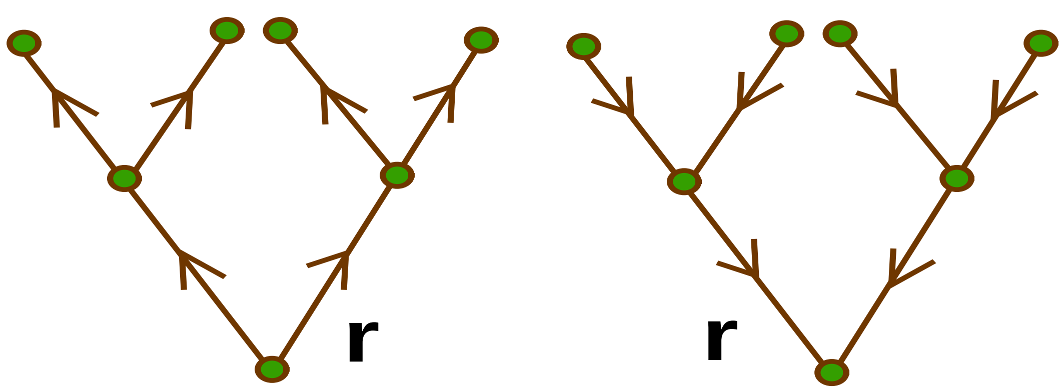
Definition: For the purpose of this section, we write:

$$\begin{aligned} L_{\text{in}} &= (EW)(E^T - B^T) \\ L_{\text{out}} &= (-BW)(E^T - B^T) \\ \underline{L} &= (EW - BW)(E^T - B^T) \\ &= (E - B)W(E^T - B^T) \end{aligned}$$

Definition: A spanning **out**-tree rooted at vertex r (**SOTR**) is a graph such that
- if $i \neq r$, then **in**-degree at i equals 1.
- **in**-degree at r equals 0.
- no directed cycles.

For a **SITR**: swap “out" and “in".

Figure: Left: **out**-tree rooted at r, and right: **in**-tree.



Definition: A spanning **undirected** tree rooted at r (**SUTR**) is a connected graph with no cycles. (No loose vertices.)

And To Each Their Tree

$$\begin{aligned} L_{\textbf{in}} &= (EW)(E^T - B^T) \\ L_{\textbf{out}} &= (-BW)(E^T - B^T) \\ \underline{L} &= (EW - BW)(E^T - B^T) \end{aligned}$$

$$(EW)_{ij} = \sum_k E_{ik} W_{kj}$$

So the effect of the diagonal matrix W is to multiply the ith edge (column) by the ith entry W_{ii}.

Definition: The **weight** $W(T)$ of a tree T is the product of the weights of all its edges. Allow arbitrary (positive) weights. The weighted adjacency matrix is denoted by S and the diagonal row-sum matrix of S is denoted by D.

Definition: For a Laplacian L, let $\mathcal{T}_r$ be the **appropriate** set of spanning trees rooted at r. By this we mean:

- For L_{in}, it is the SOTR's
- For L_{out}, it is the SITR's
- For $\underline{L}$, it is the SUTR's.

Matrix Tree Theorems

Definition: Assume G has n vertices. Let I_r be the set V of all vertices **except** r.

Theorem 2 (Matrix Tree): L a Laplacian. Then

$$q_r := \det L[I_r, I_r] = \sum_{T_r \in \mathcal{T}_r} W(T_r)$$

Observation 1: If G has $k > 1$ reaches, then no SORTs. DII Thm 9: L has eval 0 with mult. $k > 1$. Reducing L by 1 column and row will give $\det L[I_r, I_r] = 0$.

Exercise: Show that for a digraph G with one reach, if r is not in a cabal, then $\det L[I_r, I_r] = 0$.

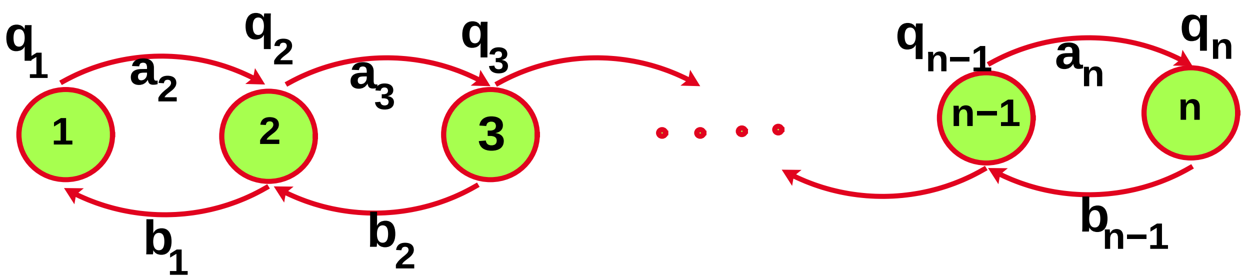
The proofs of the cases where $L = L_{\text{in}}$ or $L = L_{\text{out}}$ are almost identical (just swap “in" and “out"). In the undirected case: reaches are connected components.

Theorem 3: Furthermore

$$\sum_r q_r L_{ri} = 0$$

Observation 2: Thus the **weight** of rooted trees at vertex r has a probabilistic interpretation. (Gives stationary probability measure under rw.)

Exercises Using Path Graph



Exercise: For the graph above write out L_{in}.

Exercise: Let q_k the weight of out-trees rooted in vertex k. Show that $q_k = \prod_{k+1}^{n} a_i \prod_{i=1}^{k-1} b_i$.

Denote by q the row-vector $(q_1, q_2, \cdots q_n)$.

Exercise: Show that $qL_{\text{in}} = 0$.

Exercise: Repeat exercises on this page, but now for L_{out} and $\underline{L}$.

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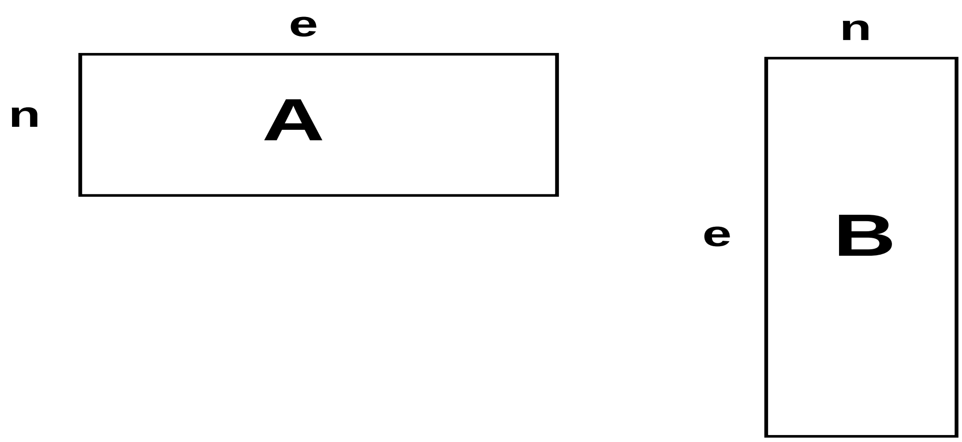
PROOF OF MATRIX TREE FOR L_{in}

First Use Cauchy-Binet



Definition (DI): I (K) subset of the row (column) labels of matrix A. $A[I,K]$ consists of the entries of A in $I \times K$.

Exercise: $L = AB$ where A and B matrices as depicted above. Show that matrix multiplication implies

$$L[I,J] = A[I, \text{all}]B[\text{all}, J]$$

Now let $|I| = |J| = k$. By Cauchy-Binet (Thm 3 of DI):

$$\det((AB)[I,J]) = \sum_{K,|K|=k} \det(A[I,K]) \det(B[K,J])$$

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

Proposition: $I_r := V \setminus \{r\}$. Then $\det\left(L_{\text{in}}[I_r, I_r]\right)$ equals

$$\sum_{K,|K|=n-1} \det((EW)[I_r, K]) \det((E^T - B^T)[K, I_r])$$

Assume K Not a Tree

Recall: **SOTR** is a graph such that

1. if $i \neq r$, then in-degree at i equals 1.

2. in-degree at r equals 0.

3. no directed cycles.

$$\det\left(L_{\text{in}}[I_r, I_r]\right) = \sum_K \det((EW)[I_r, K]) \det((E^T - B^T)[K, I_r])$$

In RHS, each choice of K selects ***n* – 1 edges**.

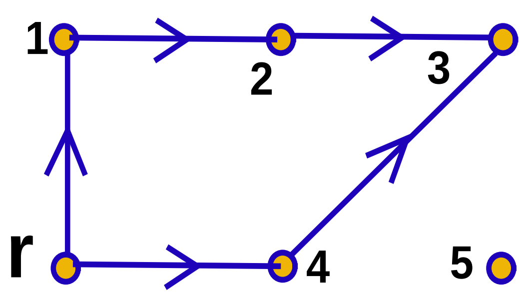
If the $n - 1$ edges K <u>do not</u> form a SOTR:

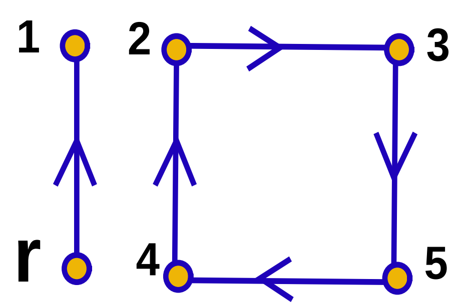
Fail 1 $\Rightarrow \exists\, i \neq r$ with in-degree 0 $\Rightarrow E$ has zero row, or

Fail 2 $\Rightarrow$ in-degree at r not 0 $\Rightarrow$ same as fail 1, or

Fail 3 $\Rightarrow \partial$(cycle)$= 0 \Rightarrow \ker(E^T - B^T)$ has dim > 0.

Example w. 6 vertices and 5 edges: Left: column 5 of





$E[I_r, K]$ is 0. Right: $(E^T - B^T)[\{2,3,4,5\},\{2,3,4,5\}]$ has row sum 0.

Total contribution: zero!

Assume K a Tree

If the $n-1$ edges of K do form a SOTR:
Relabel vertices and edges so that:
1. If $j > i$, then path from $r \rightsquigarrow i$ does not pass through j.
2. And then so that edge i ends in vertex i.

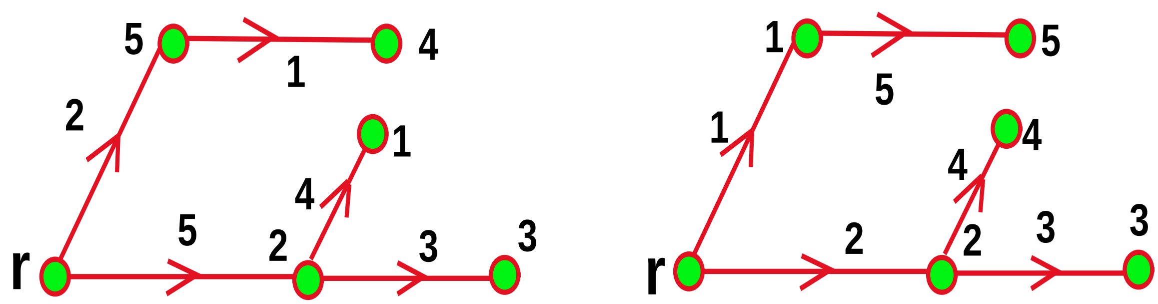
For each K, same permutations are done in two factors:

$$\sum_{K, |K|=n-1} \det((EW)[I_r, K]) \det((E^T - B^T)[K, I_r])$$

Thus the permutations have no net effect: $(-1)^{\text{even}}$!

Result: $E[I_r, K]$ is the identity, and $B[I_r, K]$ is upper tridiag with 0 on diag.

Example of SOTR w. 6 vertices and 5 edges: Left: Before



permutations. Right: After.

Total contribution: The weight of the tree!

Exercise: Repeat proof for L_{out} (trivial) and $\underline{L}$ (needs minor adaptation).

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TREES,
UNICYCLES,
PROBABILITY

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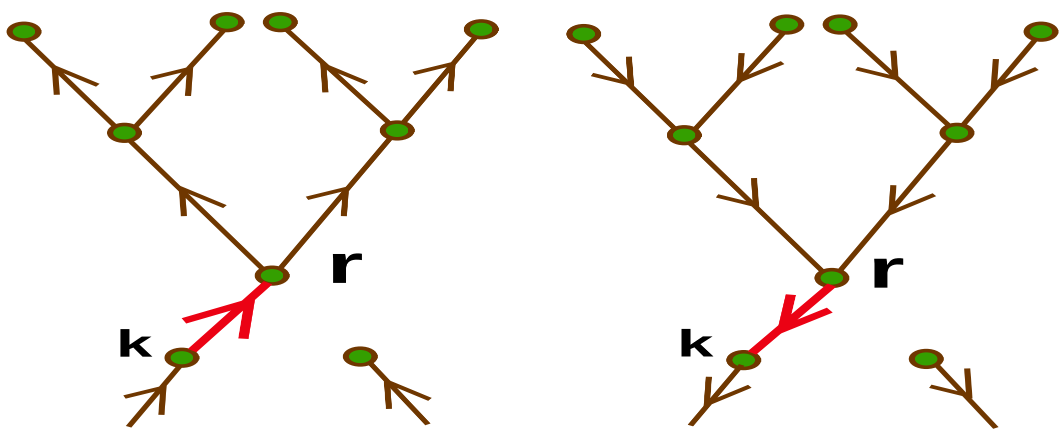
Lots of Unicycles, and to Each ...

Definition: An **augmented** spanning **out**-tree rooted at vertex r (**ASOTR**) is a
SOTR plus 1 extra edge $k \to r$ such that $(L_{\text{in}})_{rk} > 0$.
Similarly, an **ASITR** is a
SITR plus 1 extra edge $r \to k$ such that $(L_{\text{out}})_{rk} > 0$.

Left: Augmented **out**-tree. Right: Augmented **in**-tree.



Definition: An augm. spanning undirected tree rooted at r (**ASUTR**) is a SUTR with 1 extra edge from r to a neighbor.

Remark: These graphs contain **1 cycle**! They are most commonly called **cycle-rooted trees** or **unicycles**.

Definition: For a Laplacian L, let $\mathcal{A}_r$ be the **appropriate** set of augm. spanning trees rooted at r. By this we mean:
- For L_{in}, it is the ASOTR's
- For L_{out}, it is the ASITR's
- For $\underline{L}$, it is the ASUTR's.

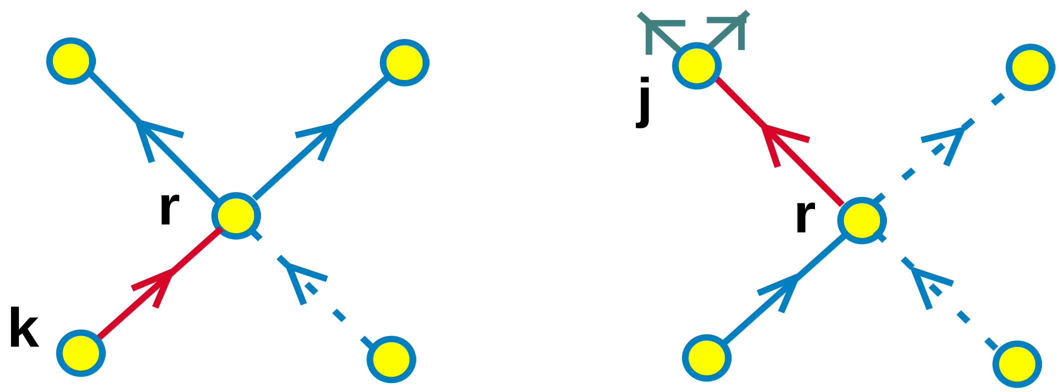
Counting Unicycles at Vertex r

Exercise: Show that a unicycle contains exactly 1 cycle. (*Hint: contract along the spanning tree. The cycles are the remaining edges.*)

Two ways to compute the weight of the L_{in}-appropriate r-rooted unicycles (ASOTR's) for a given graph G (see figure).

RECALL: S is the weighted (by W) adjacency matrix. The diagonal row-sum matrix is D.

Left(**1**): To SOTR at r, add edge from *parent* k of r to r.
Right(**2**): To SORT at *child* j of r, add edge from r to j.



Total weight of unicycles rooted at r is denoted by u_r.

$$\text{From 1:} \quad \mathbf{u_r = \sum_k q_r S_{rk} = q_r D_{rr}}$$

(Proof: The row-sum of S is given by D.)

$$\text{From 2:} \quad \mathbf{u_r = \sum_j q_j S_{jr}}$$

Proof of Theorem 3

EASY ! Equate the two expressions:

$$0 = q_r D_{rr} - \sum_j q_j S_{jr} = [q(D - S)]_r = \left[q L_{\text{in}} \right]_r$$

which proves Thm 3 for L_{in}.

DONE!

Remark: If S is a rw walk matrix, then D is identity and q is the stationary probability measure.

Exercise: Prove Theorem 3 for L_{out} and $\underline{L}$.

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