Optimal Cycles and LP/IP

Bala Krishnamoorthy
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Optimal ~~Cycles~~ Chains and LP/IP

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OHCP

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Given p-cycle c in simplicial complex K, find homologous cycle x that is "optimal."

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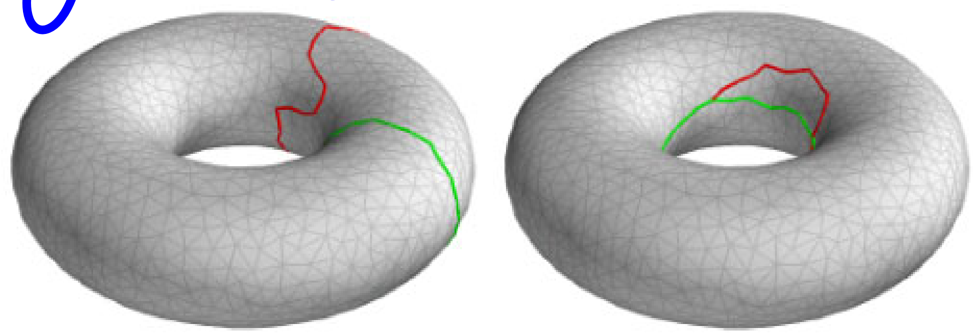

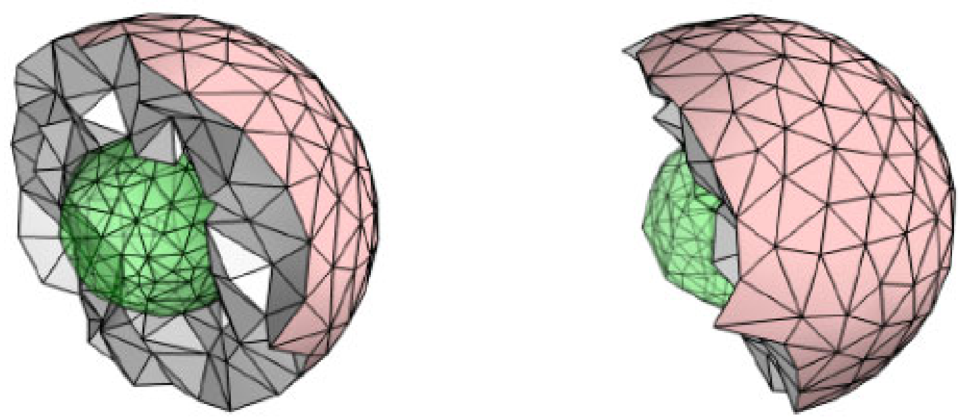

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The Optimal Homologous Chain Problem:

Given p-chain c in simplicial complex K, find "homologous" cycle x that is "optimal".

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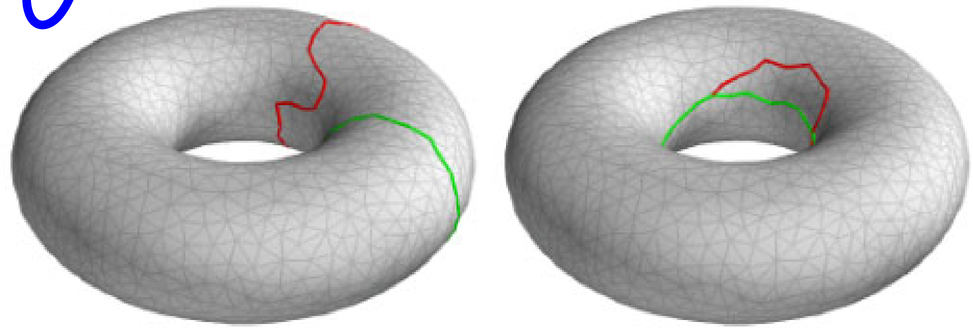

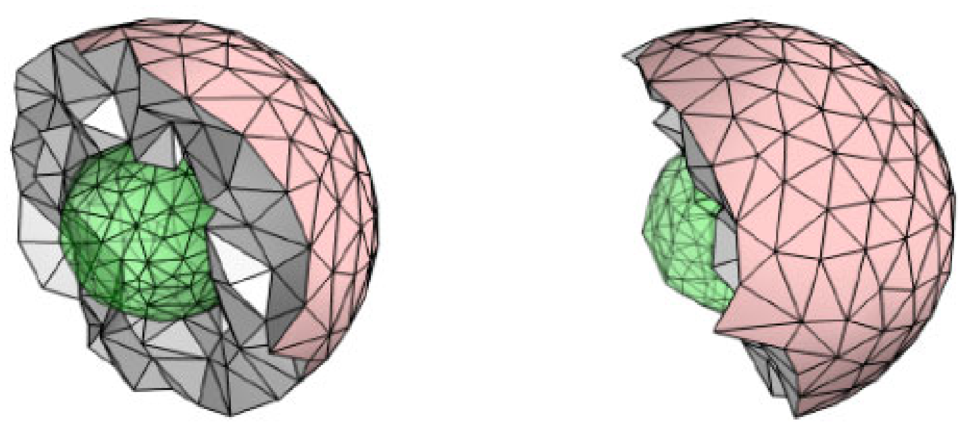

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OBCP

The **O**ptimal **B**ounding **C**hain **P**roblem:

Given p-boundary c in simplicial complex K, find $(p+1)$-chain s bounding c that is "optimal".

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MSFN

Ibrahim, K, Vixie (2013)

Multiscale Simplicial Flat Norm:

Given p-chain c in simplicial complex K, find "homologous" chain x that is "optimal".

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$\sum w_i |x_i| + \lambda \sum v_j s_j$

$\lambda \geq 0$

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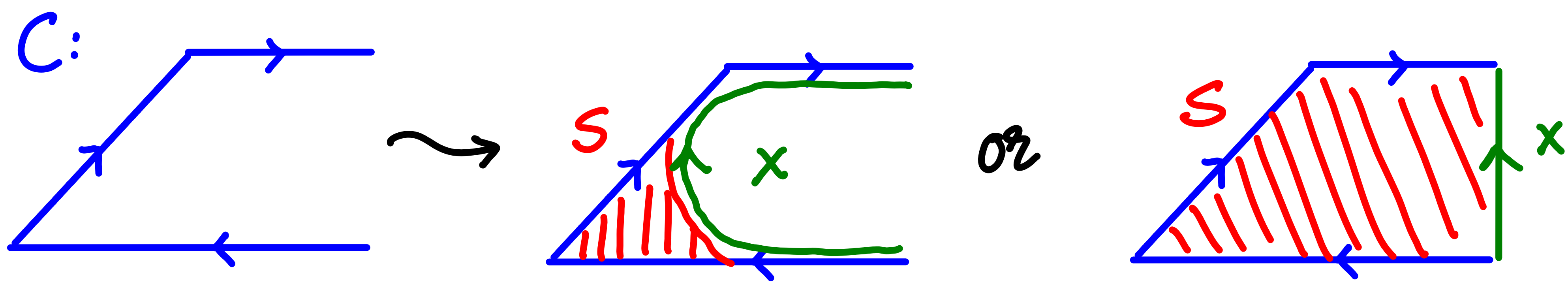

$X = C - \partial S$

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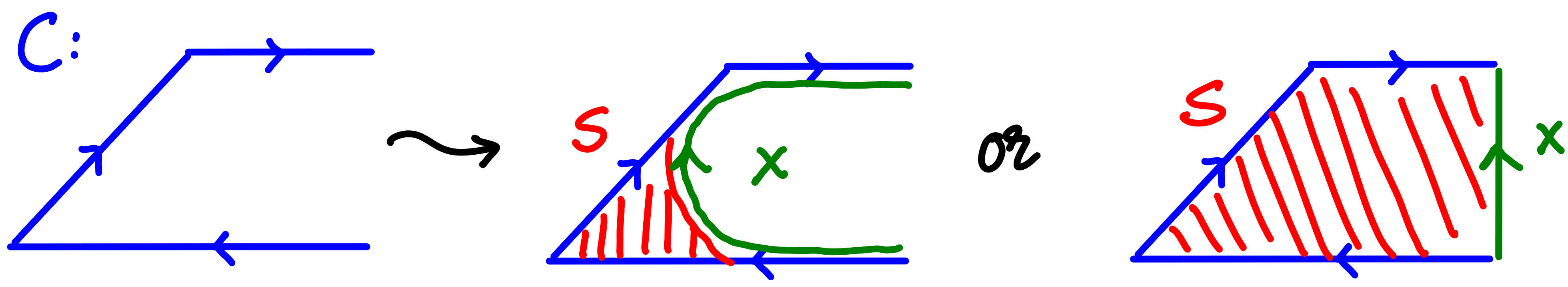

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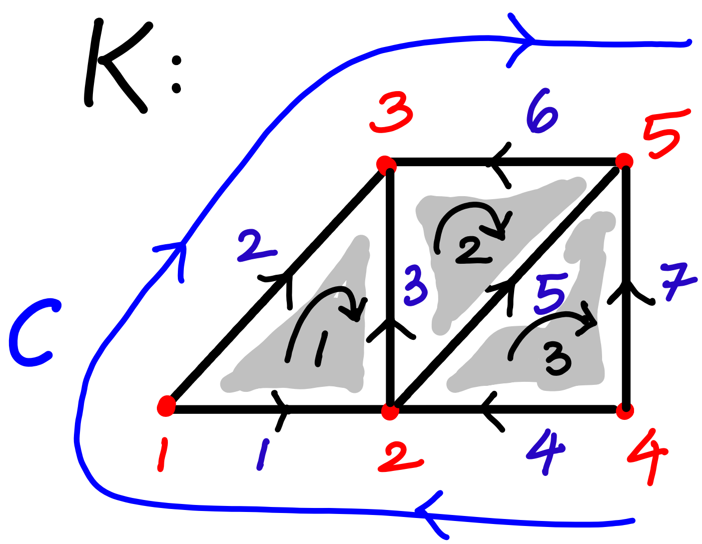
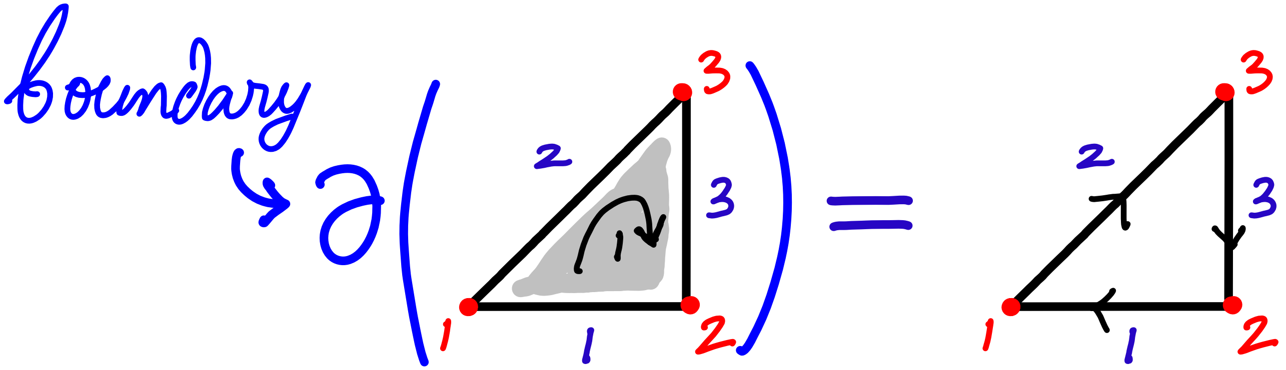
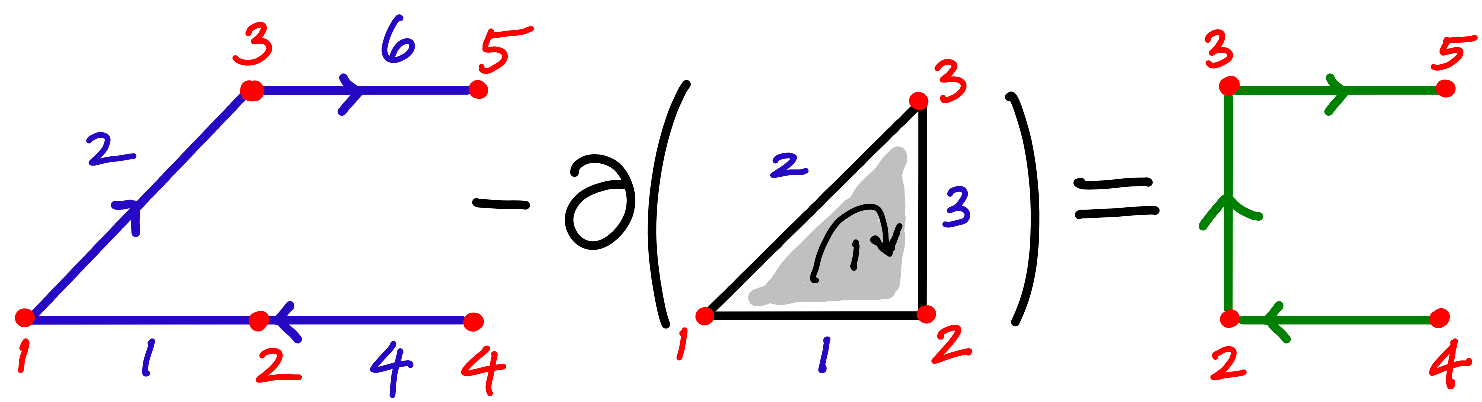


$$w_i = \begin{cases} 1, & i = 1,3,4,6,7 \\ \sqrt{2}, & i = 2,5 \end{cases} \Bigg\} \text{ lengths}$$

$$v_j = \frac{1}{2},\ j = 1,2,3 \ \Big\} \text{ areas}$$

MSFN Example





for $\lambda = 2.5$,

$$F_\lambda = 3 + \frac{\lambda}{2}$$

$$= 4.25$$

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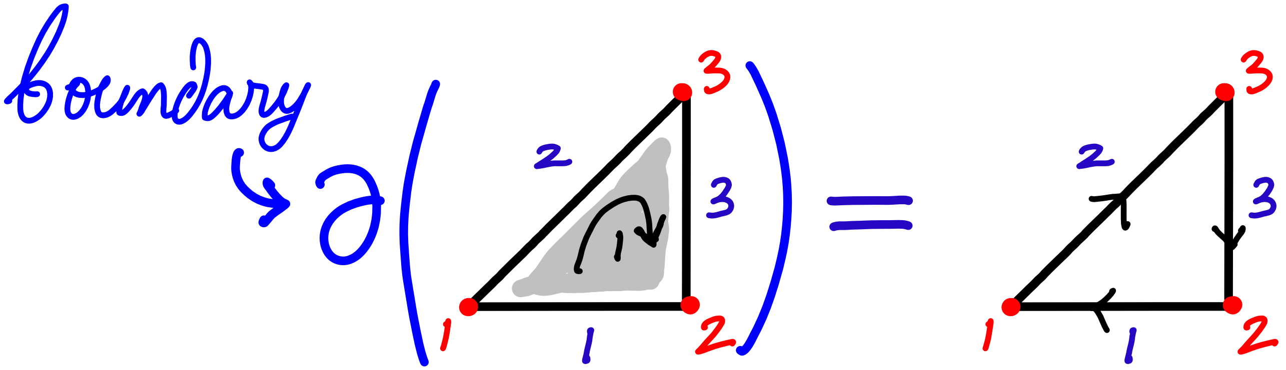

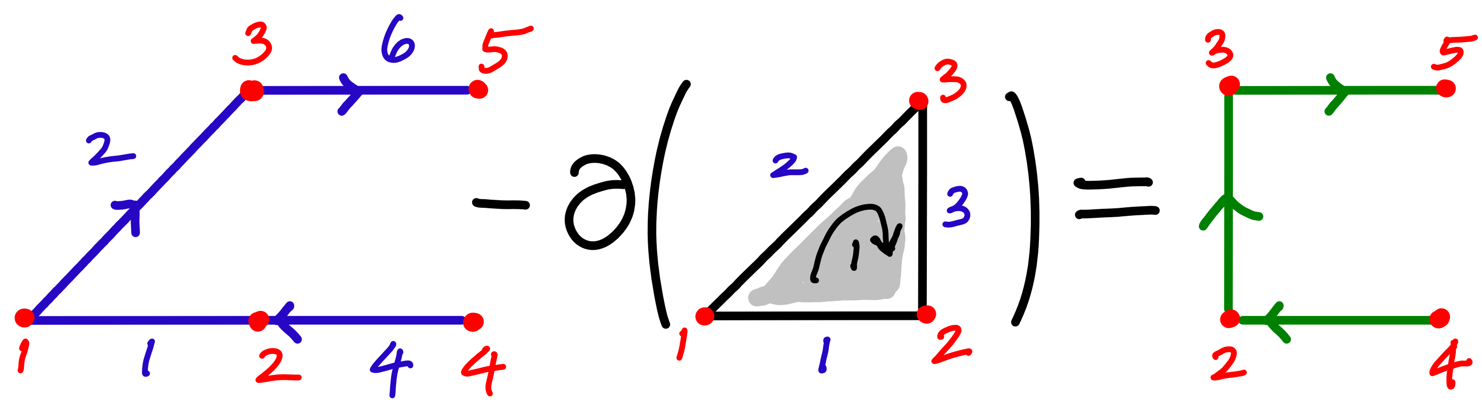

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$F_\lambda = 3 + \frac{\lambda}{2}$
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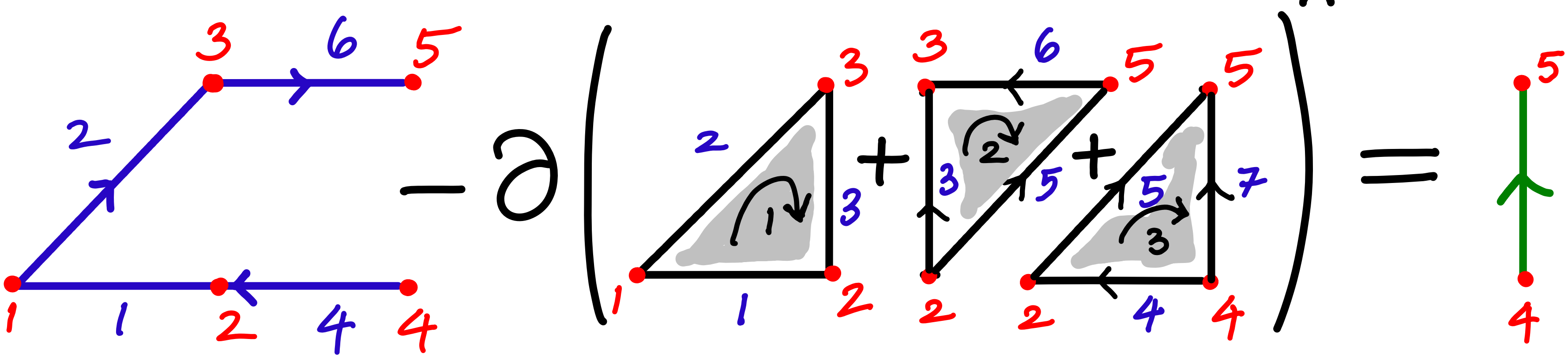
for $\lambda = 1$, $F_\lambda = 1 + \frac{3\lambda}{2} = 2.5$

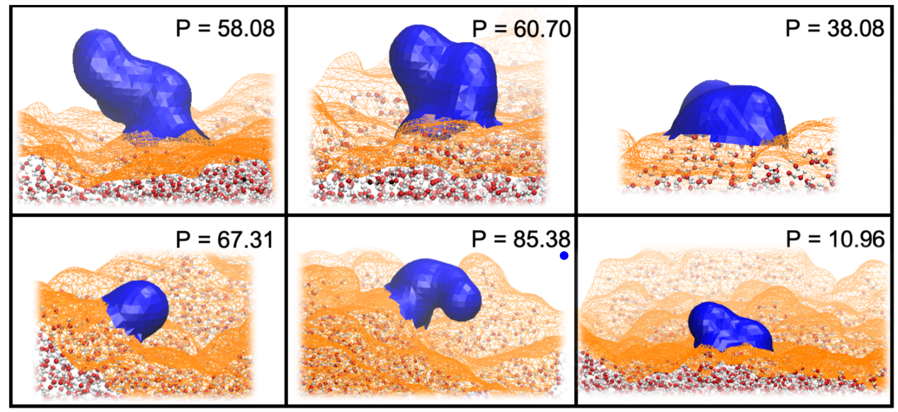


MSFN: APPLICATIONS

* protrusions in chemistry

E Alvarado, Z Liu, M Servis, BK, A Clark

JCTC 2020



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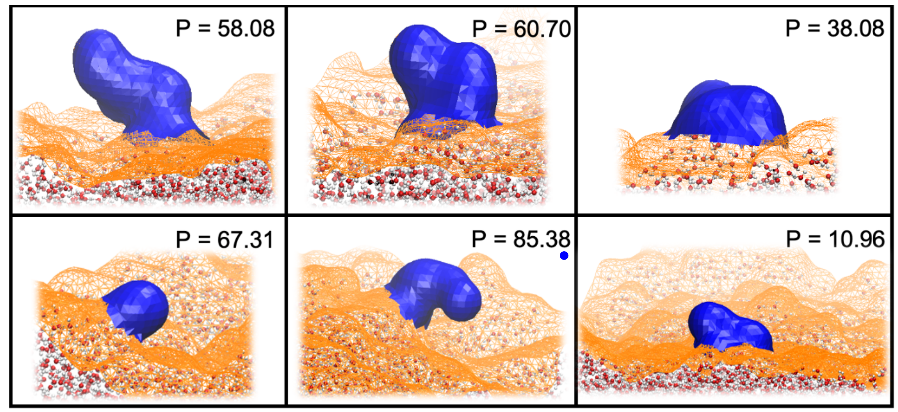
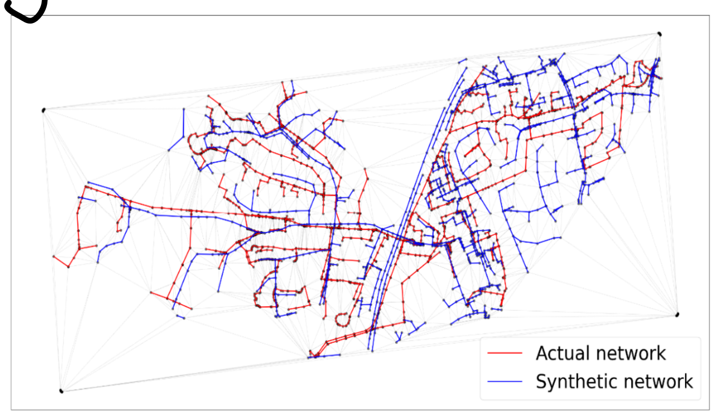
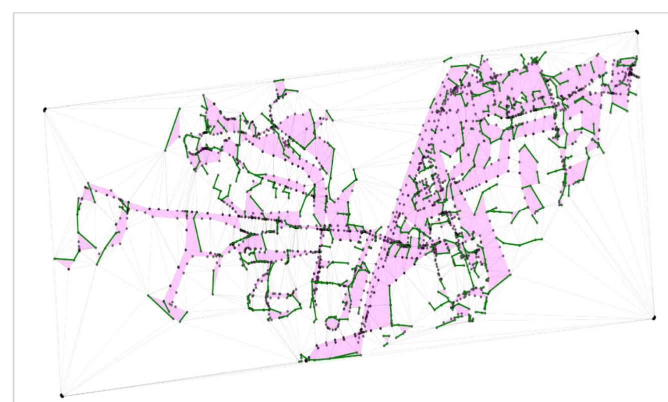


* validating synthetic power networks

  K Lyman, R Meyur, BK, M Halappanavar

  IJCGA 2025





OHCP under Persistence

* volume-optimal cycles: Obayashi, 2018
* minimal persistent cycles: Dey, Hou, Mandal, 2020 (over $\mathbb{Z}_2$)

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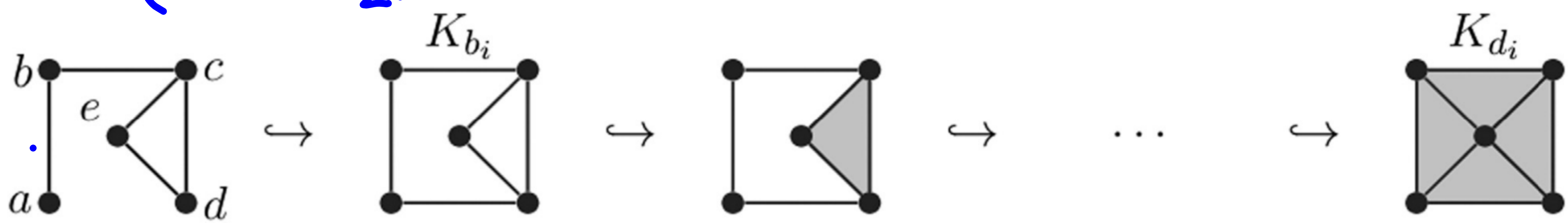

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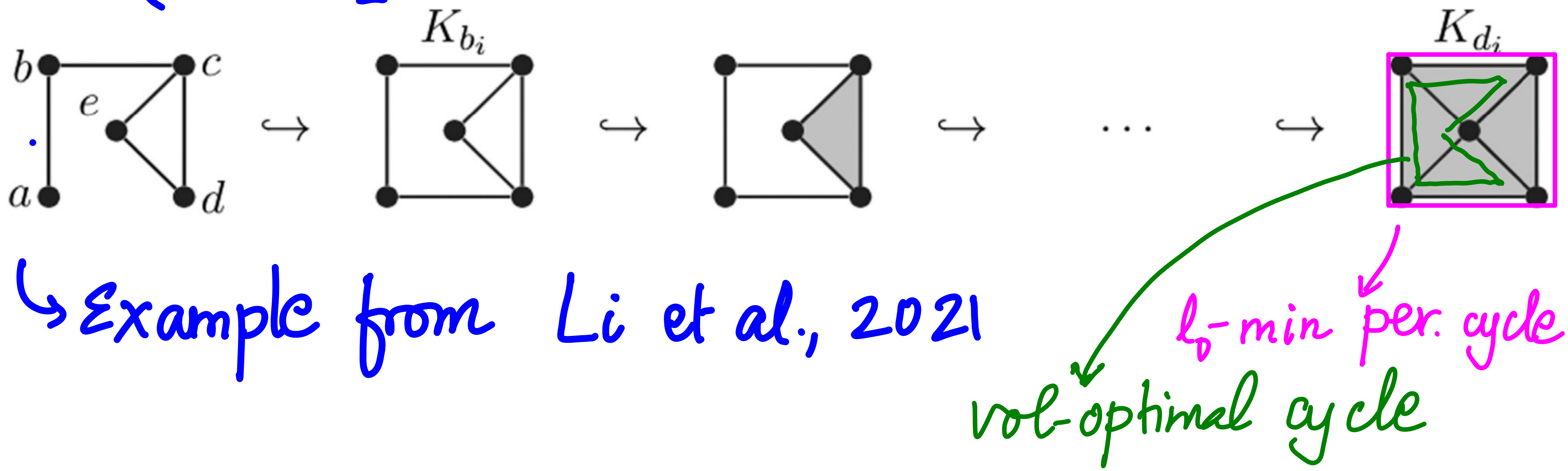

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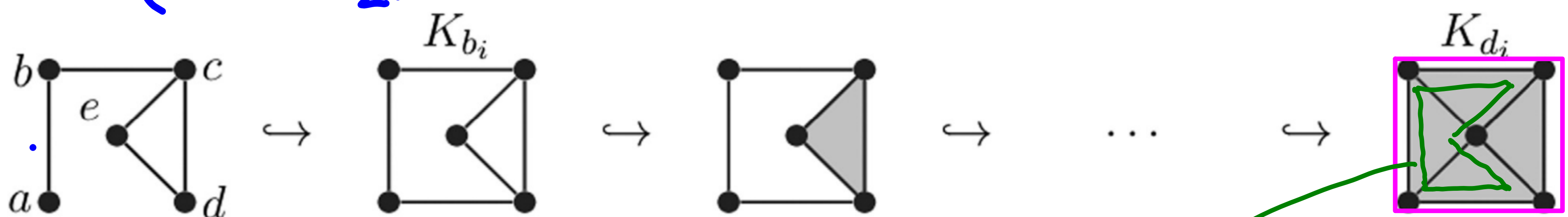

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ℓ_0-min per. cycle

vol-optimal cycle

! Today: OHCP in a single simplicial complex with homology over $\mathbb{Z}$

OHCP as an Integer Program

$$\min_{x,y} \sum_i w_i |x_i| \quad \text{such that} \qquad \text{(OHCP)}$$

$$x = c + [\partial_{p+1}]s, \; x \in \mathbb{Z}^m, \; s \in \mathbb{Z}^n \quad (w_i \geq 0)$$

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$$x = c + [\partial_{p+1}]s, \; x \in \mathbb{Z}^m, \; s \in \mathbb{Z}^n \quad (w_i \geq 0)$$

$$\min \sum_i w_i (x_i^+ + x_i^-)$$

$$\text{s.t.} \quad x^+ - x^- = c + [\partial_{p+1}](s^+ - s^-) \qquad \text{(IP)}$$

$$x^+, x^-, s^+, s^- \geq 0 \quad x^+, x^- \in \mathbb{Z}^m, \; s^+, s^- \in \mathbb{Z}^n$$

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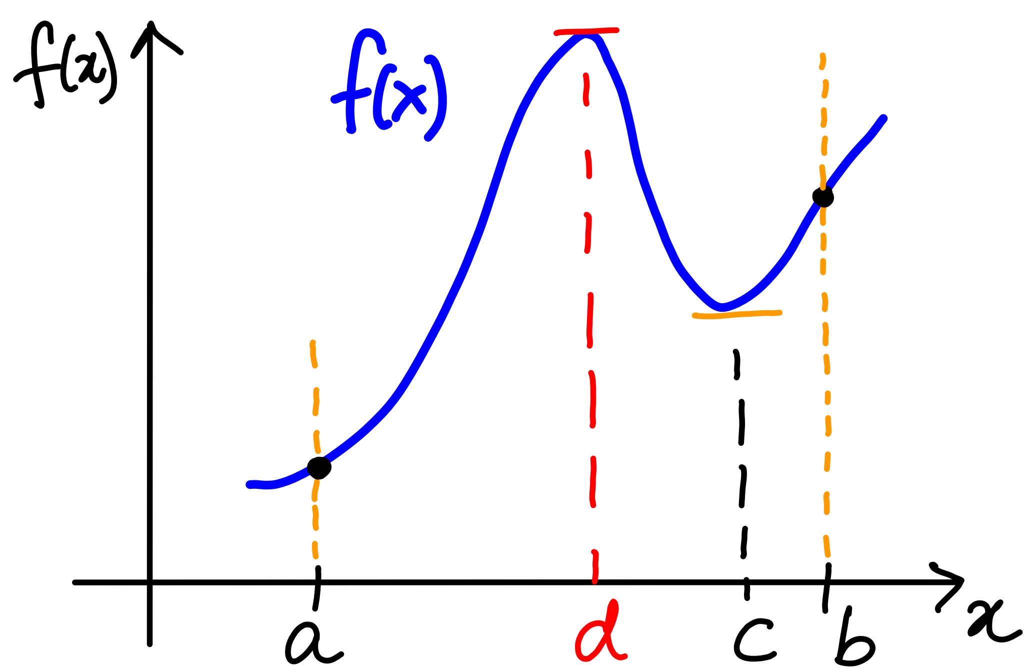
ignore to get LP

LINEAR PROGRAMMING (LP)

Optimization in Calculus I

$$\min_{a \le x \le b} f(x)$$

$f'(x) = 0, \ f''(x) > 0$



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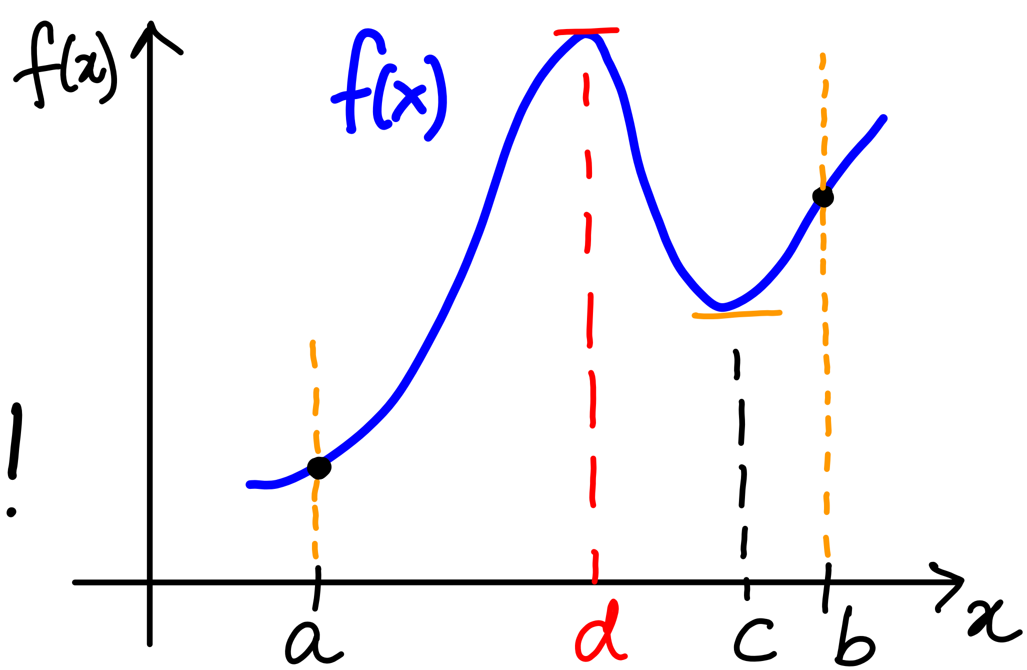

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also check end points!

Here, minimum is at $x=a$

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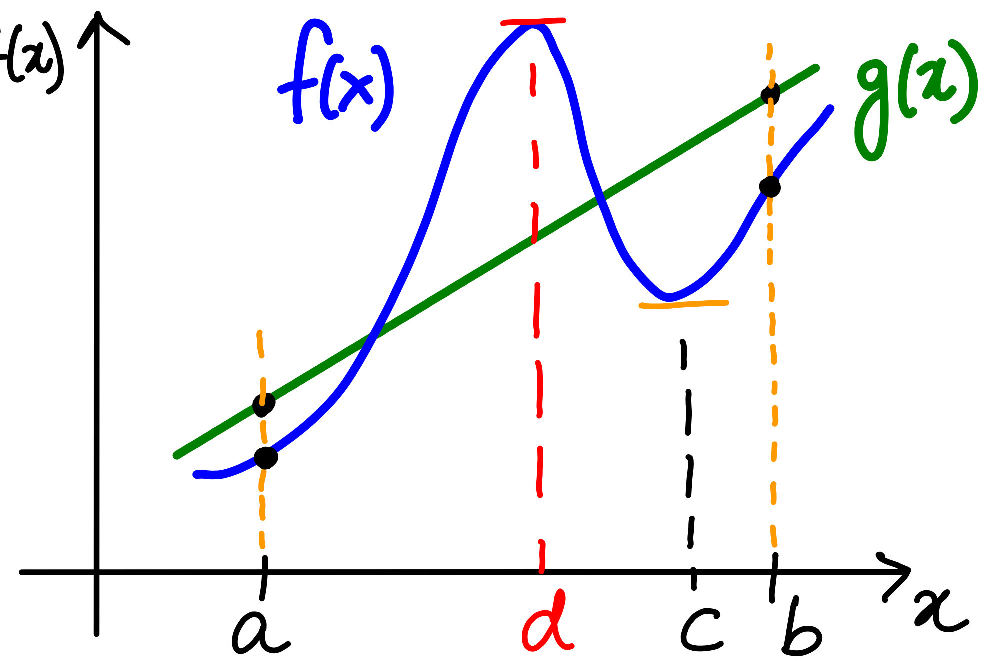

$\left\{\begin{matrix}\min g(x) \\ a \le x \le b\end{matrix}\right\}$ where $g(x)$ is linear?

Need to check ONLY the end points!

LINEAR PROGRAMMING (LP)

Extend linear case to high dimensions $\Rightarrow$ LP
(also called linear optimization)

$$\begin{aligned}
\max \quad & x_1 + x_2 \\
\text{s.t.} \quad & 5x_1 - x_2 \leq 7 \\
& 3x_1 - 4x_2 \geq -3 \\
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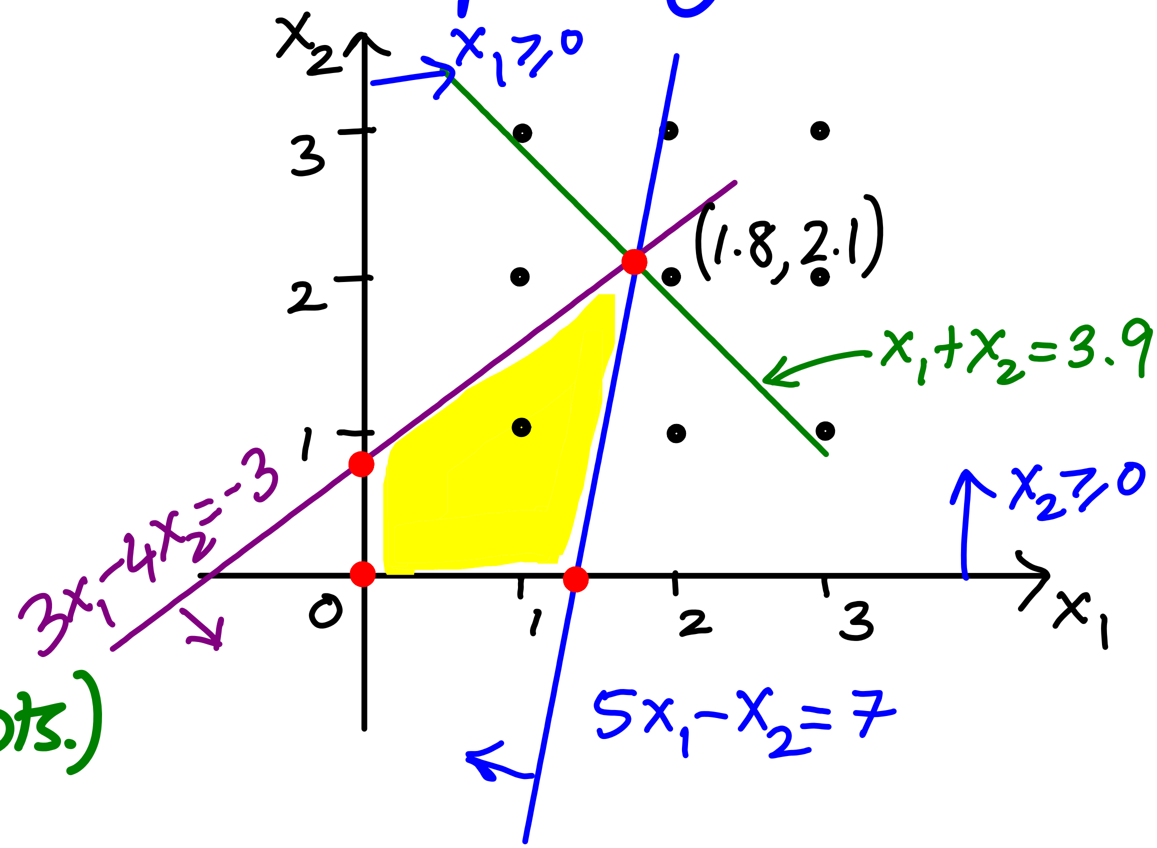

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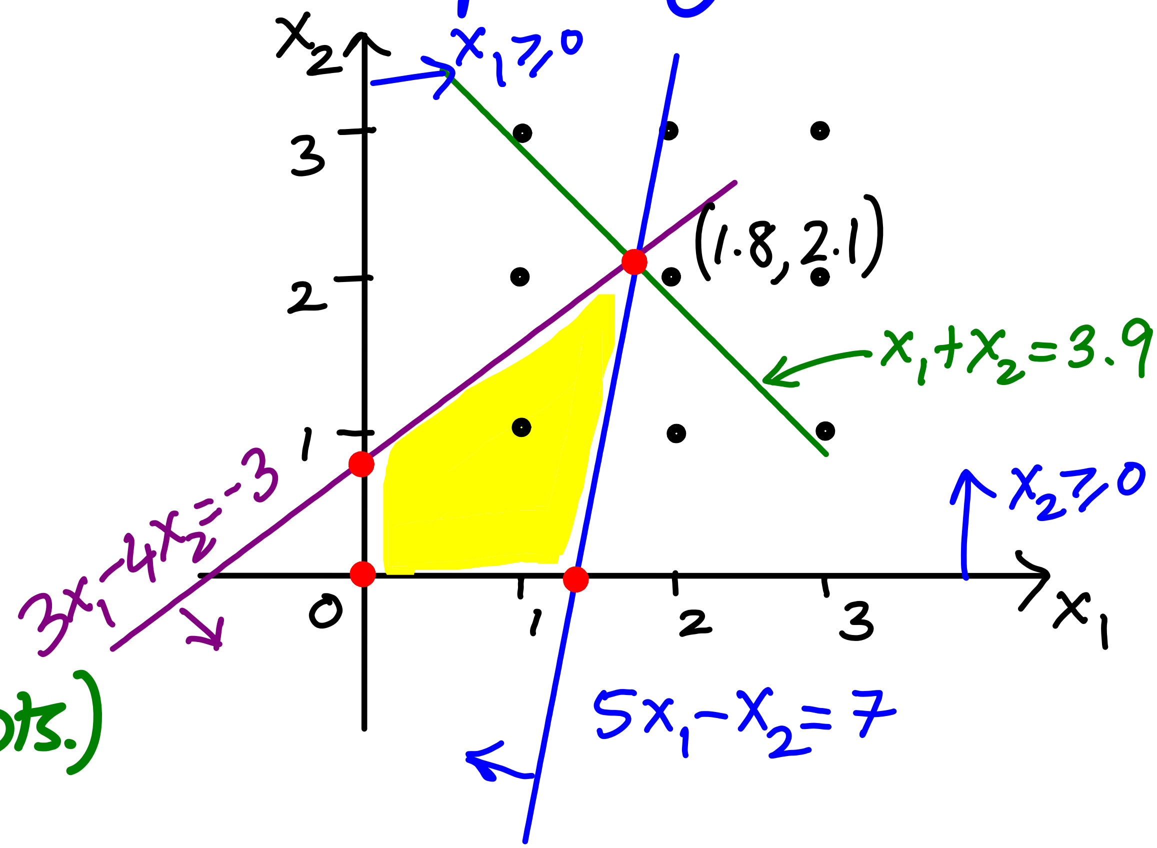

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Require $x_j \in \mathbb{Z} \Rightarrow$ integer programming (IP)

IP and Total Unimodularity

$$\min \{ c^T x \mid Ax = b, x \geq 0, x \in \mathbb{Z}^n \} \quad \text{(IP)}$$

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In particular, $A_{ij} \in \{-1, 0, 1\} \; \forall i,j$.

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e.g., node-arc incidence matrix of directed graph

OHCP AND TU OF $[\partial_{p+1}]$

total unimodularity

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The constraint matrix of above LP is TU iff $[\partial_{p+1}]$ is TU.

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OBCP, MSFN as well

WHEN IS $[\partial_{p+1}]$ TU?

Dey, Hirani, K, 2010: $[\partial_{p+1}]$ is TU iff K has "no relative torsion."
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✓ $\dim(K) = d$, K in $\mathbb{R}^d$

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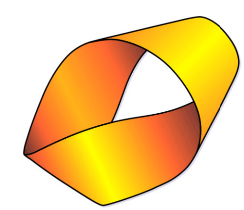

✓ $[\partial_2]$ is TU $\Leftrightarrow$ K has "no Möbius strip"
(DHK '11)

DUAL GRAPH: MAX FLOW

* Chen & Freedman, 2008 (OHCP, $\mathbb{Z}_2$)
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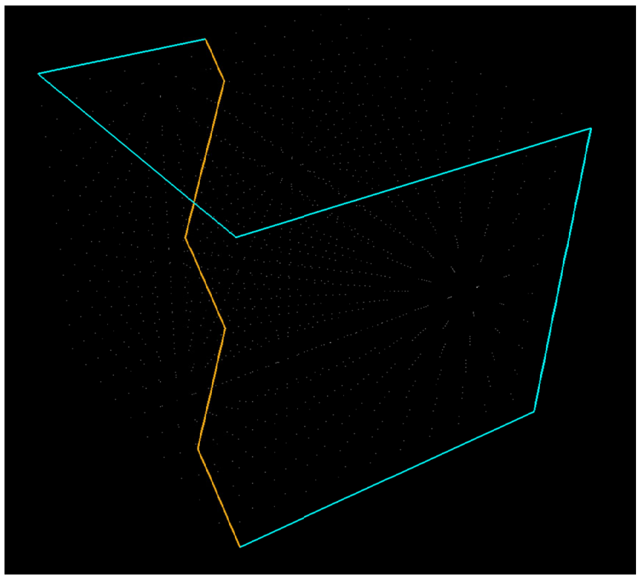
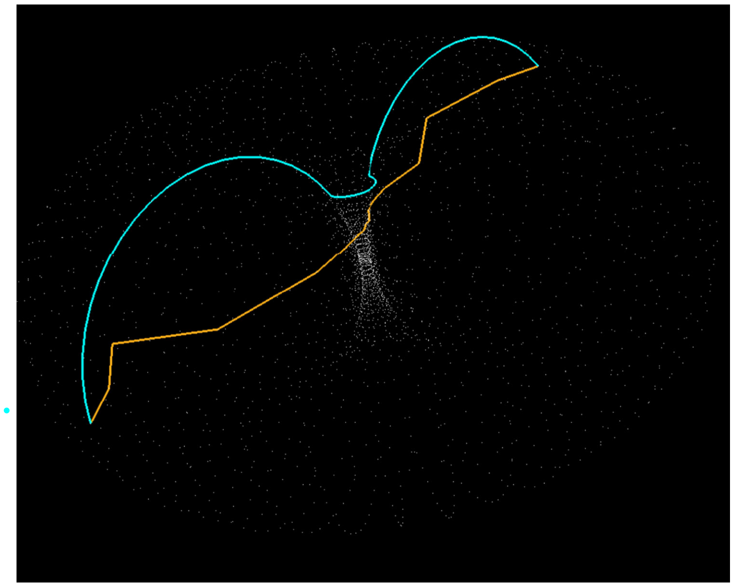
Q: What happens when boundary matrix is not TU?

MSFN IN CODIM. 2





— C

— X

K: 2-skeleton of solid cube 2-skeleton of solid torus

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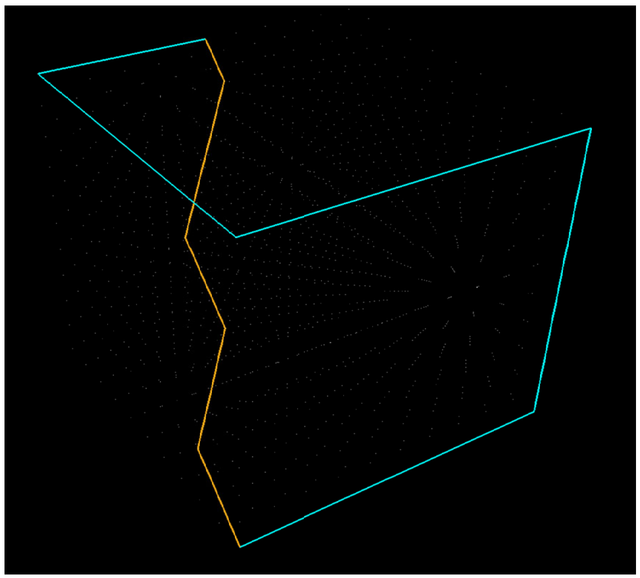

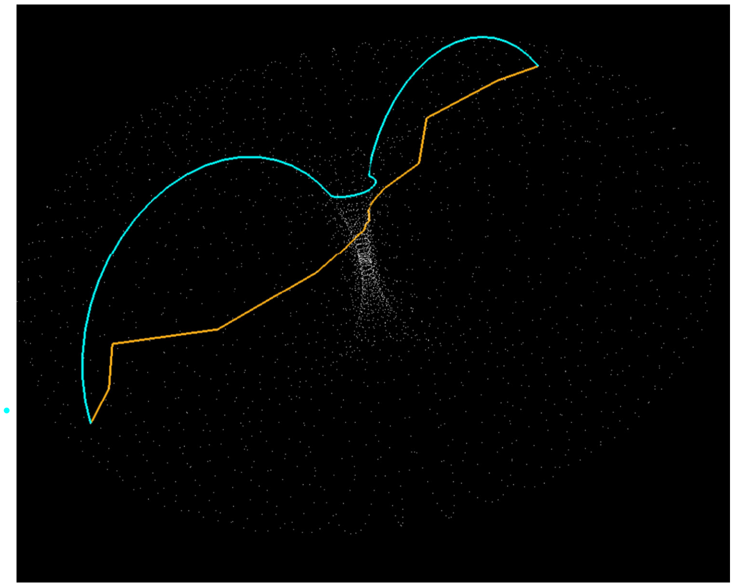

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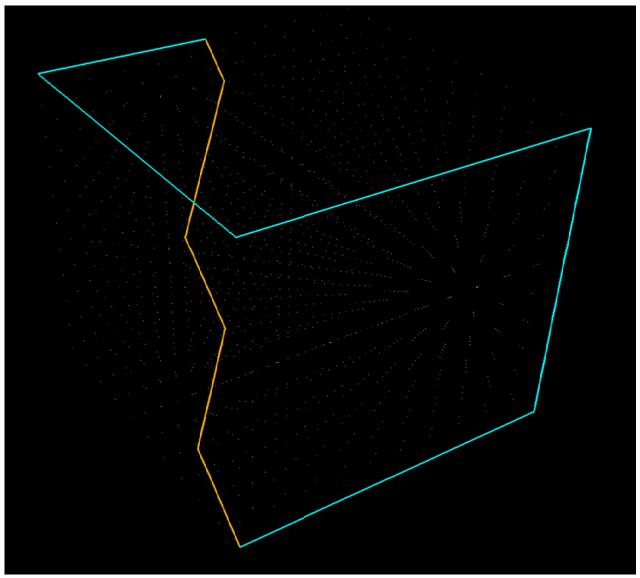

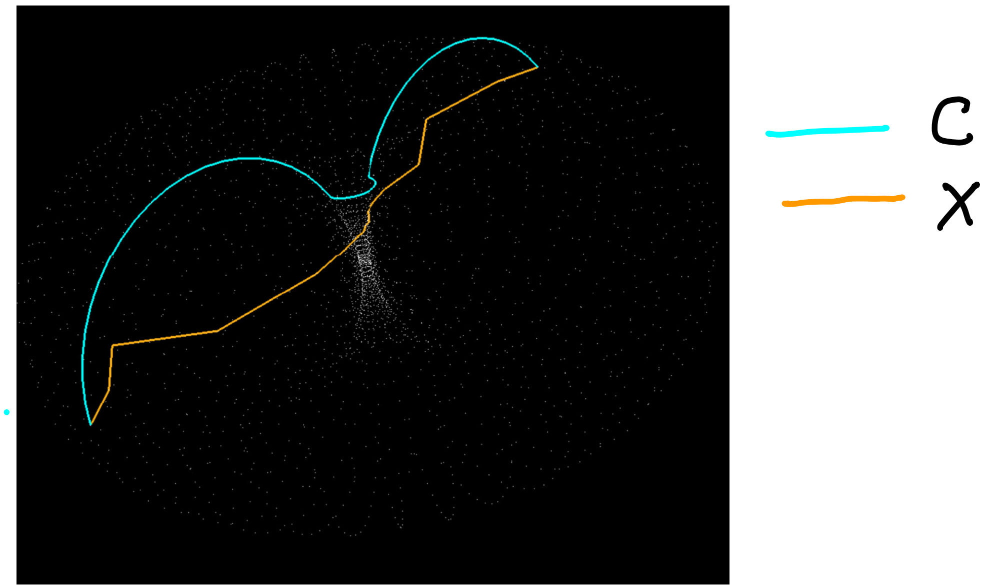

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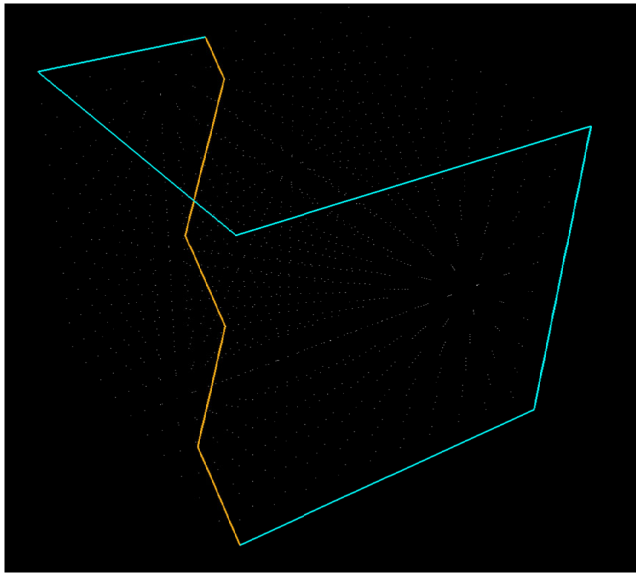
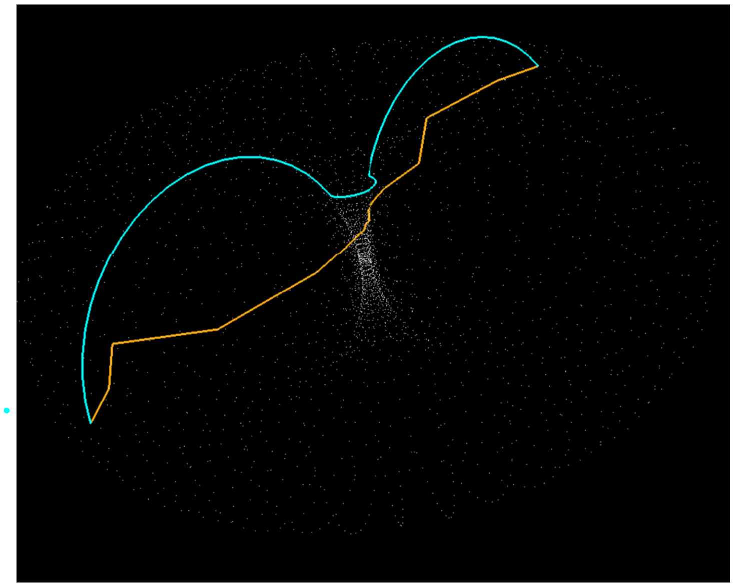
Q1: When/why does MSFN LP in codim. 2 give integer solutions for free?

MSFN IN CODIM. 2





K: 2-skeleton of solid cube 2-skeleton of solid torus

$[\partial_2]$ is not TU, but MSFN LP gives integer soln!

Q1: When/Why does MSFN LP in Codim. 2 give integer solutions for free?

— Li et al, 2021: mostly $\{-1,0,1\}$ sol.'s Why?

NON-TU NEUTRALIZED K

— K, G Smith, 2018

✓ Define a condition when simplicial complex K is non total-unimodularity neutralized (NTUN)

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✓ property of K (independent of weights on simplices and input chain)

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<u>Theorem</u> Every OHCP LP on K has an integer optimal solution if every elementary chain in each relative torsion in K has a "neutralizing chain" in K.

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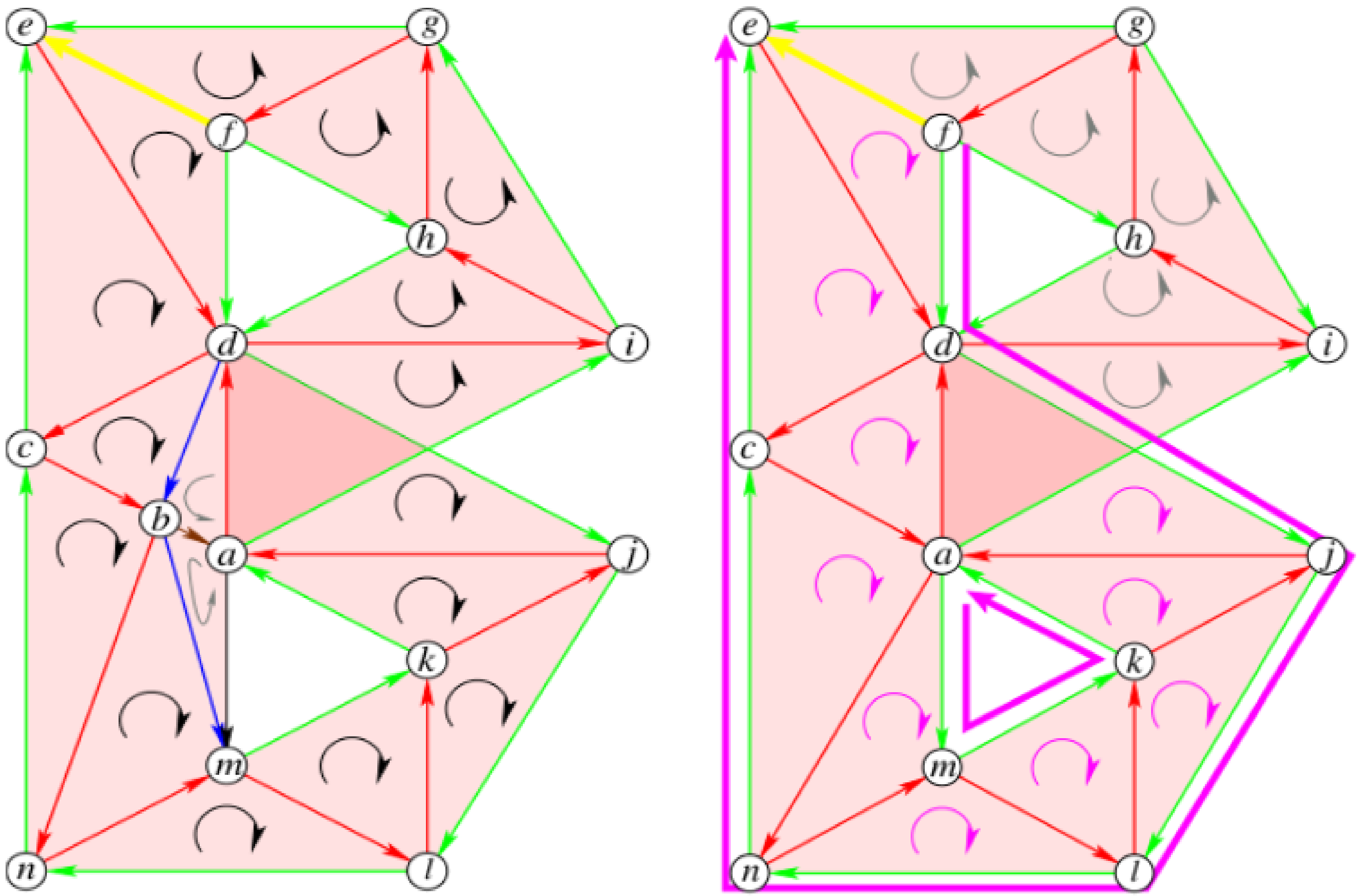
TU OR NOT ?



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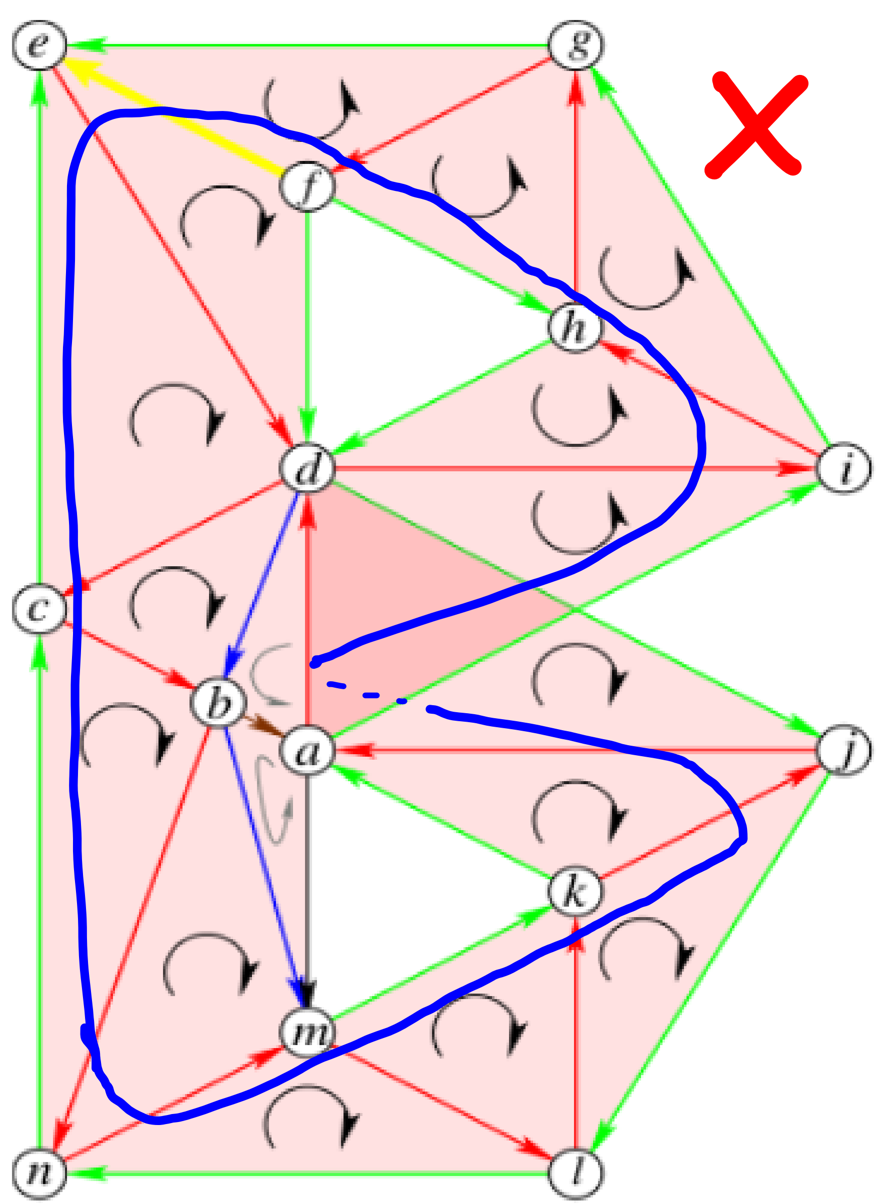

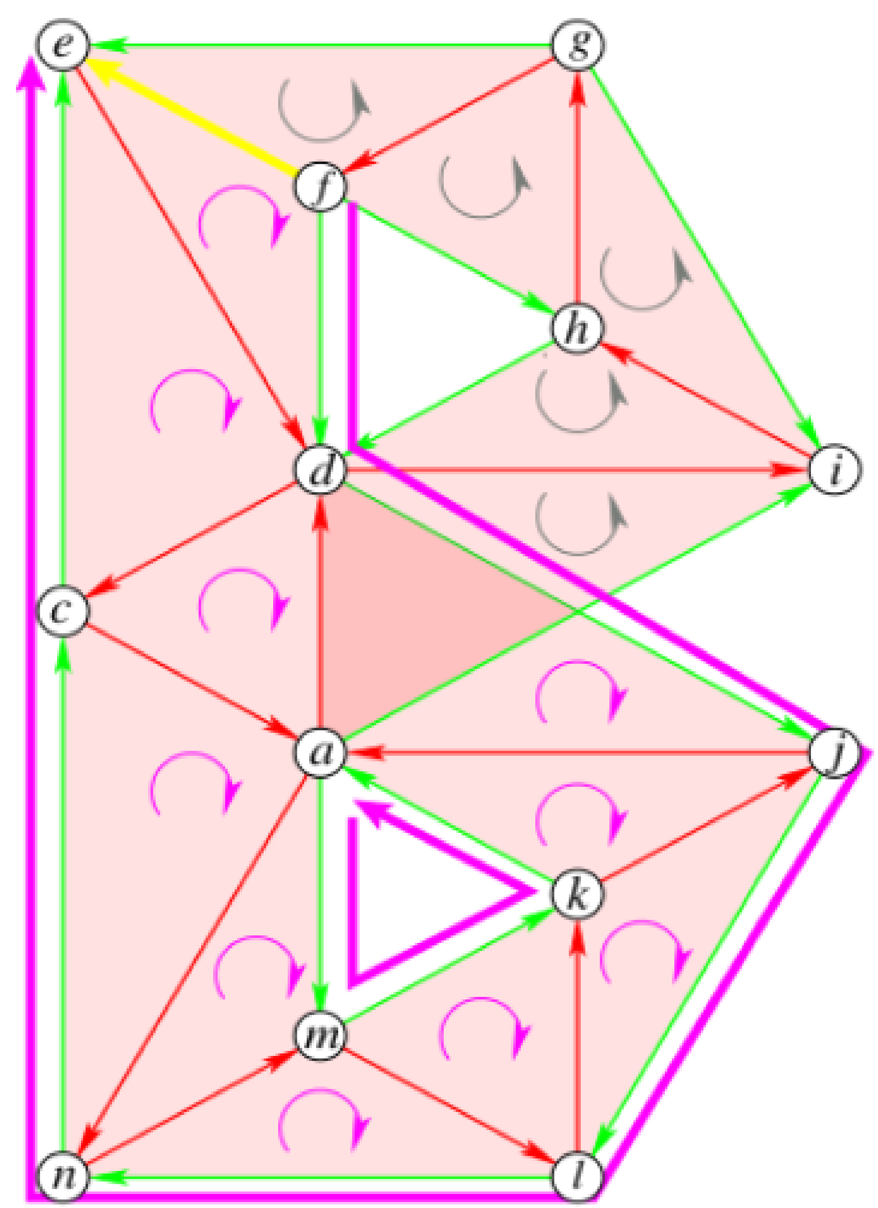

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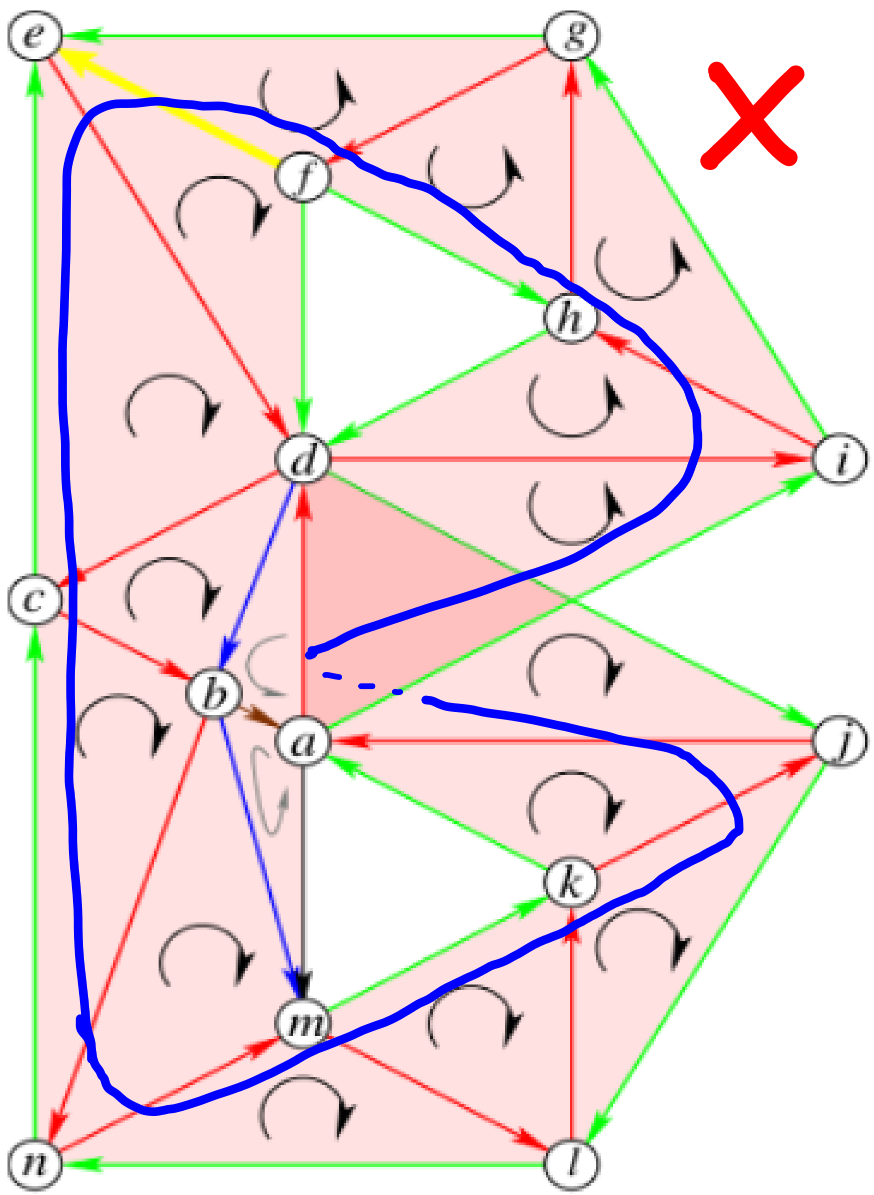

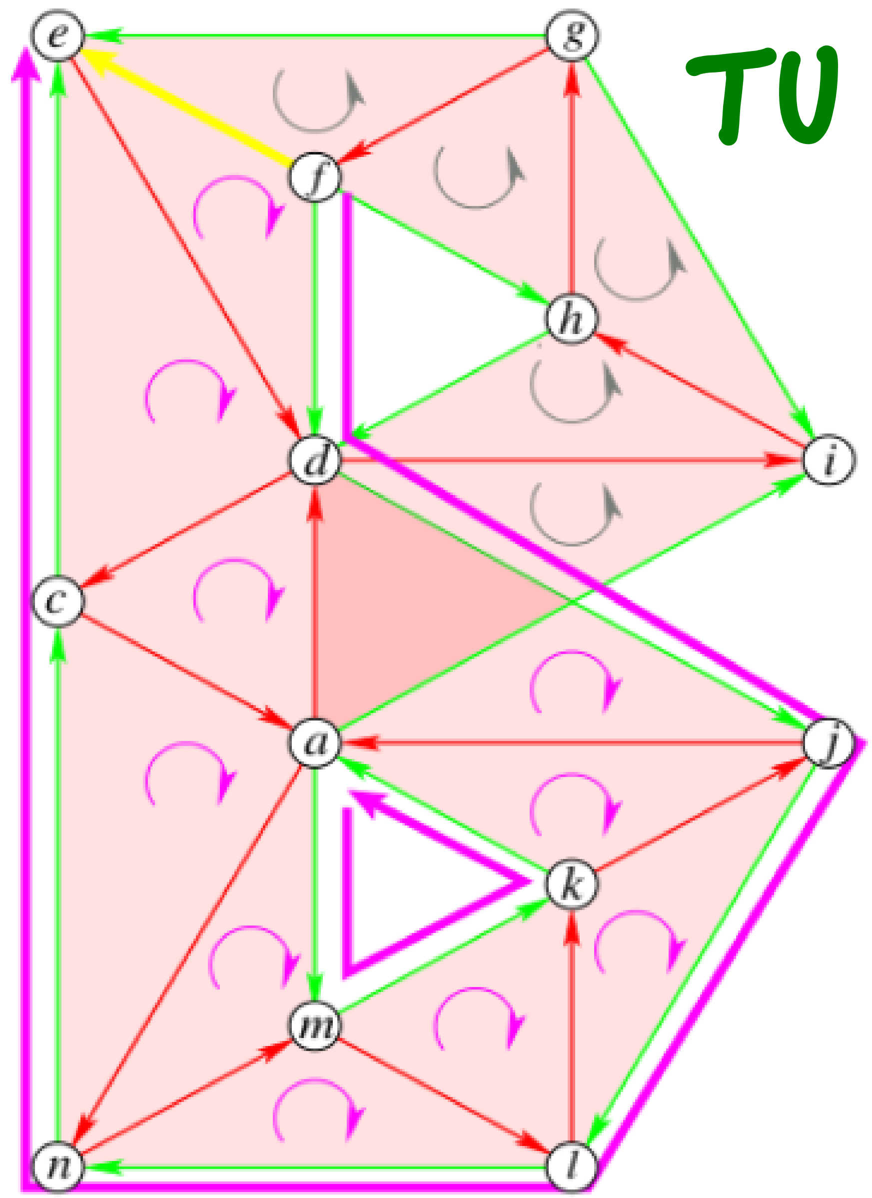

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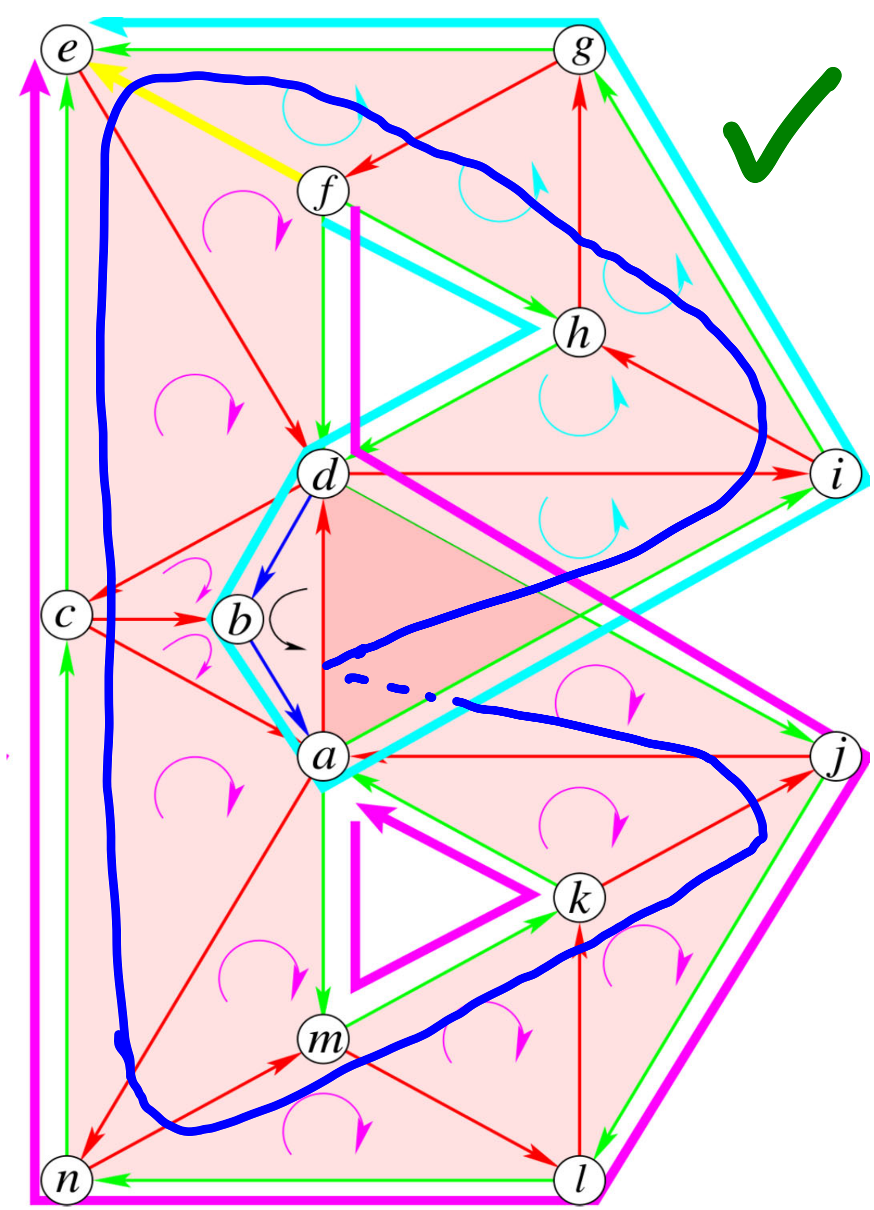
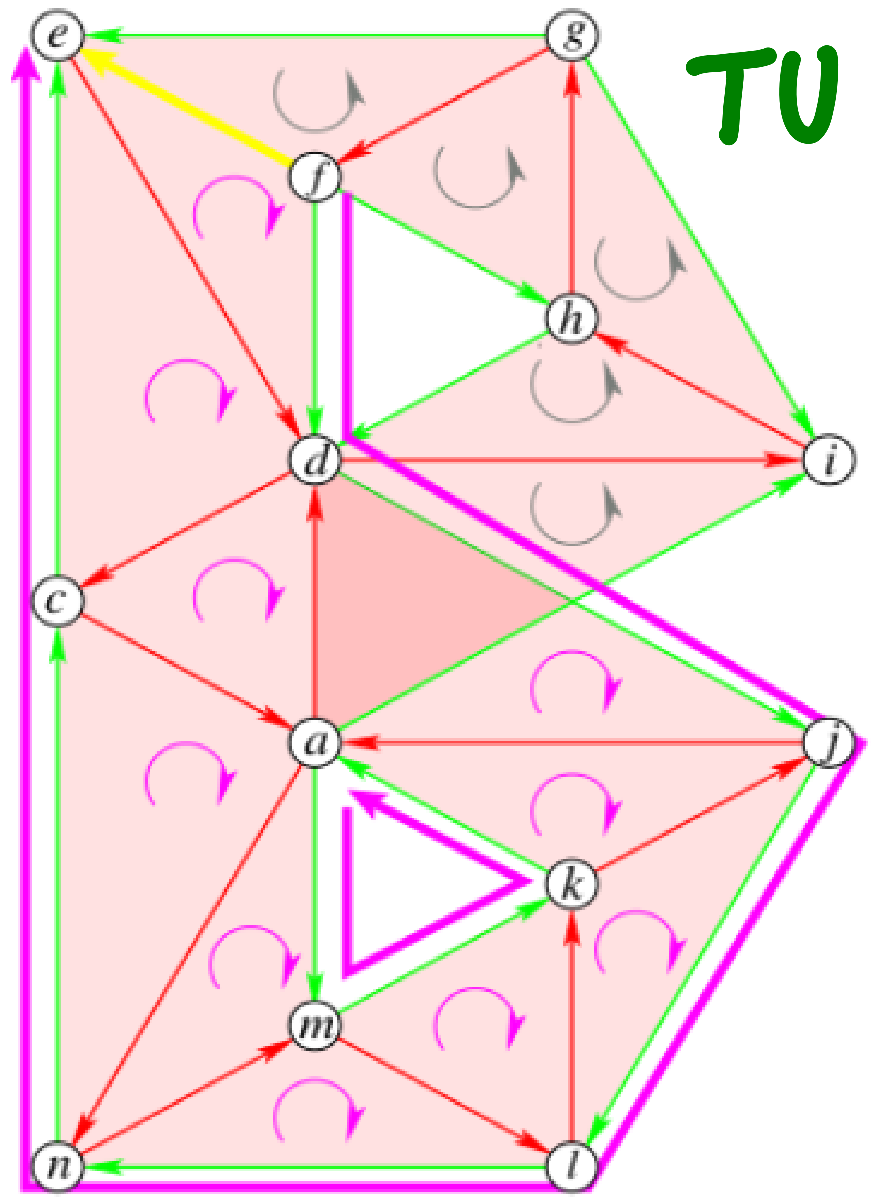
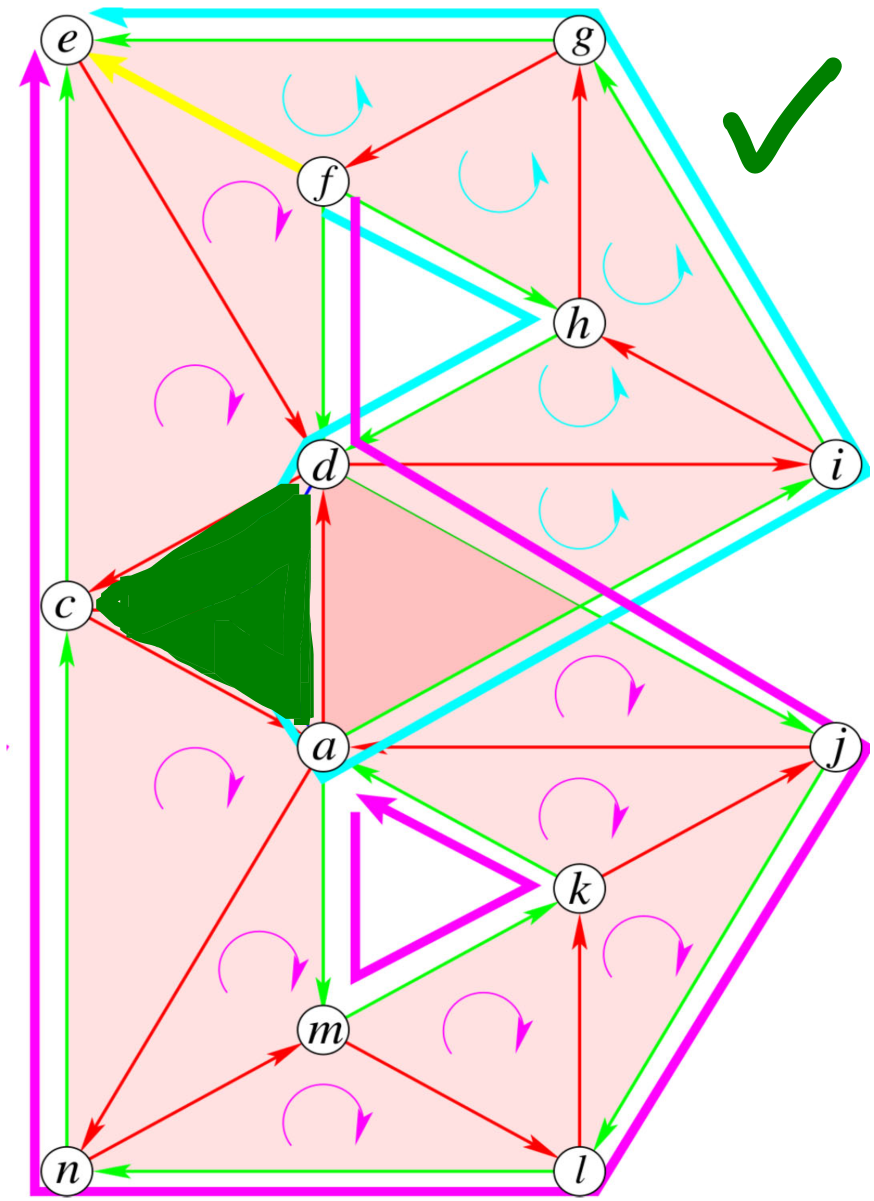


TU



NEUTRALIZING CHAIN



a disc whose boundary consists of an odd number of red (heavy/manifold) edges

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Q2: NTUN result for MSFN ?

MEDIAN SHAPE

Hu, Hudelson, K, Tumurbaatar, Vixie, 2019

* flat distance between T, T' : $\mathbb{F}_\lambda(T, T') = \mathbb{F}_\lambda(T - T')$

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  flat norm w/ scale λ

* median of $\{T_i\}$:

$$\hat{T} = \underset{T}{\arg\min} \sum_i \mathbb{F}_\lambda(T - T_i)$$

MEDIAN SHAPE : LP

$$\min \left[\quad [\mathbf{w} \;\; \mathbf{w} \;\; \lambda\mathbf{v} \;\; \lambda\mathbf{v}] \;\; [\mathbf{w} \;\; \mathbf{w} \;\; \lambda\mathbf{v} \;\; \lambda\mathbf{v}] \;\; \cdots \;\; [\mathbf{w} \;\; \mathbf{w} \;\; \lambda\mathbf{v} \;\; \lambda\mathbf{v}] \right] \mathbf{x}$$

s.t.

$$\begin{bmatrix} [I \;\; -I] & [-I \;\; I \;\; -B \;\; B] & & & \\ [I \;\; -I] & & [-I \;\; I \;\; -B \;\; B] & & \\ \vdots & & & \ddots & \\ [I \;\; -I] & & & & [-I \;\; I \;\; -B \;\; B] \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \\ \vdots \\ \mathbf{t}_N \end{bmatrix}$$

$$\left[\mathbf{t}^+ \;\; \mathbf{t}^- \;\; \mathbf{r}_1^+ \;\; \mathbf{r}_1^- \;\; \mathbf{s}_1^+ \;\; \mathbf{s}_1^- \;\; \mathbf{r}_2^+ \;\; \mathbf{r}_2^- \;\; \mathbf{s}_2^+ \;\; \mathbf{s}_2^- \;\; \cdots \;\; \mathbf{r}_N^+ \;\; \mathbf{r}_N^- \;\; \mathbf{s}_N^+ \;\; \mathbf{s}_N^- \right] \geq \mathbf{0}.$$

$B = [\partial_{p+1}]$

MEDIAN SHAPE : LP

$$\min \begin{bmatrix} [\,\mathbf{w} & \mathbf{w} & \lambda\mathbf{v} & \lambda\mathbf{v}\,] & [\,\mathbf{w} & \mathbf{w} & \lambda\mathbf{v} & \lambda\mathbf{v}\,] & \cdots & [\,\mathbf{w} & \mathbf{w} & \lambda\mathbf{v} & \lambda\mathbf{v}\,] \end{bmatrix} \mathbf{x}$$

s.t.

$$\begin{bmatrix} \begin{bmatrix} I & -I \end{bmatrix} & \begin{bmatrix} -I & I & -B & B \end{bmatrix} & & \\ \begin{bmatrix} I & -I \end{bmatrix} & & \begin{bmatrix} -I & I & -B & B \end{bmatrix} & \\ \vdots & & & \ddots \\ \begin{bmatrix} I & -I \end{bmatrix} & & & \begin{bmatrix} -I & I & -B & B \end{bmatrix} \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \\ \vdots \\ \mathbf{t}_N \end{bmatrix}$$

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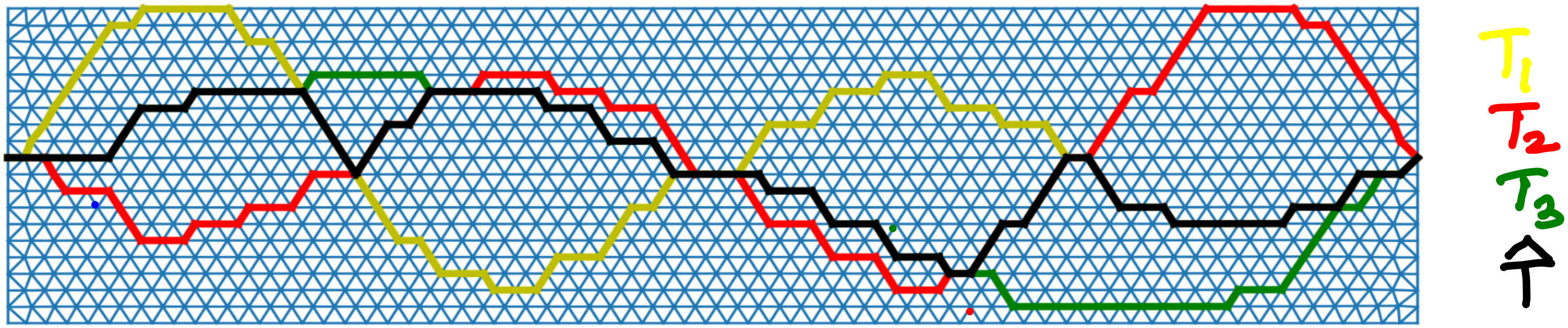
✗ constraint matrix not TU even if $[\partial_{p+1}]$ is

MEDIAN SHAPE: EXAMPLES



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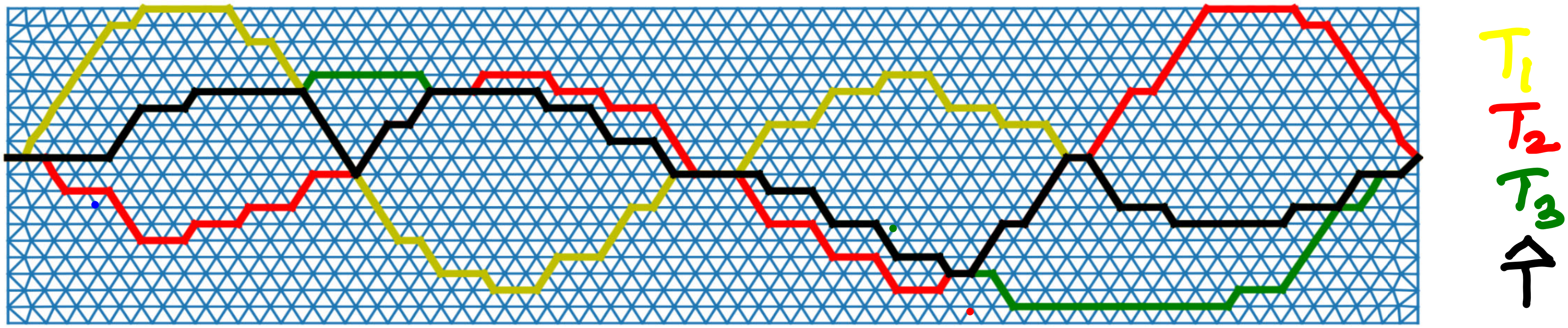

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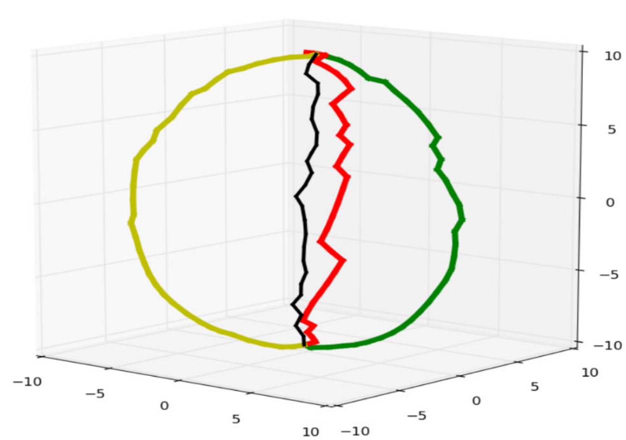

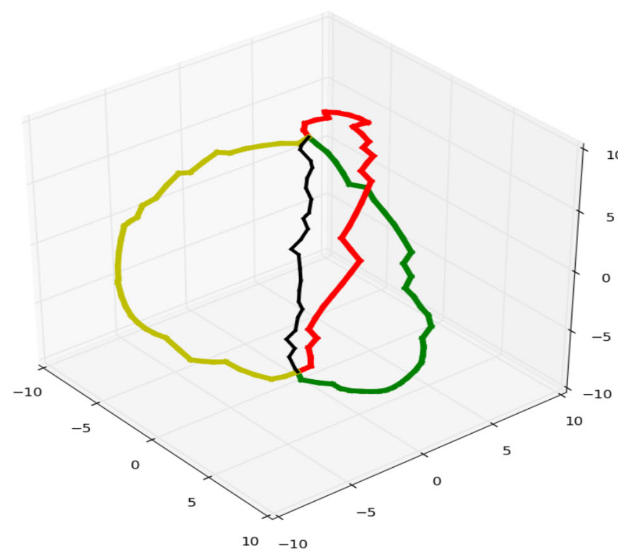

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MEDIAN SHAPE: QUESTIONS

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Q4: Network flow (dual graph) model for median shape?

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Thank You!