Characterizing PSSs through graph theory

S. Kerleau, C. Royer, D. Cornaz

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Dauphine | PSL
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LAMSADE
UMR CNRS 7243
laboratoire d'analyse et modélisation de systèmes pour l'aide à la décision

Why should we care ?

Question

How to minimize a smooth function f ? (∇f is not available).

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Through direct search:

- **Inputs**: $x \in \mathbb{R}^n$, $M = \{c_1, \ldots, c_s\} \subset \mathbb{R}^n$.
- Compare $f(x)$ to each $f(x + \alpha c_i)$.
- If $f(x)$ is the smallest, decrease α.
- Otherwise, $x \leftarrow x_0 + \alpha c_i$.

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If the elements of M are *'well spread'* in $\mathbb{R}^n$, the algorithm converges.

Positive spanning sets and positive bases

Definition

A **PSS** is a set of vectors well spread in $\mathbb{R}^n$.
A **positive basis** is minimal for this property.

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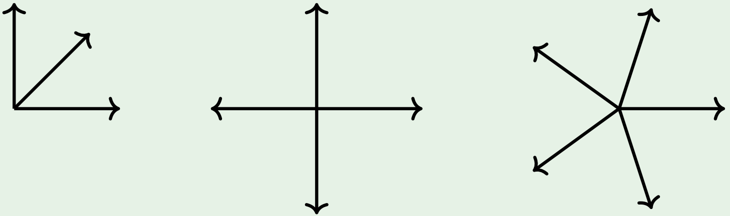
Examples in $\mathbb{R}^2$



One of these is not a PSS...

Positive spanning sets and positive bases

Definition

A **PSS** is a matrix M such that $y^\top M \leq 0^\top$ implies $y = 0$.
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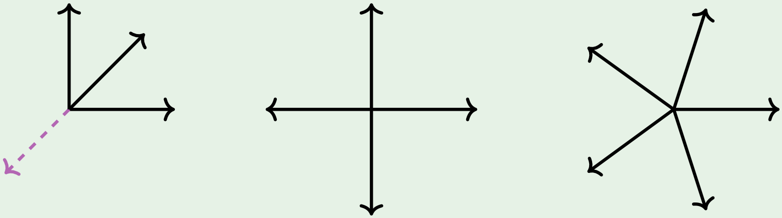

No close neighbor for the dashed vector.

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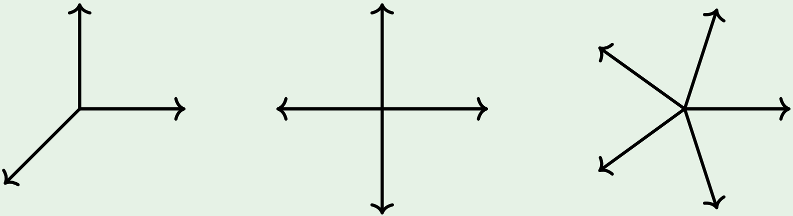

Which is not a positive basis ?

Positive spanning sets and positive bases

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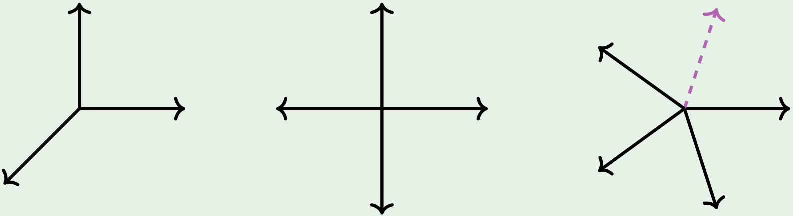
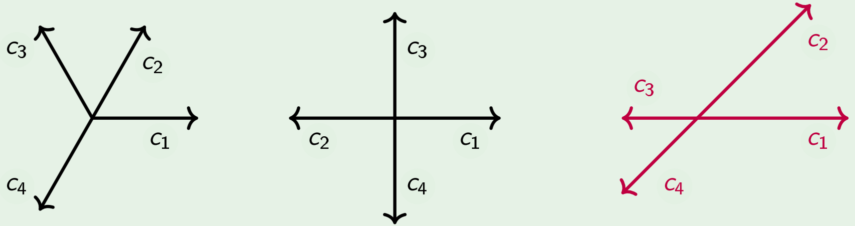


The dashed vector can be removed.

Structural equivalence

Quiz

Examples in $\mathbb{R}^2$

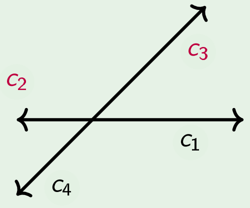


Which set is 'equivalent' to the red ?

We're looking for transformations that leave the 'positively spanning' property invariant.

Quiz

Examples in $\mathbb{R}^2$



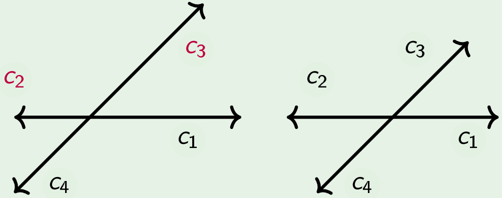
Reorder the elements.

Definition (Structural equivalence $\equiv$)

M is **structurally equivalent** to N if $M = \quad NP \quad$ where P is a permutation matrix,

Quiz

Examples in $\mathbb{R}^2$



Rescale them.

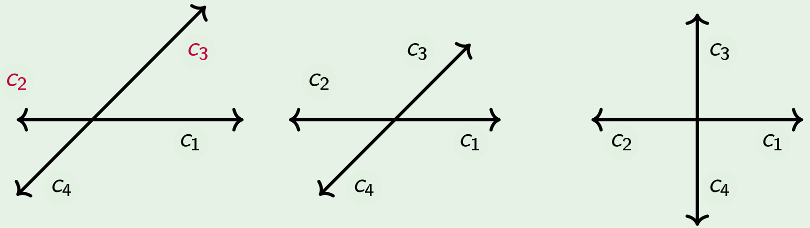
Definition (Structural equivalence $\equiv$)

M is **structurally equivalent** to N if $M = \quad NPD$ where P is a permutation matrix, D is diagonal with positive entries

Structural equivalence

Quiz

Examples in $\mathbb{R}^2$



Change bases.

Definition (Structural equivalence $\equiv$)

M is **structurally equivalent** to N if $M = BNPD$ where P is a permutation matrix, D is diagonal with positive entries and B is invertible.

An algebraic approach

Remark

- *If* $M \equiv N$*:* $\begin{cases} M \text{ PSS} & \iff & N \text{ PSS.} \\ M \text{ positive basis} & \iff & N \text{ positive basis.} \end{cases}$.

An algebraic approach

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- *M positive basis* $\implies n+1 \leq |M| \leq 2n.$

An algebraic approach

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- M *positive basis* $\implies n+1 \leq |M| \leq 2n$.
- $\begin{bmatrix} I_n & -1_n \end{bmatrix}$ *and* $\begin{bmatrix} I_n & -I_n \end{bmatrix}$ *are positive bases, where* $-1_n = \begin{bmatrix} -1 \\ \dots \\ -1 \end{bmatrix}$.

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- $\begin{bmatrix} I_n & -1_n \end{bmatrix}$ *and* $\begin{bmatrix} I_n & -I_n \end{bmatrix}$ *are positive bases, where* $-1_n = \begin{bmatrix} -1 \\ \dots \\ -1 \end{bmatrix}$.
- *PSSs span* $\mathbb{R}^n$ *with positive combinations.* *obviously...*

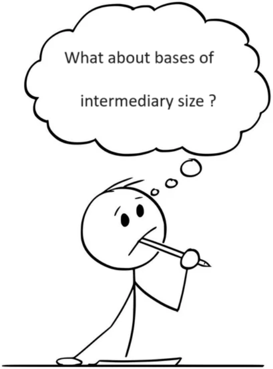
Characterizing positive bases

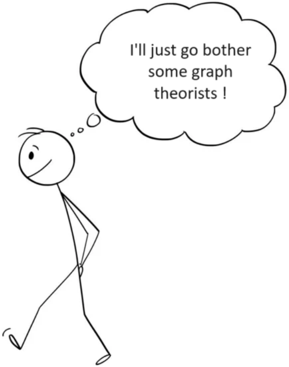
Proposition

M *positive basis and* $|M| = n+1 \implies M \equiv \begin{bmatrix} I_n & -1_n \end{bmatrix}$.
M *positive basis and* $|M| = 2n \implies M \equiv \begin{bmatrix} I_n & -I_n \end{bmatrix}$.

Application

In $\mathbb{R}^3$, *any non-minimal PSS of size* 5 *satisfies* $M \equiv \begin{bmatrix} 1 & 0 & 0 & -1 & \times \\ 0 & 1 & 0 & -1 & \times \\ 0 & 0 & 1 & -1 & \times \end{bmatrix}$.


What about bases of
intermediary size ?

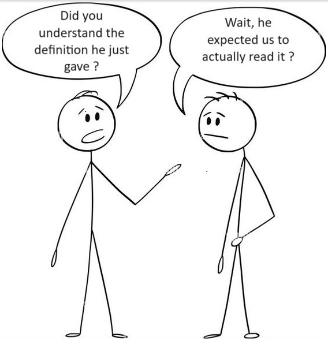

I'll just go bother
some graph
theorists !

Nec matrices

Definition (Negative echelon column matrix)

$\mathrm{N} \in \mathbb{R}^{n \times s}$ is a **nec matrix** if there exists a sequence $z_0 = 1 < z_1 < z_2 < \cdots < z_{s-1} \leq n$ of integers satisfying

1. For all $j \in [\![1, s-1]\!]$, for all $i \in [\![z_j, n]\!]$, $\mathrm{N}_{i,j} = 0$.
2. For all $j \in [\![1, s-1]\!]$, for all $i \in [\![z_{j-1}, z_j - 1]\!]$, $\mathrm{N}_{i,j} < 0$.
3. $\mathrm{N}_{i,s} < 0$, for all $i \geq z_{s-1}$.



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Example

$$\begin{bmatrix} -1 & \times & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}, \quad \begin{bmatrix} -1 & \times & \times & \times \\ -1 & \times & \times & \times \\ 0 & -1 & \times & \times \\ 0 & -1 & \times & \times \\ 0 & 0 & -1 & \times \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad \begin{bmatrix} -1 & \times & \times \\ -1 & \times & \times \\ 0 & -1 & \times \\ 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}.$$

Nec and PSS

Theorem

$M \equiv \begin{bmatrix} I_n & N & X \end{bmatrix}$ *(with N nec)* $\implies$ M PSS

Proof.

Simply note that $-1_n \in cone(M)$! □

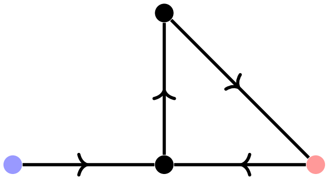
Example

$$\begin{bmatrix} -1 & \times & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & \times & \times & \times \\ -1 & \times & \times & \times \\ 0 & -1 & \times & \times \\ 0 & -1 & \times & \times \\ 0 & 0 & -1 & \times \\ 0 & 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & \times & \times \\ -1 & \times & \times \\ 0 & -1 & \times \\ 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}.$$

Strong edge-connection

Definition (Strongly connected)

A digraph G is **strongly connected** if for each two vertices u and v, an oriented path joins u to v.



Not strongly connected: no path from red to blue.

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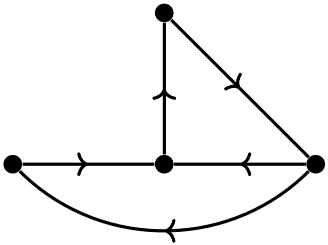
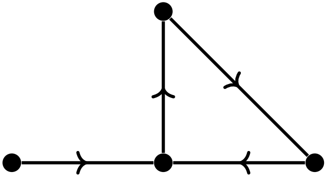


A strongly connected digraph G.

Ears

Definition (Ear)

An **ear** is a directed path with no vertices in G, except the extremities.



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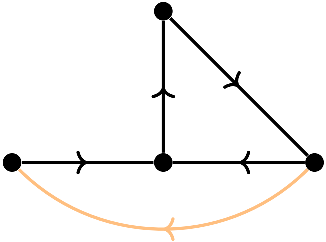

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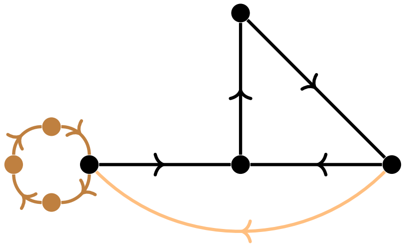

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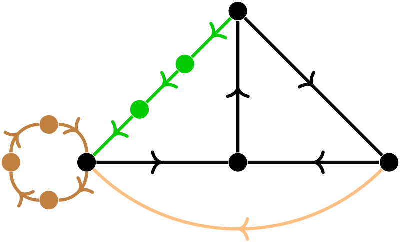

Three ears of the black digraph G.

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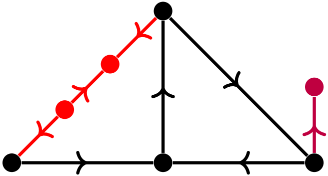

Not ears !

Ear-decomposition

Characterization

G strongly connected $\iff$ *G can be built from a sequence of ears.*

An ear-decomposition of the boat G.

Ear-decomposition

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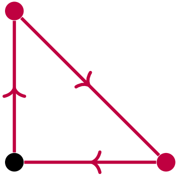

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Ear-decomposition

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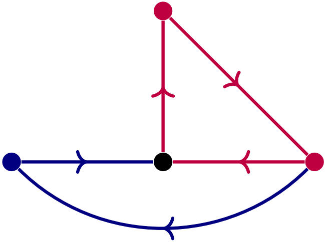

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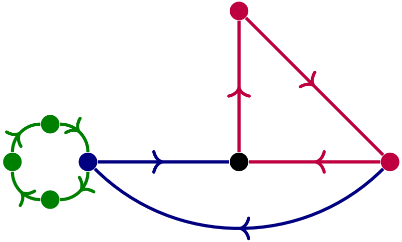
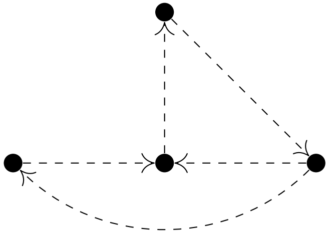


An ear-decomposition of the boat G.

Network matrices

PSSs arise from strongly connected digraphs through **network matrices**.

G = 

Draw your favourite connected digraph G.

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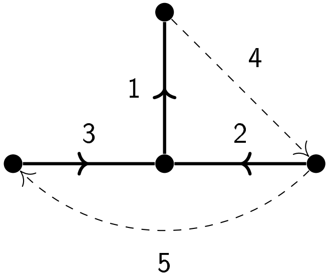
G = 

Choose a spanning tree. That's your basis.

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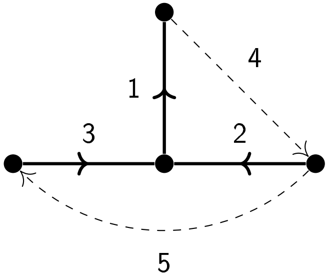
G = 

$$M = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

The n^{th} column is the n^{th} arc expressed in the basis.

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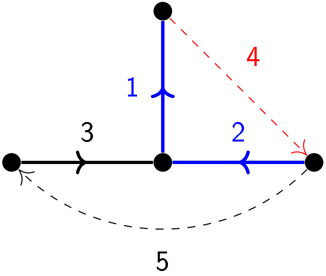
G = 

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arcs: $-1-2=4$ **columns:** $-c_1-c_2=c_4$

Network matrices

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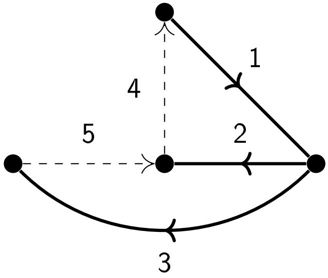
$G =$



$$M = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

All network matrices are equivalent.

Network matrices

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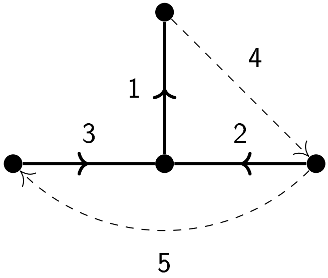
G =



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G is strongly connected $\implies$ M is a PSS.

Network matrices

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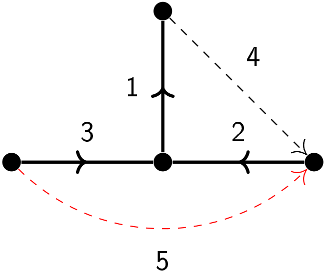
G = 

$$M = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & -1 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

G is **not** strongly connected $\implies$ M is **not** a PSS.

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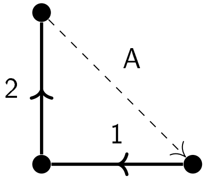
Strongly connected $\iff$ PSS ?

G strongly connected $\iff$ G associated to $\begin{bmatrix} \mathtt{I}_n & N & X \end{bmatrix}$.

Let's prove it.

Strongly connected $\iff$ PSS ?

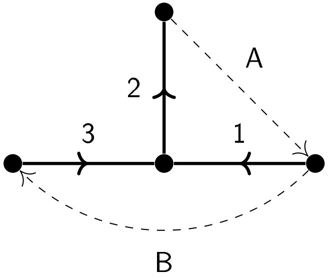
G cycle $\implies$ network matrix $\begin{bmatrix} \mathrm{I}_n & -\mathbb{1}_n \end{bmatrix}$.



$$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}$$

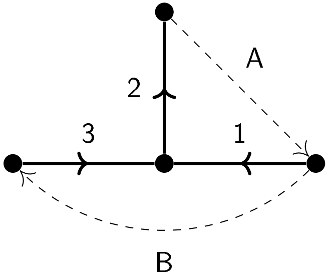
Strongly connected $\iff$ PSS ?

Add an ear. What happens ?



Strongly connected $\iff$ PSS ?

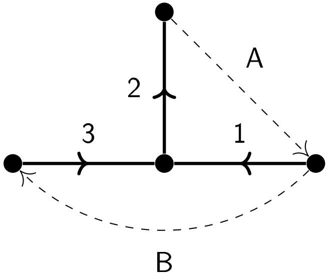
The previous matrix is contained in the new one...



$$\begin{bmatrix} 1 & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

Strongly connected $\iff$ PSS ?

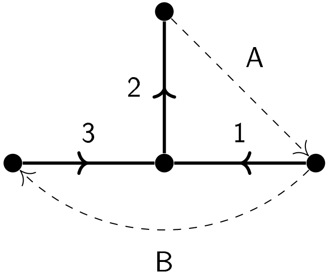
...with zeros ending its columns.



$$\begin{bmatrix} 1 & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

Strongly connected $\iff$ PSS ?

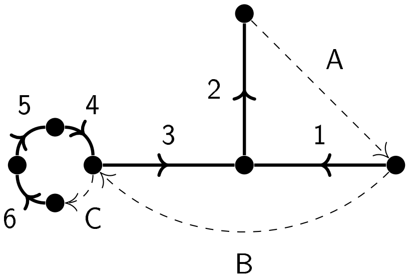
The new column ends with -1.



$$\left[\begin{array}{c|cc} & -1 & 1 \\ I_3 & -1 & 0 \\ & 0 & -1 \end{array}\right]$$

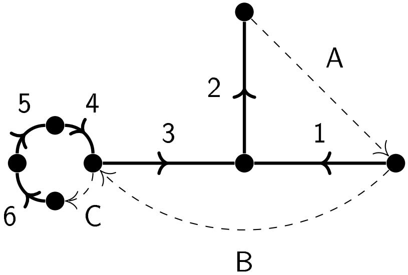
Strongly connected $\iff$ PSS ?

Add another ear.



Strongly connected $\iff$ PSS ?

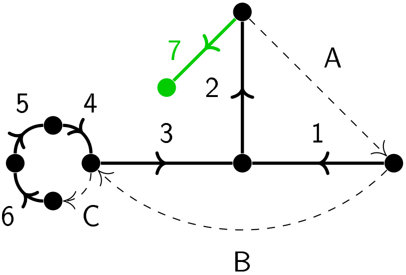
Same phenomenon ! **nec** matrix !



$$\left[\begin{array}{cccc} & -1 & 1 & 0 \\ & -1 & 0 & 0 \\ & 0 & -1 & 0 \\ I_6 & 0 & 0 & -1 \\ & 0 & 0 & -1 \\ & 0 & 0 & -1 \end{array}\right]$$

Strongly connected $\iff$ PSS ?

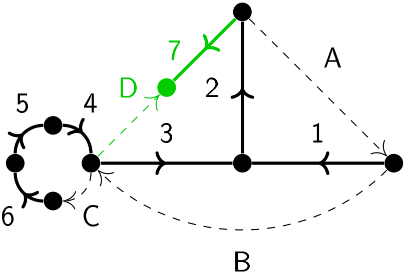
Non-ears break the pattern.



$$\begin{bmatrix} I_7 & \begin{matrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{matrix} \end{bmatrix}$$

Strongly connected $\iff$ PSS ?

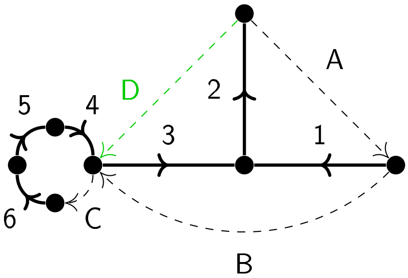
Non-ears break the pattern.



$$\begin{bmatrix} & -1 & 1 & 0 & 0 \\ & -1 & 0 & 0 & 1 \\ & 0 & -1 & 0 & 1 \\ I_7 & 0 & 0 & -1 & 0 \\ & 0 & 0 & -1 & 0 \\ & 0 & 0 & -1 & 0 \\ & 0 & 0 & 0 & 1 \end{bmatrix}$$

Strongly connected $\iff$ PSS ?

Trivial ears add useless columns.



$$\left[\begin{array}{cc} I_6 & \begin{matrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \end{matrix} \end{array}\right]$$

Graphs and PSSs

Theorem

Graph strongly connected $\iff$ its network matrices are PSSs !

Remark

Characterizations of strongly connected digraphs can be restated in the language of linear algebra !

Restating properties

Characterization

G strongly connected $\iff$ *a network matrix is* $\begin{bmatrix} I & N & X \end{bmatrix}$ *(N nec).*

G not strongly connected $\iff$ *it is* $\begin{bmatrix} I & N & X \\ 0 & 0 & A \end{bmatrix}$ *(A non-negative).*

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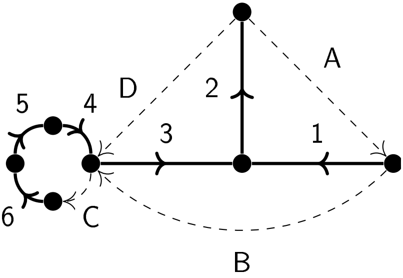

G is strongly connected.

$$\overset{I}{}\quad\overset{N}{}\quad\overset{X}{}$$

$$\left[\begin{array}{c|ccc|c} & -1 & 1 & 0 & 0 \\ & -1 & 0 & 0 & -1 \\ I_6 & 0 & -1 & 0 & -1 \\ & 0 & 0 & -1 & 0 \\ & 0 & 0 & -1 & 0 \\ & 0 & 0 & -1 & 0 \end{array}\right]$$

Restating properties

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G strongly connected $\iff$ *a network matrix is* $\begin{bmatrix} I & N & X \end{bmatrix}$ *(N nec).*

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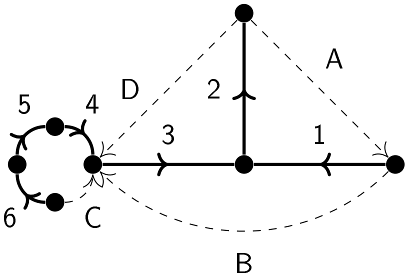


G is not strongly connected.

$$\begin{array}{cccc} I & N & X & \\ \left[\begin{matrix} I_3 \\ O_3 \end{matrix}\right. & \begin{matrix} -1 & 1 \\ -1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{matrix} & \begin{matrix} 0 & 0 \\ 0 & -1 \\ 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{matrix} & \left.\begin{matrix} O_3 \\ I_3 \end{matrix}\right] \\ 0 & 0 & A & \end{array}$$

Restating properties

Characterization

G strongly connected $\iff$ *a network matrix is* $\begin{bmatrix} I & N & X \end{bmatrix}$ *(N nec).*

G not strongly connected $\iff$ *it is* $\begin{bmatrix} I & N & X \\ 0 & 0 & A \end{bmatrix}$ *(A non-negative).*

The property can be generalized !

Characterization

M *PSS* $\iff$ $M \equiv \begin{bmatrix} I & N & X \end{bmatrix}$ *(N nec).*

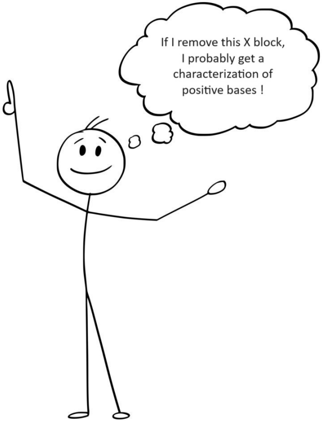
M *not PSS* $\iff$ $M \equiv \begin{bmatrix} I & N & X \\ 0 & 0 & A \end{bmatrix}$ *(A non-negative).*

A very nice conjecture

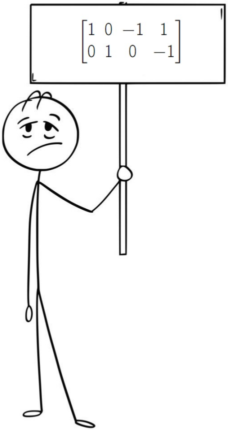
Characterization

M PSS $\iff$ *it is equivalent to* $\begin{bmatrix} I & N & X \end{bmatrix}$ *(N nec).*

M not PSS $\iff$ *it is equivalent to* $\begin{bmatrix} I & N & X \\ 0 & 0 & A \end{bmatrix}$ *(A non-negative).*



…well, maybe not



Nec matrices

Definition (Negative echelon column matrix)

$N \in \mathbb{R}^{n \times s}$ is a **nec matrix** if

1. Each column ends with zeros. except the last.
2. Each has less zeros than its predecessor.
3. Each has a block of -1 above the zeros. the first column starts with it.
4. The other values are arbitrary. Not for positive bases !

Example

$$\begin{bmatrix} -1 & \times & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & -1 & \times \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}, \quad \begin{bmatrix} -1 & \times & \times & \times \\ -1 & \times & \times & \times \\ 0 & -1 & \times & \times \\ 0 & -1 & \times & \times \\ 0 & 0 & -1 & \times \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad \begin{bmatrix} -1 & \times & \times \\ -1 & \times & \times \\ 0 & -1 & \times \\ 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}.$$

Creating a basis

$$
\left[\begin{array}{c|cccc}
 & -1 & \times & \times & \times \\
 & -1 & \times & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
\mathrm{I}_{10} & 0 & 0 & -1 & \times \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1
\end{array}\right]
\begin{array}{l}
\left.\right\} X_2 \\
\left.\right\} X_3 \\
\left.\right\} X_1
\end{array}
$$

We see three 'arbitrary' blocks.

Creating a basis

$$
\left[\begin{array}{c|cccc}
 & -1 & \times & \times & \times \\
 & -1 & \times & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
\mathrm{I}_{10} & 0 & 0 & -1 & \times \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1
\end{array}\right]
\begin{array}{l}
\left.\vphantom{\begin{array}{c}1\\1\end{array}}\right\} X_2 \\
\left.\vphantom{\begin{array}{c}1\\1\\1\end{array}}\right\} X_3 \\
\} X_1 \\
\\ \\ \\ \\
\end{array}
$$

Let's list the restrictions on these blocks.

Creating a basis

$$
\left[\begin{array}{c|cccc}
 & -1 & \times & \times & \times \\
 & -1 & \times & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
\mathrm{I}_{10} & 0 & 0 & -1 & \times \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1
\end{array}\right]
\begin{array}{l}
X_2 \\ \\ \\ X_3 \\ \\ X_1 \\ \\ \\ \\ \\
\end{array}
$$

- Vectors in $cone(X_i)$ do not have one positive coordinate.

Creating a basis

$$
\left[\begin{array}{c|cccc}
 & -1 & \times & \times & \times \\
 & -1 & \times & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
\mathrm{I}_{10} & 0 & 0 & -1 & \times \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1
\end{array}\right]
$$

X_2 (rows 1–2, columns 2–4 of the right block), X_3 (rows 3–5, columns 3–4), X_1 (row 6, column 4)

- Vectors in $cone(X_i)$ do not have one positive coordinate.
- Vectors in $cone(X_i)$ are not negative.

Creating a basis

$$\left[\begin{array}{c|cccc} & -1 & \times & \times & \times \\ & -1 & \times & \times & \times \\ & 0 & -1 & \times & \times \\ & 0 & -1 & \times & \times \\ \mathrm{I}_{10} & 0 & -1 & \times & \times \\ & 0 & 0 & -1 & 0 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \end{array}\right] \begin{array}{l} \left.\right\} X_2 \\ \\ \left.\right\} X_3 \end{array}$$

- Vectors in $cone(X_i)$ do not have one positive coordinate.
- Vectors in $cone(X_i)$ are not negative.

$\Longrightarrow$ In X_1, each cross is a 0.

Creating a basis

$$\left[\begin{array}{c|cccc} & -1 & \times & \times & \times \\ & -1 & \times & \times & \times \\ & 0 & -1 & \times & \times \\ & 0 & -1 & \times & \times \\ & 0 & -1 & \times & \times \\ \mathrm{I}_{10} & 0 & 0 & -1 & \color{red}{0} \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \end{array}\right] \begin{array}{l} \}\, X_2 \\ \\ \}\, X_3 \\ \\ \\ \\ \\ \\ \\ \\ \end{array}$$

- The max entry of $x \in cone(X_i)$, when positive, is <u>not</u> unique.
- Vectors in $cone(X_i)$ are not negative.

Creating a basis

$$
\left[\begin{array}{ccccc}
 & -1 & 3 & 9 & 2 \\
 & -1 & 3 & 9 & 2 \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
 & 0 & -1 & \times & \times \\
\mathrm{I}_{10} & 0 & 0 & -1 & 0 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1 \\
 & 0 & 0 & 0 & -1
\end{array}\right]
\quad X_3 \text{ (boxed block of } \times \text{ entries)}
$$

- The max entry of $x \in cone(X_i)$, when positive, is <u>not</u> unique.
- Vectors in $cone(X_i)$ are not negative.

$\implies$ Columns of X_2 are positive multiples of a same $y \in \{1_2, -e_1, -e_2\}$.

Creating a basis

$$\left[\begin{array}{c|cccc} & -1 & 3 & 9 & 2 \\ & -1 & 3 & 9 & 2 \\ & 0 & -1 & 0 & 0 \\ & 0 & -1 & -3 & 5 \\ & 0 & -1 & -3 & 5 \\ I_{10} & 0 & 0 & -1 & 0 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \\ & 0 & 0 & 0 & -1 \end{array}\right]$$

- The max entry of $x \in cone(X_i)$, when positive, is not unique.
- Vectors in $cone(X_i)$ are not negative.

There are no other restrictions !

Characterizing bases

Definition (Critical set)

$K(\mathbb{R}^n)$ is the set of vectors v satisfying condition 1 or 2.

1. $\mathrm{v} \leq 0_n \quad \& \quad \exists i, v_i = 0.$
2. $\exists i, j, v_i = v_j = \max_{k \leq n} v_k > 0.$

Characterizing bases

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2. $\exists i, j, v_i = v_j = \max\limits_{k \leq n} v_k > 0.$

Theorem

$$\left[\begin{array}{c|ccc} & -1 & & \\ & \dots & X_{n_1} & \\ & -1 & & \\ I_n & & -1 & \\ & 0 & \dots & X_{n_2} \\ & & -1 & \\ & & 0 & \dots \end{array}\right] \textit{ is a basis } \iff \forall i, cone(X_{n_i}) \subset K(\mathbb{R}^{n_i}).$$

...recursive

Near-maximal bases

Proposition

$$|M| = 2n-1 \iff M \equiv \begin{bmatrix} \multirow{3}{*}{I_n} & -1 & 0 \\ & -1 & x^\top \\ & 0 & -I_{n-2} \end{bmatrix}, \ x \in \mathbb{R}^{n-2}, \ x \leq 0_{n-2}.$$

Example

Basis of size 7 in $\mathbb{R}^4$ $\iff$ equivalent to $\begin{bmatrix} \multirow{4}{*}{I_4} & -1 & 0 & 0 \\ & -1 & x & y \\ & 0 & -1 & 0 \\ & 0 & 0 & -1 \end{bmatrix}, \ \begin{cases} x \leq 0 \\ y \leq 0 \end{cases}.$

Near-minimal bases

Proposition

$$|M| = n+2 \iff M \equiv \begin{bmatrix} I_n & \begin{matrix} -1_k \\ 0_{n-k} \end{matrix} & \begin{matrix} x \\ -1_{n-k} \end{matrix} \end{bmatrix}, \quad \begin{cases} 1 \leq k < n, x \in \mathbb{R}^k \\ x \leq 0, x_1 = 0 \end{cases}.$$

Example

Basis of size 5 in $\mathbb{R}^3$ $\iff$ equivalent to $\begin{bmatrix} & -1 & 0 \\ \mathrm{I}_3 & -1 & x \\ & 0 & -1 \end{bmatrix}, x \leq 0.$

Conclusion

In a nutshell

- Digraphs are pretty cool.
- The notion of PSS generalizes that of strongly connected digraph.
- Knowing so allows to find new properties of PSSs.

Perspectives

- Characterizing blocks with even more rows.
- Characterizing blocks with few columns.
- Characterizing PkSSs in a similar fashion.

Thanks

for your attention !