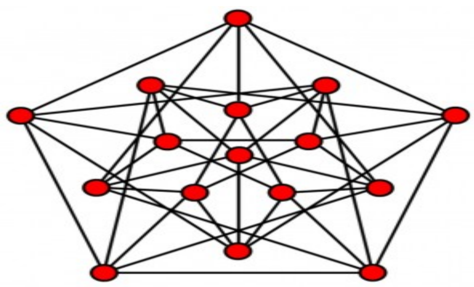
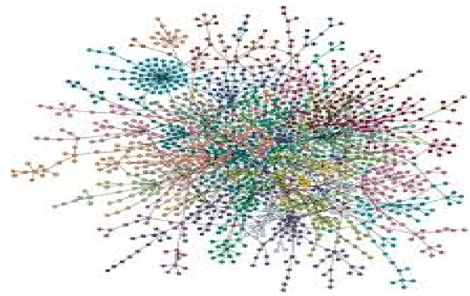
Pescara, Italy, July 2019





DIGRAPHS IV
The Matrix Tree Theorem

Based on various sources.

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Conference Website:
www.sci.unich.it/mmcs2019

SUMMARY:

* 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

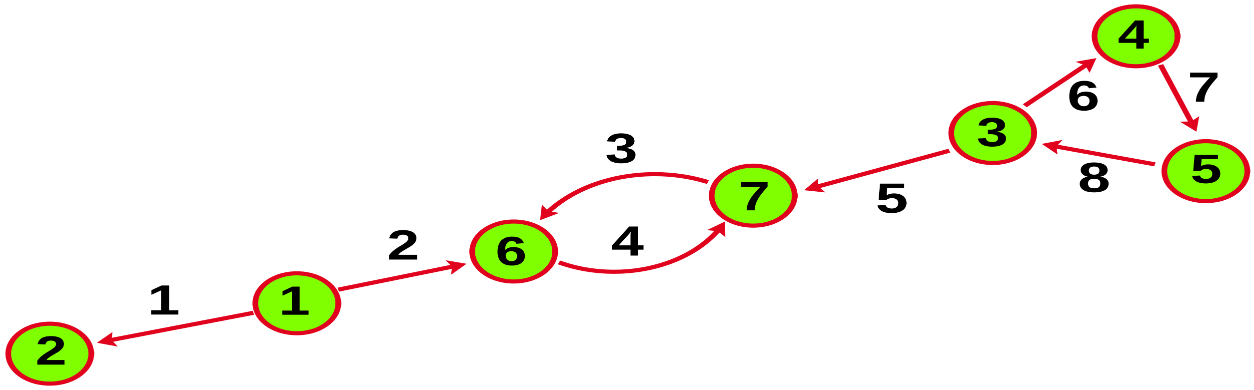
Matrix Tree Theorems

Proof of Matrix Tree Theorems

Trees and Unicycles

BOUNDARY OPERATORS

The Boundary Matrices



Definition: Given a digraph G, define matrices B (for Begin) and E (for End)

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

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

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

Edges are columns. vertices are rows.

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

$$\boldsymbol{\partial := E - B}$$

From Boundary to Adjacency

Let V the set 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 1: Check the facts as well as the ones mentioned for BB^T and BE^T.

... and on to Laplacians

The Lemma immediately implies:

Theorem 1: In the notation of DI, we have:

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

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:

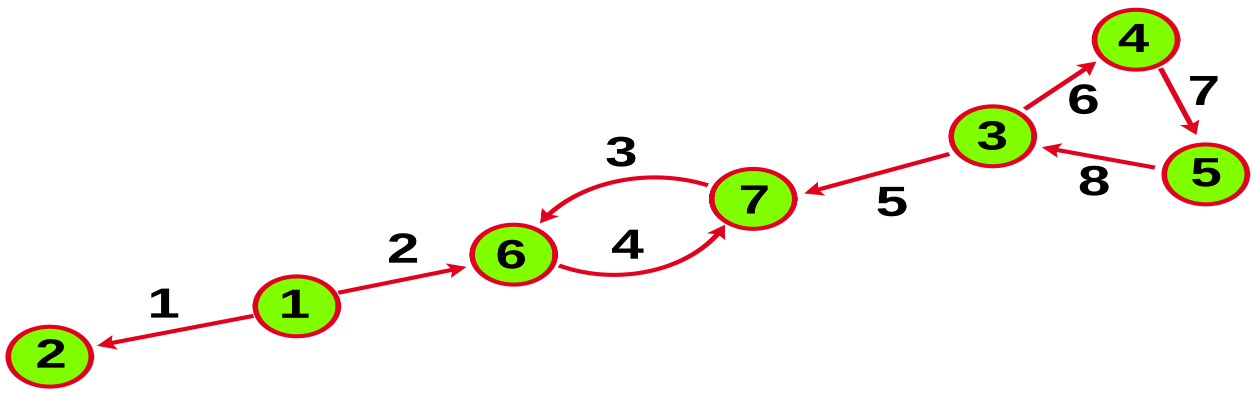
Corollary: We have:

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

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

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

Example



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

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

And $\underline{L} = L_{\text{in}} + L_{\text{out}}$ is symmetric.

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)

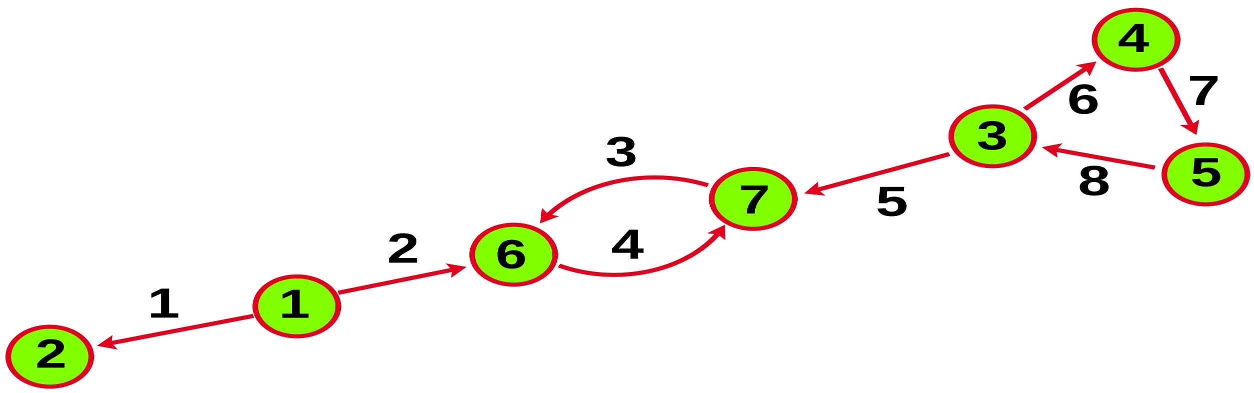
Remark: Note that

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

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

Be careful: The symbol $\mathcal{L}_{\text{in}}$ 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



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

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

Notice that the sum of these two is NOT symmetric. Edge 6 has received two different weights.

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FORMULATION OF THE MATRIX TREE THEOREM

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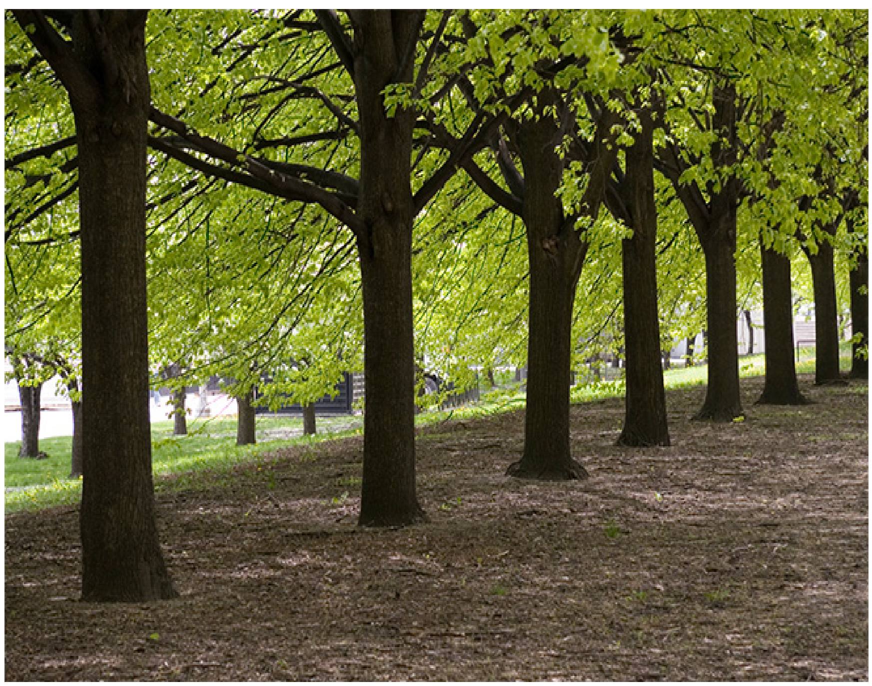


Lots of Trees

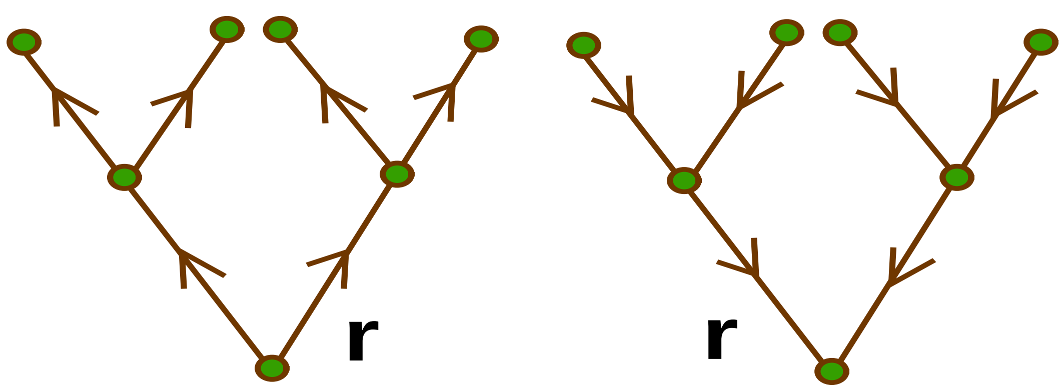
Definition: For the purpose of this section, we write:

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

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.

Definition: For a Laplacian L, let $\mathcal{W}_r$ 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 of all vertices **except** r.

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

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

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

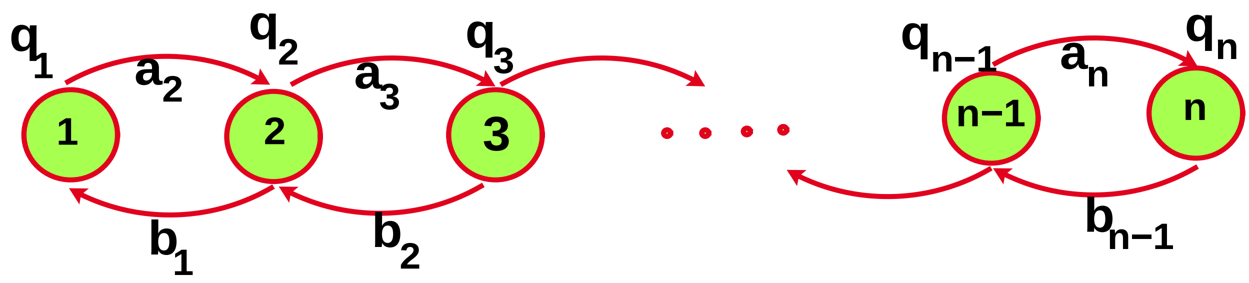
The proofs of the cases where $L = L_{\text{in}}$ or $L = L_{\text{out}}$ are almost identical (just swap "in" and "out"). The undirected is slightly different, but the same techniques work.

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 2: For the graph above write out L_{in}, L_{out}, and $\underline{L}$.

Exercise 3: Let q_k the weight of out-trees rooted in vertex k. Show that $q_k = \prod_{k+1}^{n} a_i \prod_{i=1}^{k-1} b_i$.

Exercise 4: Show that $qL_{\text{in}} = 0$.

Exercise 5: Repeat exercises 2 and 3 for L_{out}, and $\underline{L}$.

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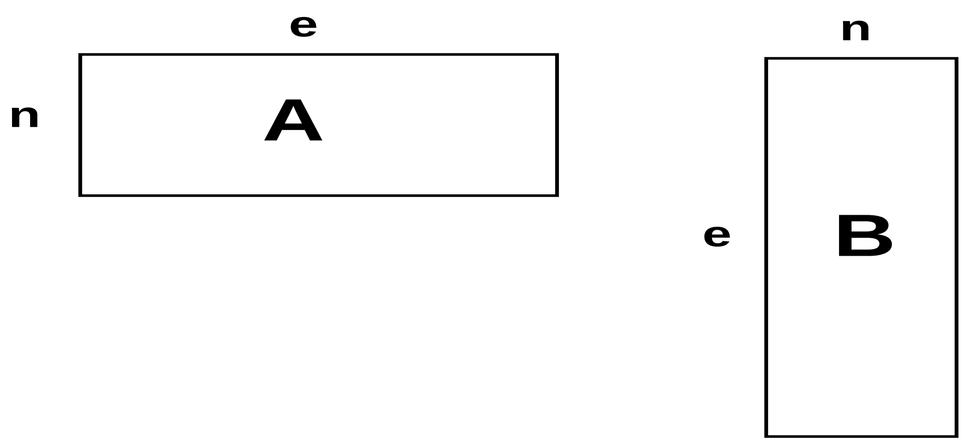
PROOF OF MATRIX TREE THEOREMS

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 6: $L = AB$ 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: $I_r := V \backslash \{r\}$. Then $\det(L_{\text{in}}[I_r, I_r])$ equals

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

Assume No 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.

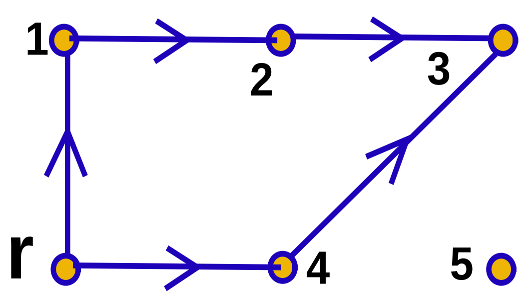
$$\det\left(L_{\text{in}}[I_r, I_r]\right) = \sum_K \det((EW)[I_r, K]) \det((E^T - B^T)[K, I_r])$$

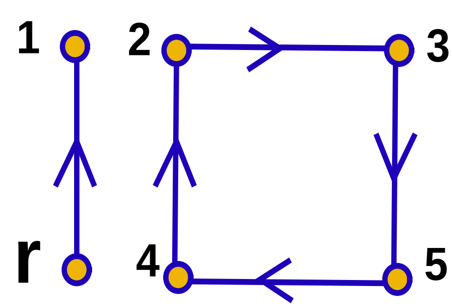
In RHS, each choice of K selects $n-1$ edges.

If the $n-1$ edges K do not form a SOTR:

They fail 1. or 2. $\Longrightarrow$ E has column of zeroes, or they fail 3. $\Longrightarrow$ $(E^T - B^T)$ contains a cycle-Laplacian.

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 Tree

If the $n-1$ edges K do form a SOTR:
Relabel vertices twice, 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.

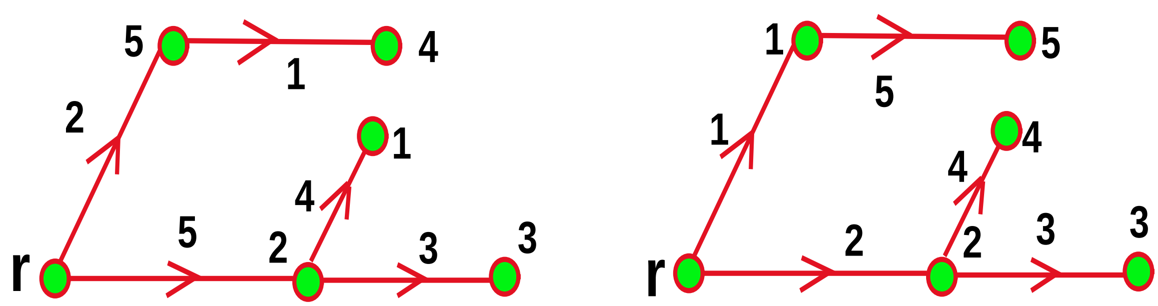
For each K, the same permutations are done in two factors:

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

Thus no net effect!

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

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



permutations. Right: After.

Total contribution: The weight of the tree!

Exercise 7: Repeat proof for L_{out} (trivial) and $\underline{L}$ (needs minor adaptation).

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TREES,
UNICYCLES,
PROBABILITY

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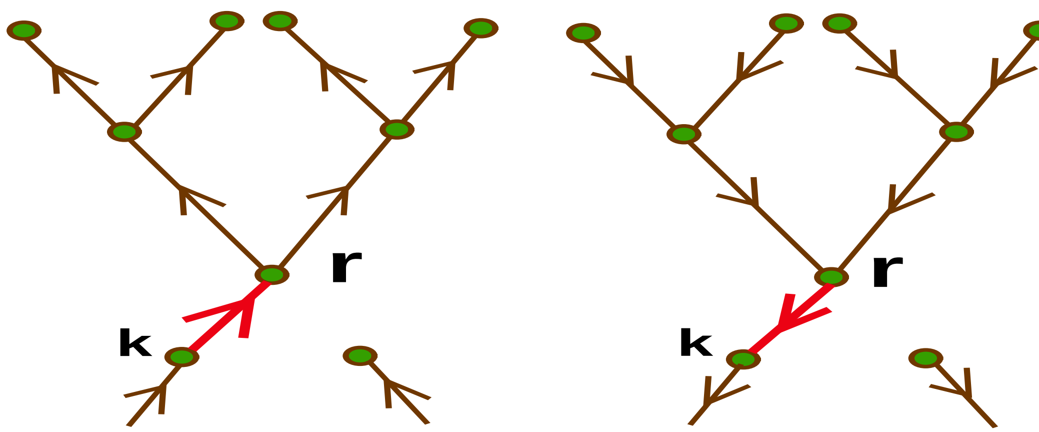
Lots of Unicycles, and to Each ...

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**.

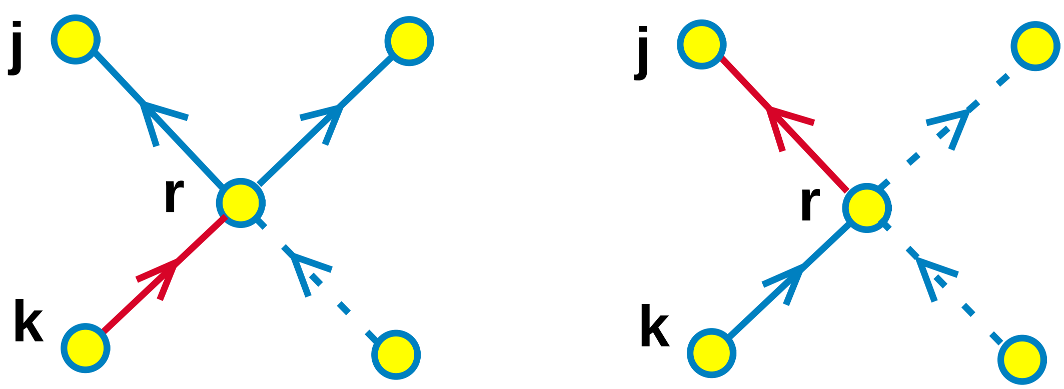
Definition: For a Laplacian L, let $\mathcal{A}_r$ be the **appropriate** set of augm. spanning trees rooted at r. By this we mean:
- For L_{in}, it is the ASOTR's
- For L_{out}, it is the ASITR's
- For $\underline{L}$, it is the ASUTR's.

Counting Unicycles

Exercise 8: 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).

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 by u_r.

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

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

Proof of Theorem 3

Equate the two expressions:

$$q_r D_{rr} - \sum_j q_j S_{jk} = qL_{\text{in}} = 0$$

which proves Thm 3 for L_{in}.

DONE!

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

Exercise 9: Prove Theorem 3 for L_{out} and $\underline{L}$.

References

[1] P. De Leenheer, *An Elementary Proof of a Matrix Tree Theorem for Directed Graphs*, **https://arxiv.org/abs/1904.12221**.