

4-22-2011

# Integer Optimization and Computational Algebraic Topology

Bala Krishnamoorthy  
*Washington State University*

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## Recommended Citation

Krishnamoorthy, Bala, "Integer Optimization and Computational Algebraic Topology" (2011). *Systems Science Friday Noon Seminar Series*. 55.

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# INTEGER OPTIMIZATION AND COMPUTATIONAL TOPOLOGY

BALA KRISHNAMOORTHY  
WASHINGTON STATE UNIVERSITY

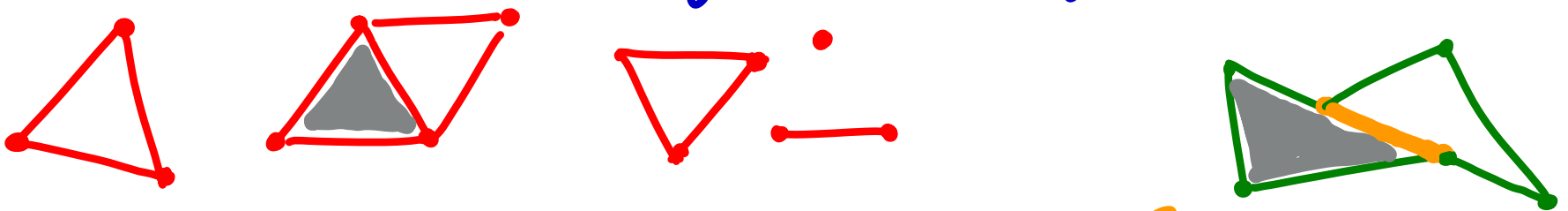
[www.wsu.edu/~kbala](http://www.wsu.edu/~kbala)

# SIMPLICIAL COMPLEX

$K$ : a collection of simplices in  $\mathbb{R}^d$  such that

(1) every face of a simplex in  $K$  is in  $K$ ;

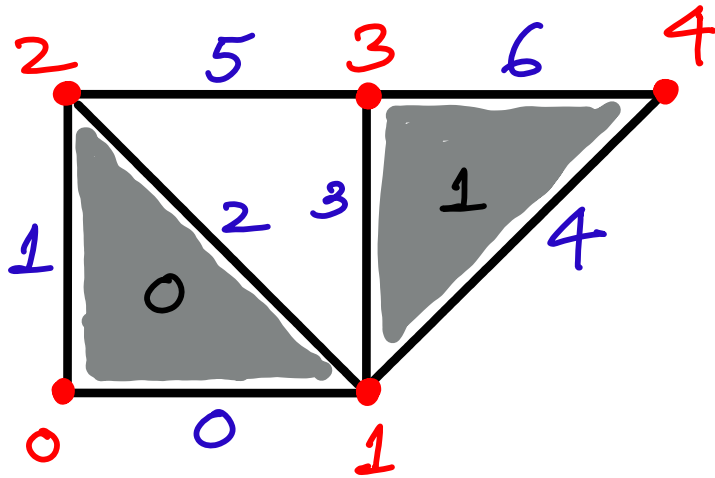
(2) intersection of two simplices of  $K$  is a face of each of them.



not a simplicial complex ←

# AN EXAMPLE

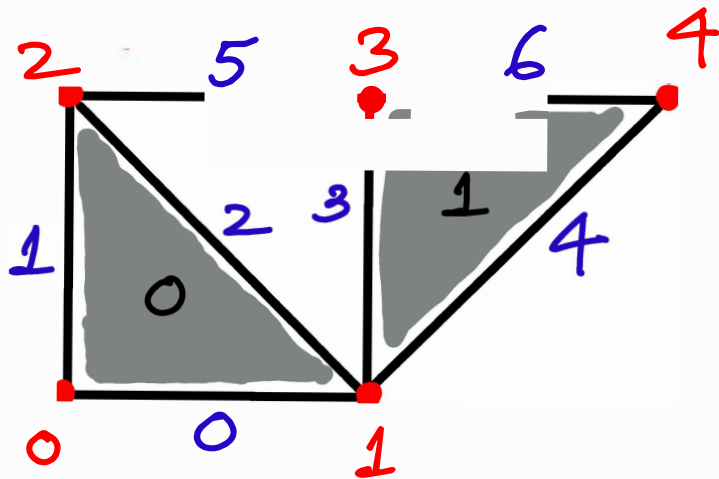
K:



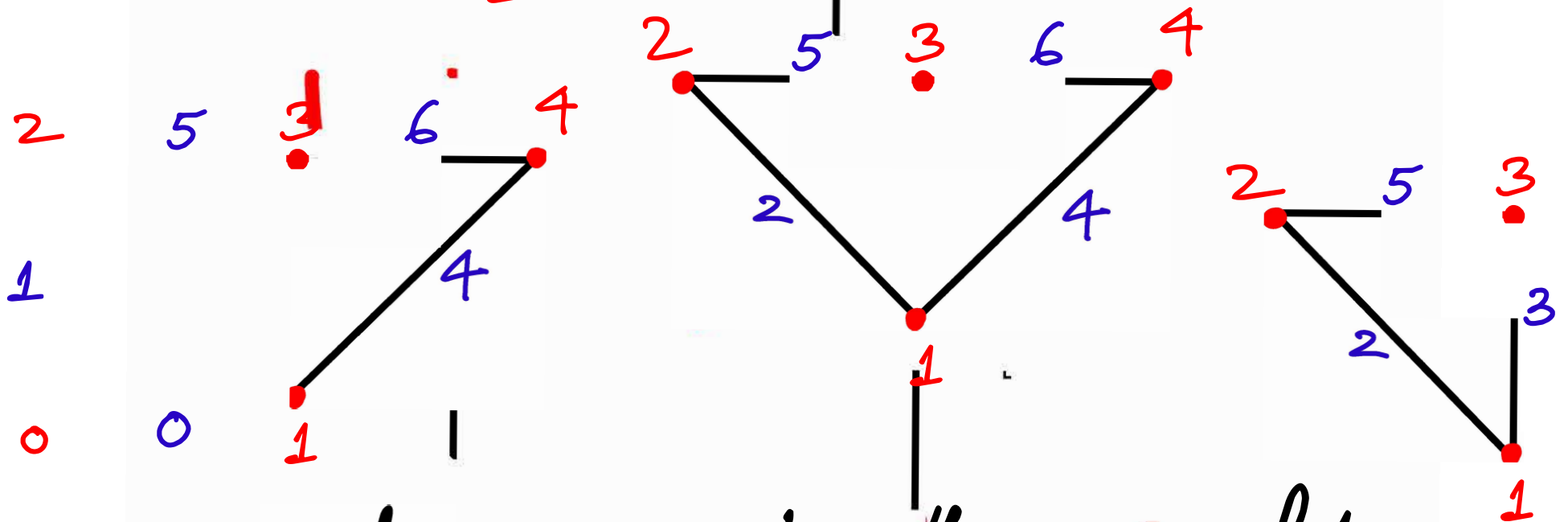
*hole in the middle*

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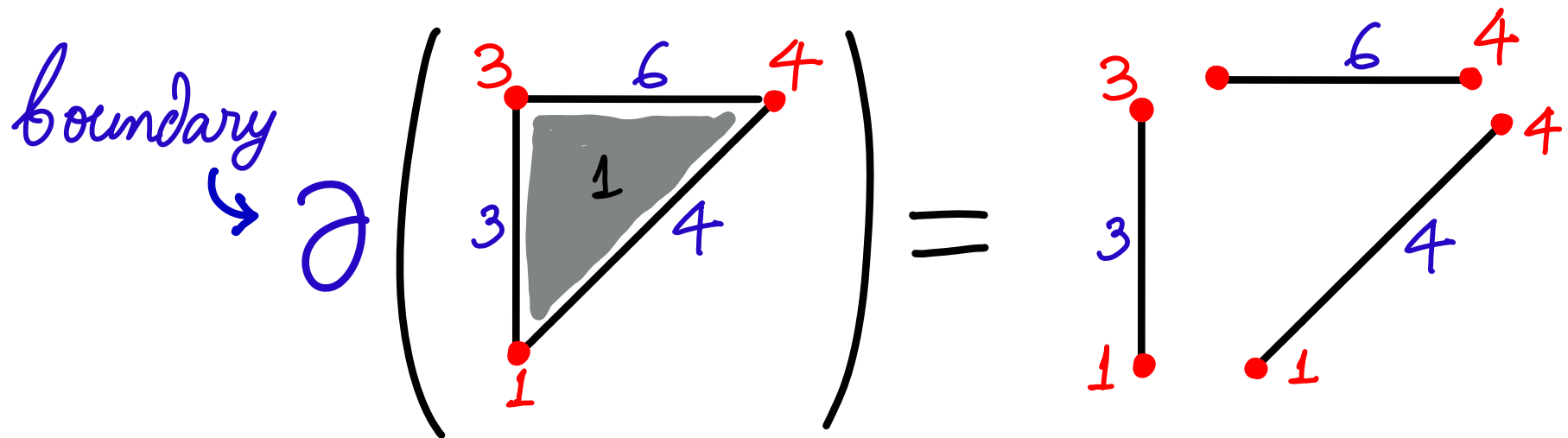
hole in the middle



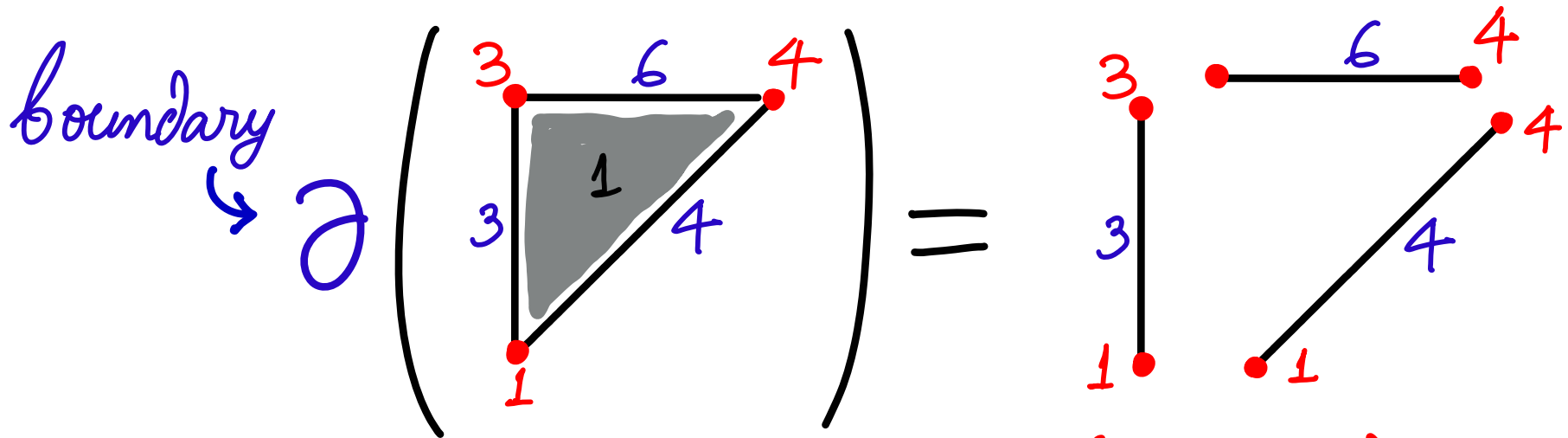
cycles representing the same hole

②

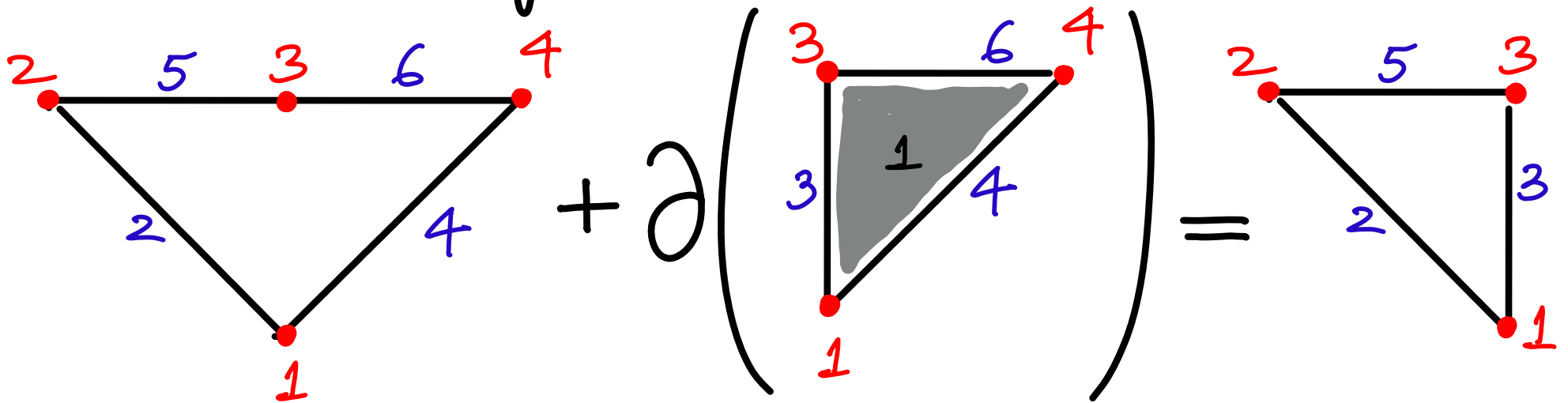
# AN EXAMPLE



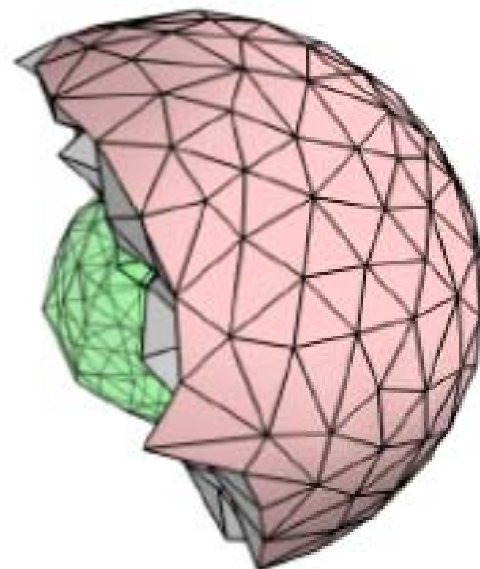
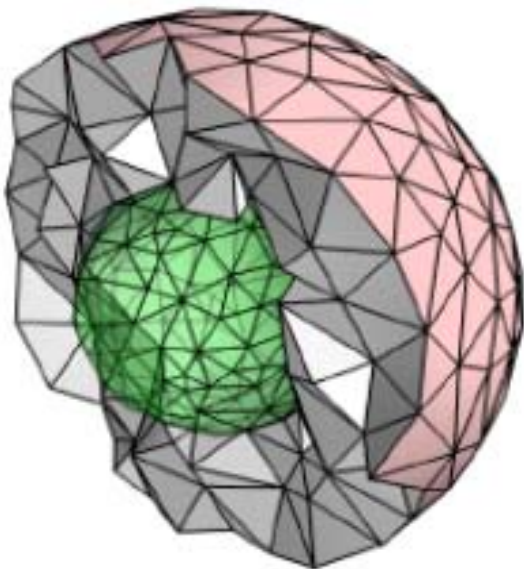
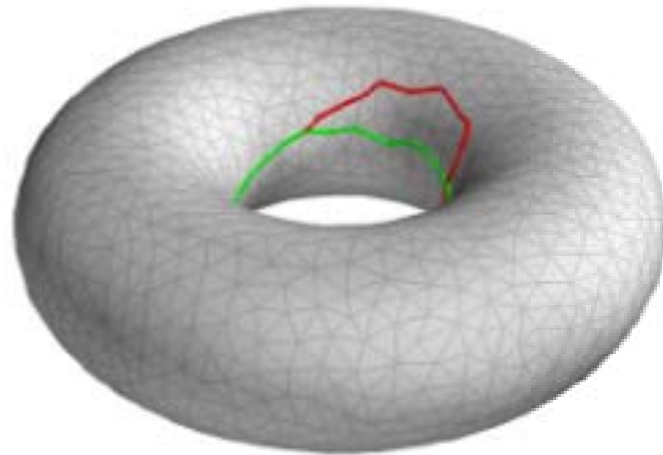
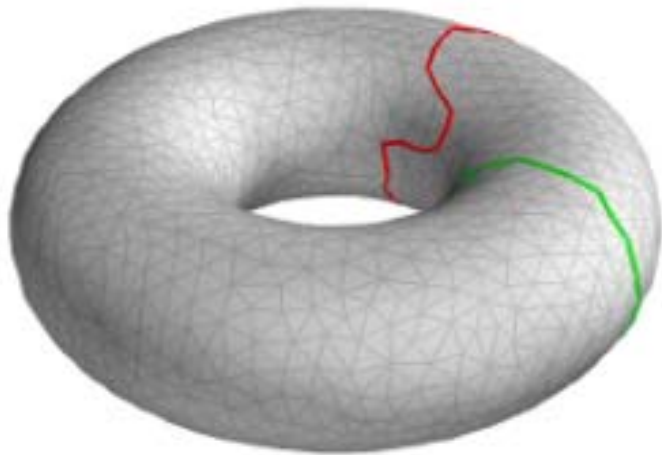
# AN EXAMPLE



add edges in  $\mathbb{Z}_2$  ( $1+1=0$ )



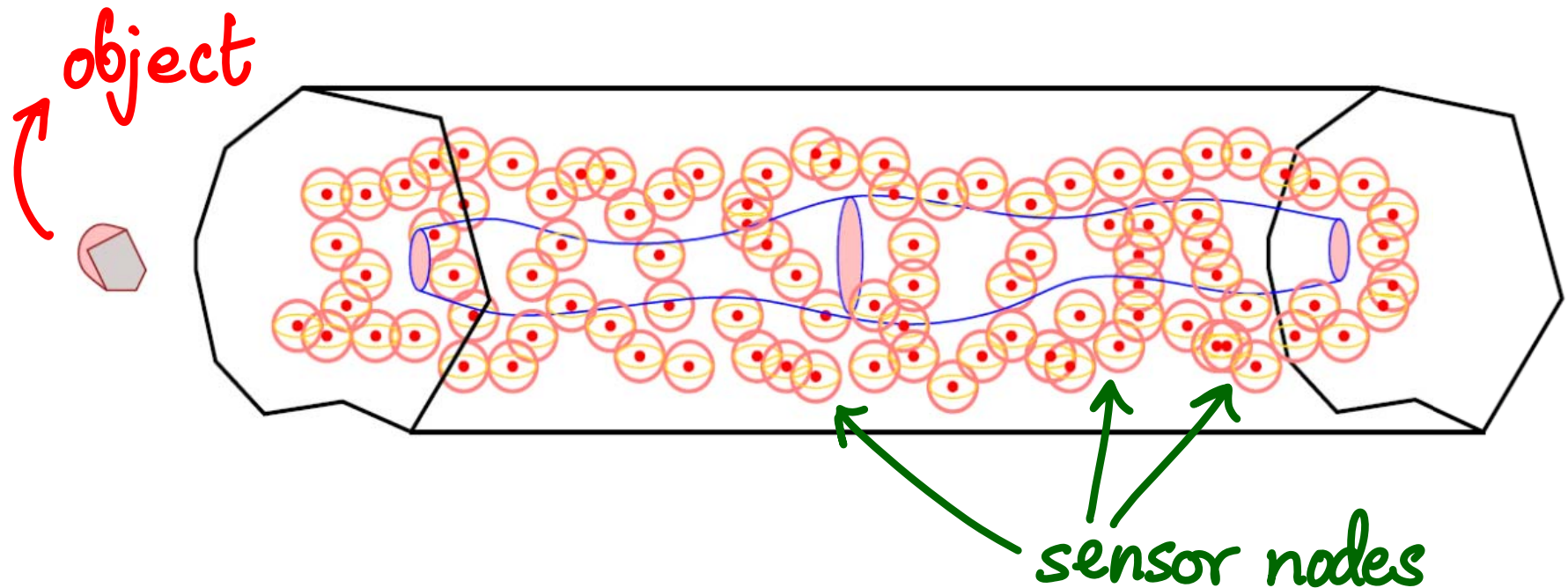
# EXAMPLES IN 3D





# APPLICATIONS

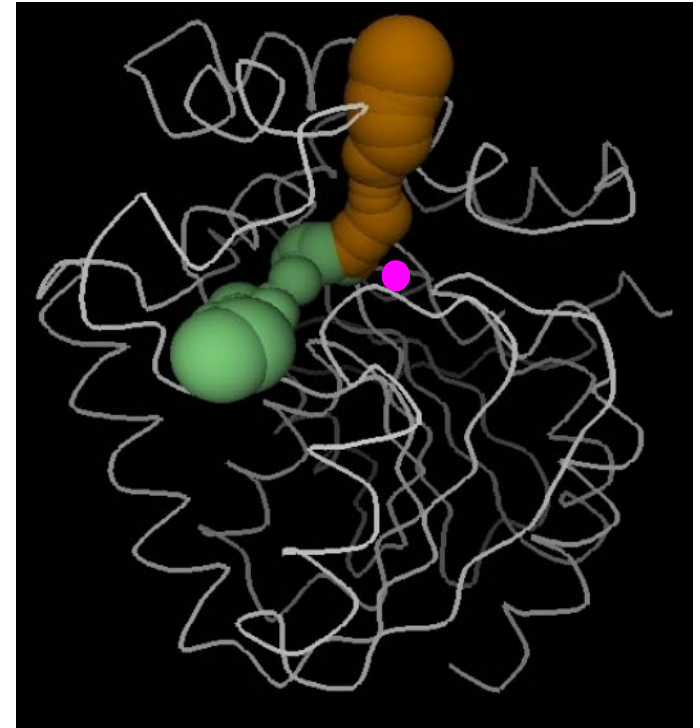
Sensor networks: object-specific coverage in 3D



Coverage guaranteed if "narrowest neck" in tunnel is smaller than object

# APPLICATIONS

tunnels in proteins —  
access to active site



(image: CAVER)

Substrate can react with protein  
if the "narrowest neck" of tunnel  
is "big enough"

# RESULTS

✗ Problem is NP-hard with addition  
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- Tamal Dey (Ohio St.)  
Anil Hirani (U. Illinois)  
STOC '10  
SICOMP '11

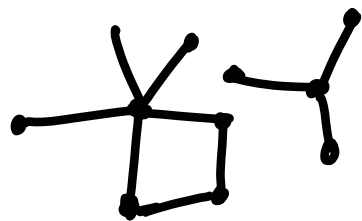
# RESULTS

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  - ✓ Addition over  $\mathbb{Z}$ : polynomial-time solvable for a large majority of  $K$  using linear programming.
  - ✓ topological characterization of total unimodularity (TU)
  - ✓ flat norm of currents in simplicial complexes
- Tamal Dey (Ohio St.)  
Anil Hirani (U. Illinois)  
STOC '10  
SICOMP '11
- Kevin Vixie,  
Sharif Ibrahim (WSU)

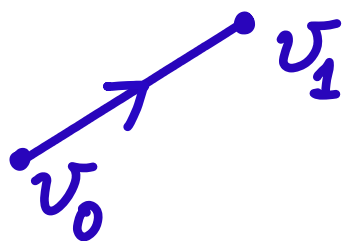
# CHAINS

Orientation of a simplex:

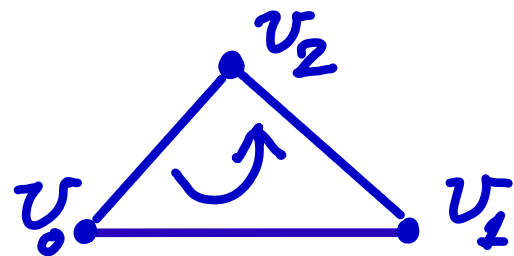
1-chain:



collection of edges



$[v_0 v_1]$  or  $[v_1 v_0]$



$[v_0 v_1 v_2]$  or  $[v_0 v_2 v_1]$

p-chain c: Function from oriented simplices to  $\mathbb{Z}$ :

$c(\sigma) = -c(\sigma')$  if  $\sigma$  and  $\sigma'$  are opposite orientations of same simplex



# CHAIN GROUPS

Add  $p$ -chains by adding their values over  $\mathbb{Z} \Rightarrow$   
 $C_p(K)$ : group of (oriented)  $p$ -chains.

Elementary chain of  $\sigma \in K$ :

$$c(\sigma) = 1,$$

$$c(\sigma') = -1, \text{ if } \sigma': \text{ opposite orientation of } \sigma$$

$$c(\tau) = 0 \quad \forall \tau \neq \sigma, \sigma'$$

Result:  $C_p(K)$  is free abelian; the elementary chains form a basis for  $C_p(K)$ .

# BOUNDARY OPERATOR

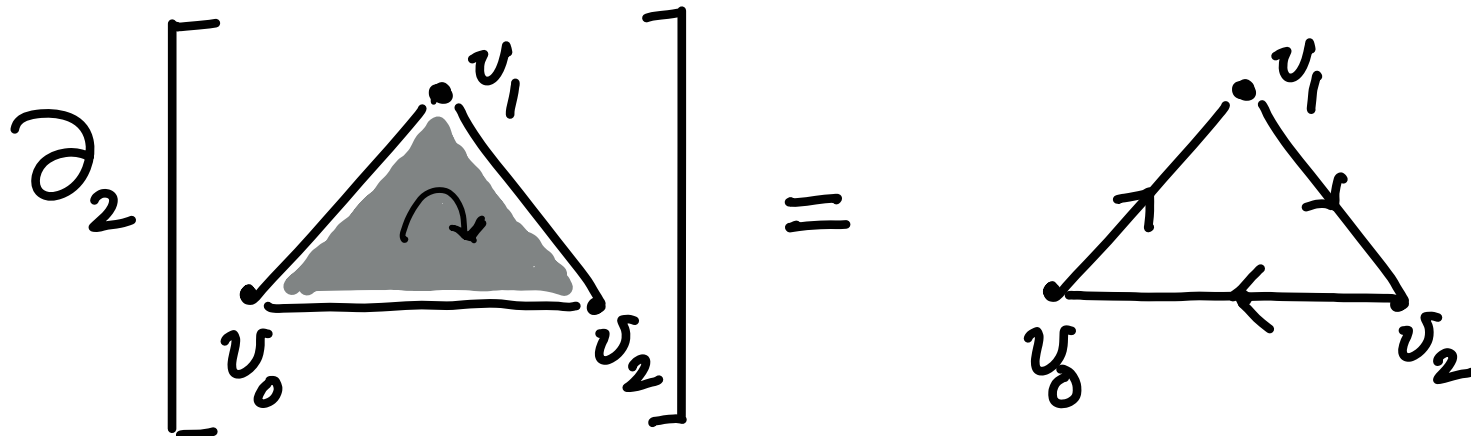
The homomorphism  $\partial_p: C_p(K) \rightarrow C_{p-1}(K)$ .

$\sigma = [v_0, \dots, v_p]$ : oriented simplex,  $p > 0$ .

$$\partial_p \sigma = \partial_p [v_0, \dots, v_p] = \sum_{i=0}^p (-1)^i [v_0, \dots, \overset{\wedge}{v_i}, \dots, v_p]$$

delete  $v_i$

e.g.,  $\partial_2 [v_0, v_1, v_2] = [v_1, v_2] - [v_0, v_2] + [v_0, v_1]$



# HOMOLOGY GROUPS

Lemma:  $\partial_{p-1} \circ \partial_p = 0$  boundary of boundary is empty

$\ker \partial_p = Z_p(K)$  group of  $p$ -cycles

$\text{im } \partial_{p+1} = B_p(K)$  group of  $p$ -boundaries

$$B_p(K) \subset Z_p(K) \subset C_p(K)$$

$$H_p(K) = Z_p(K) / B_p(K)$$

$\rightarrow$   $p^{\text{th}}$  homology group of  $K$ .  
group of  $p$ -cycles that are NOT  $p$ -boundaries

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$$B_p(K) \subset Z_p(K) \subset C_p(K)$$

Could study  $H_p(K, G)$  for  
 $G = \mathbb{Z}, \mathbb{Z}_2, \mathbb{Q}, \text{ etc.}$

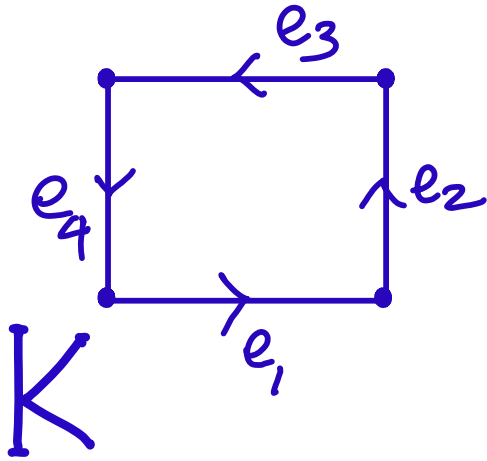
$$H_p(K) = Z_p(K) / B_p(K)$$

$\mathbb{Z}_2$ : widely used for computation.  
field, simple, intuitive

group of  $p$ -cycles that are NOT  $p$ -boundaries

$\rightarrow$   $p^{\text{th}}$  homology group of  $K$ .

# EXAMPLE



$C_1(K)$ : free abelian of rank 4  
general 1-chain:  $c = \sum_{i=1}^4 n_i e_i$   
 $c$  is a cycle  $\Leftrightarrow n_1 = n_2 = n_3 = n_4$

$\Rightarrow Z_1(K)$  is infinite cyclic, generated by  
 $e_1 + e_2 + e_3 + e_4$

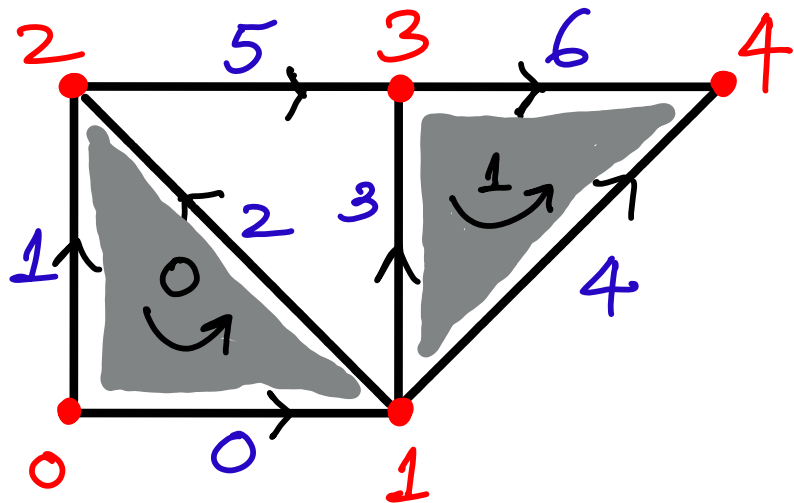
No 2-simplices in  $K \Rightarrow B_1(K)$  is trivial.

$\Rightarrow H_1(K) = Z_1(K) / B_1(K) \cong \mathbb{Z}$ .

# BOUNDARY MATRIX $[\partial_p]$

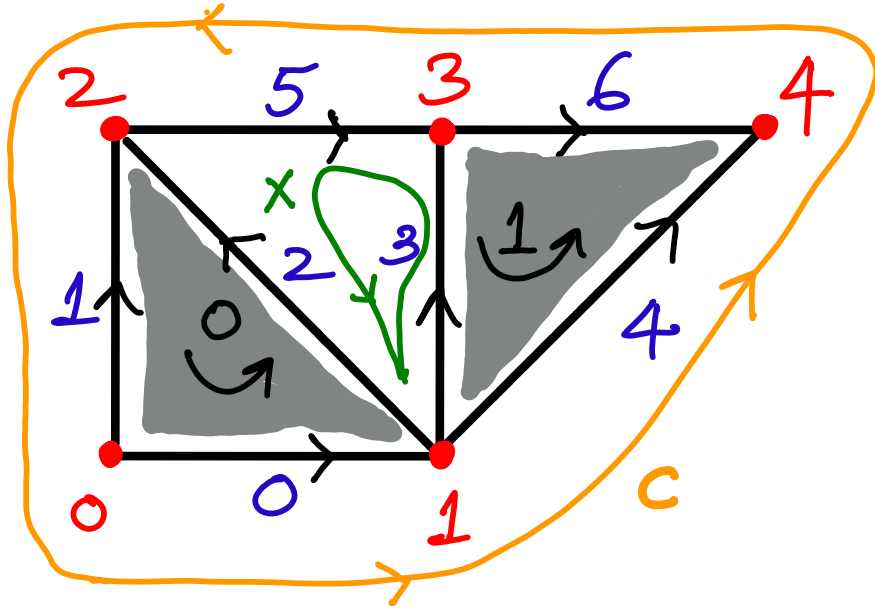
$$\partial_p: C_p(K) \rightarrow C_{p-1}(K)$$

If  $\{\sigma_i\}_{i=0}^{m-1}$  and  $\{\tau_j\}_{j=0}^{n-1}$  are elementary chain bases for  $C_{p-1}(K)$  &  $C_p(K)$ , then  $[\partial_p]$  is an  $m \times n$  matrix,  $[\partial_p]_{ij} \in \{-1, 0, 1\}$ .



$$[\partial_2] = \begin{matrix} & 0 & 1 \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix} & \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & -1 \end{bmatrix} \end{matrix}$$

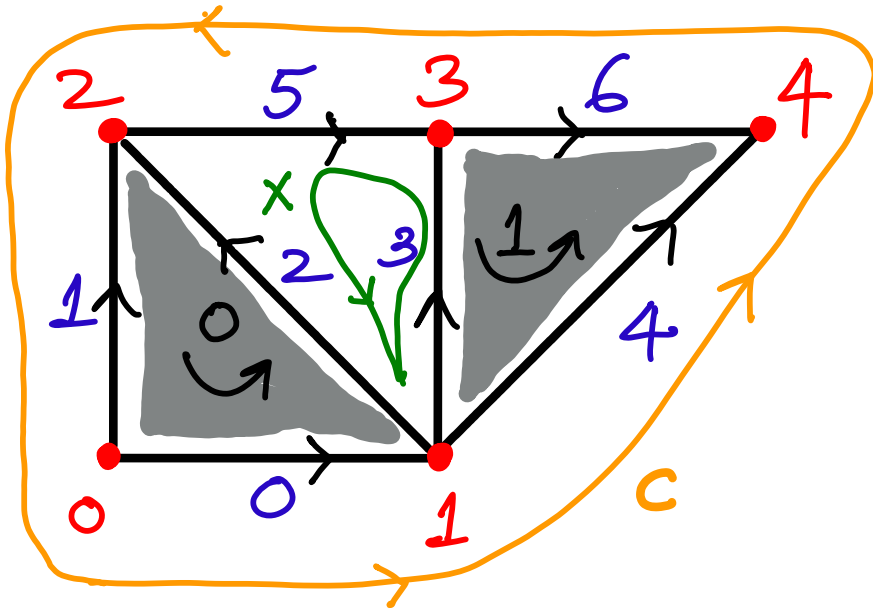
# SHORT HOMOLOGOUS CYCLES



$$C = \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

represents hole in middle, but has 5 edges.

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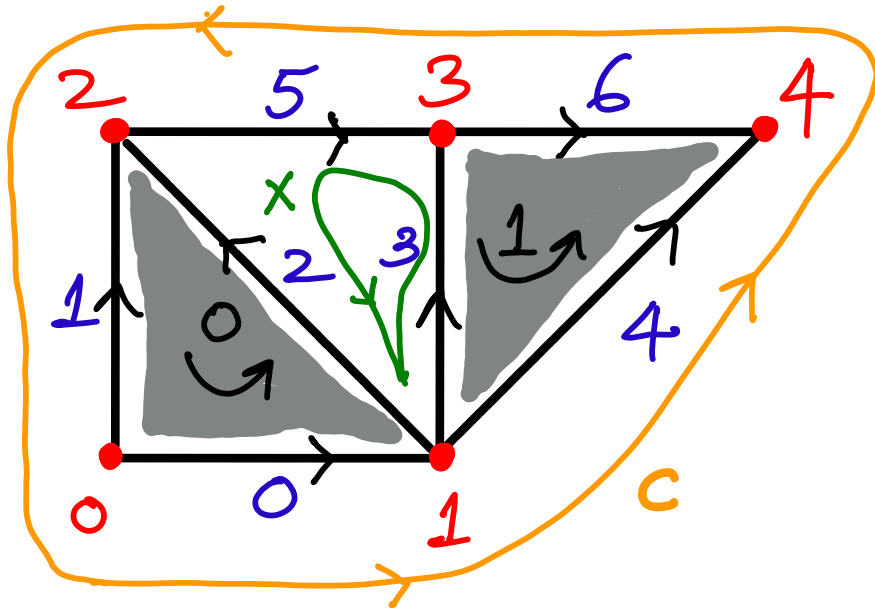
$$x = \begin{bmatrix} 0 \\ 0 \\ -1 \\ -1 \\ 0 \\ 0 \end{bmatrix}$$

is homologous to  $c$ , but is shorter (has only 3 edges)

$x$  is "tightest" cycle around the hole



# SHORT HOMOLOGOUS CYCLES



$$C = \begin{bmatrix} -1 \\ -1 \\ 0 \\ 0 \\ -1 \\ -1 \end{bmatrix} \quad X = \begin{bmatrix} 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ 0 \end{bmatrix}$$

$$X = C + [\partial_2] \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$X \sim C$  ( $X$  is homologous to  $C$ )

Can study weighted (in  $\mathbb{R}$ ) chains/cycles (instead of  $\pm 1$  weights)

$$[\partial_2] = \begin{matrix} & 0 & 1 \\ 0 & 1 & 0 \\ 1 & -1 & 0 \\ 2 & 1 & 0 \\ 3 & 0 & -1 \\ 4 & 0 & 1 \\ 5 & 0 & 0 \\ 6 & 0 & -1 \end{matrix}$$

# OPTIMAL HOMOLOGOUS CYCLE PROBLEM

OHCP: Given a  $p$ -cycle  $c$  in  $K$ , find a cycle  $c^*$  with smallest value of  $\|Wc^*\|_1$  among all cycles homologous to  $c$ .

$W = \text{diag}(w_1, \dots, w_m)$ , where  $w_i \in \mathbb{R}_{\geq 0}$  is the weight of  $p$ -simplex  $\sigma_i \in K$ .

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# OPTIMAL HOMOLOGOUS CHAIN PROBLEM

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With homology defined over  $\mathbb{Z}_2$ , OHCP is NP-hard (Chen & Freedman, 2010)

# OHCP AS AN INTEGER PROGRAM

$\min_{x, y} \|Wx\|_1$  such that

$$x = c + [a_{p+1}]y, \quad x \in \mathbb{Z}^m, \quad y \in \mathbb{Z}^n$$

# OHCP AS AN INTEGER PROGRAM

$$\min_{x, Y} \|Wx\|_1 \quad \text{such that} \quad = \sum_i |w_i| |x_i| \quad \text{piecewise linear}$$
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$$\min \sum_i |w_i| (x_i^+ + x_i^-) \quad (\text{IP})$$

$$\text{s.t.} \quad x^+ - x^- = c + [a_{p+1}]Y$$

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

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ignore to get LP relaxation  $\leftarrow$



# IP AND TOTAL UNIMODULARITY

$$\left. \begin{array}{l} \min \{ c^T x \mid Ax = b, x \geq 0, x \in \mathbb{Z}^n \} \text{ (IP)} \\ \min \{ c^T x \mid Ax = b, x \geq 0 \} \text{ (LP)} \end{array} \right\} \begin{array}{l} A \in \mathbb{Z}^{m \times n} \\ b \in \mathbb{Z}^m \end{array}$$

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$A$  is TU if every square submatrix has determinant  $-1, 0,$  or  $1$ .

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

# OHCP AND TU OF $[\partial_{p_{t+1}}]$

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

$$\text{s.t. } x^+ - x^- = c + [\partial_{p_{t+1}}]Y \quad (\text{LP})$$

$$x^+, x^- \geq 0$$

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

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

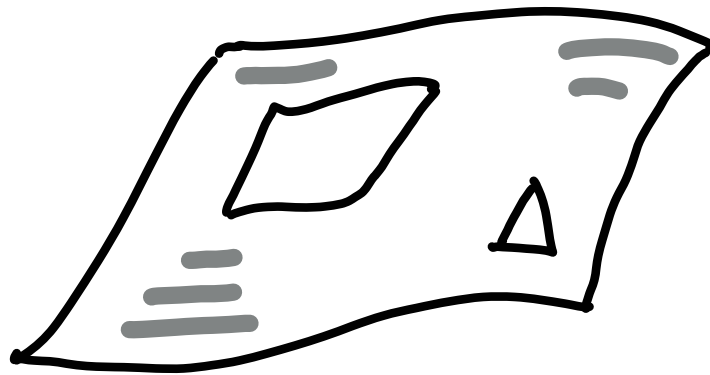
$$\begin{aligned} \min \quad & \sum_i |w_i| (x_i^+ + x_i^-) \\ \text{s.t.} \quad & x^+ - x^- = c + [\partial_{pt+1}]Y \quad (\text{LP}) \\ & x^+, x^- \geq 0 \end{aligned}$$

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

$\Rightarrow$  OHCP (with homology defined over  $\mathbb{Z}$ ) is solvable in polynomial time iff  $[\partial_{pt+1}]$  is TU.

# ORIENTABLE MANIFOLDS

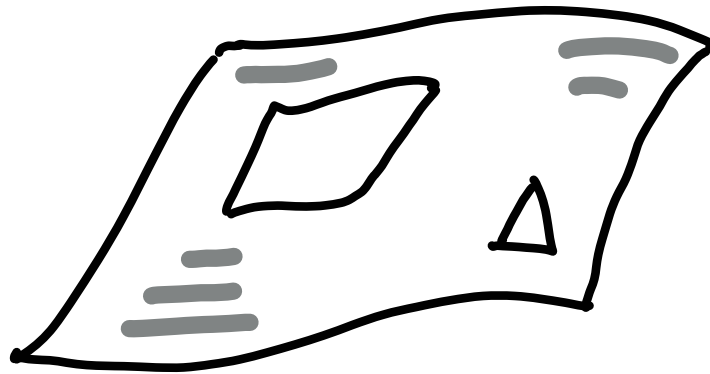
Consistent orientation of  $(p+1)$ -manifold  $M$ : Orient  $(p+1)$ -simplices s.t.  $(p+1)$ -boundary is carried by  $\partial M$ .



possibly empty

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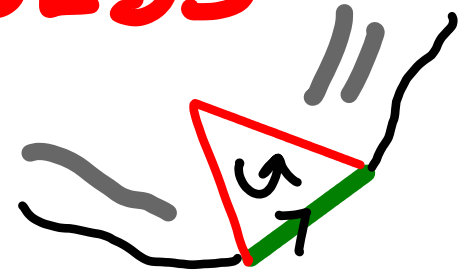
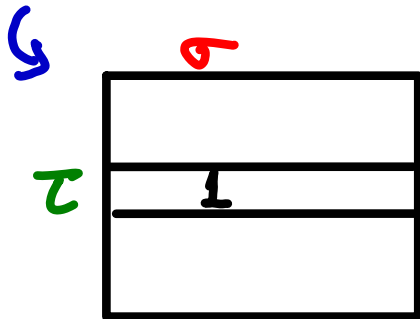
possibly empty

Theorem 1. For a finite simplicial complex triangulating a compact orientable manifold,  $[\partial_{p+1}]$  is TU.



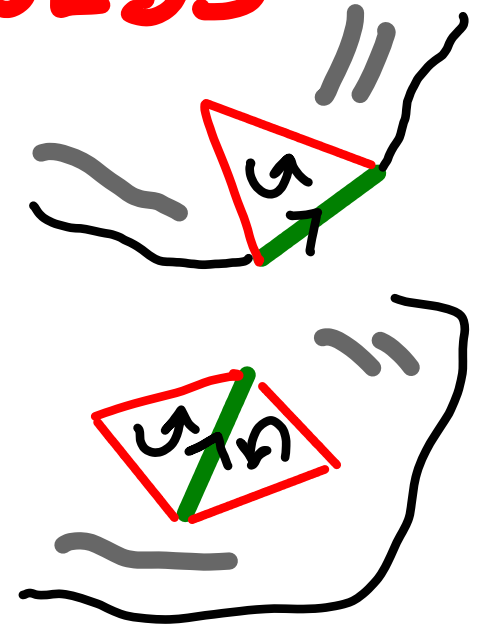
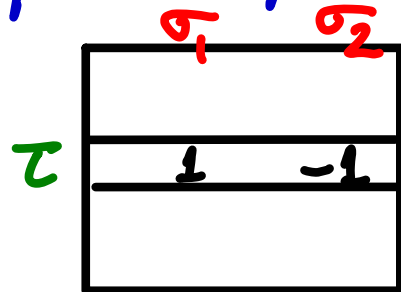
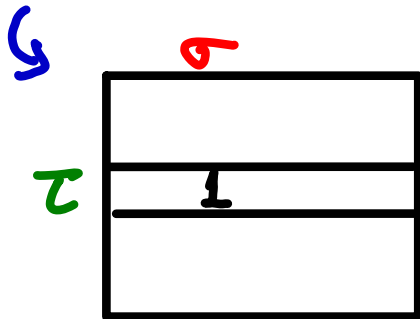
# ORIENTABLE MANIFOLDS

Proof.  $\tau$  ( $p$ -simplex): face of  
one  $\sigma$  ( $(p+1)$ -simplices)



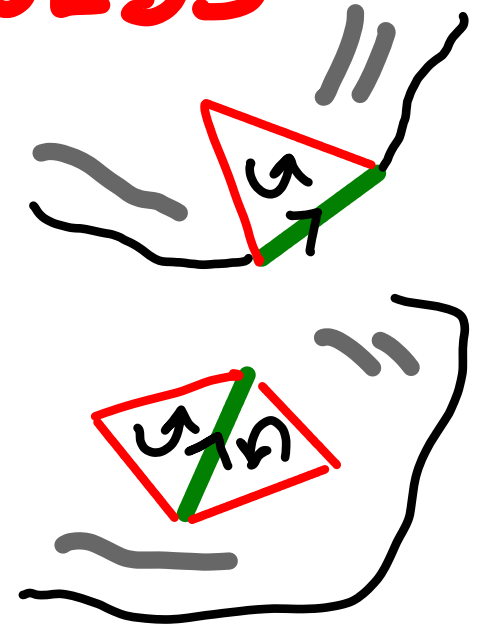
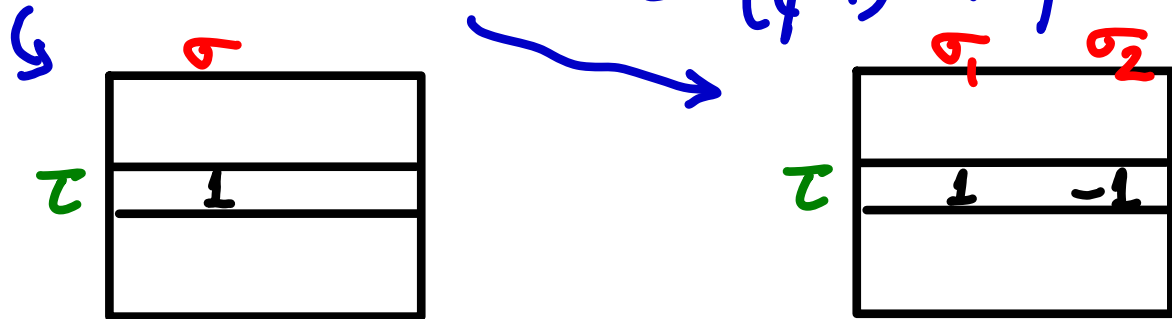
# ORIENTABLE MANIFOLDS

Proof.  $\tau$  ( $p$ -simplex): face of one or two  $\sigma$ 's ( $(p+1)$ -simplices)



# ORIENTABLE MANIFOLDS

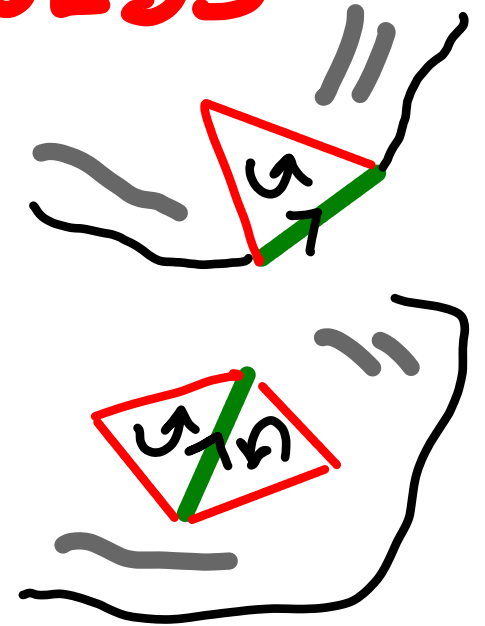
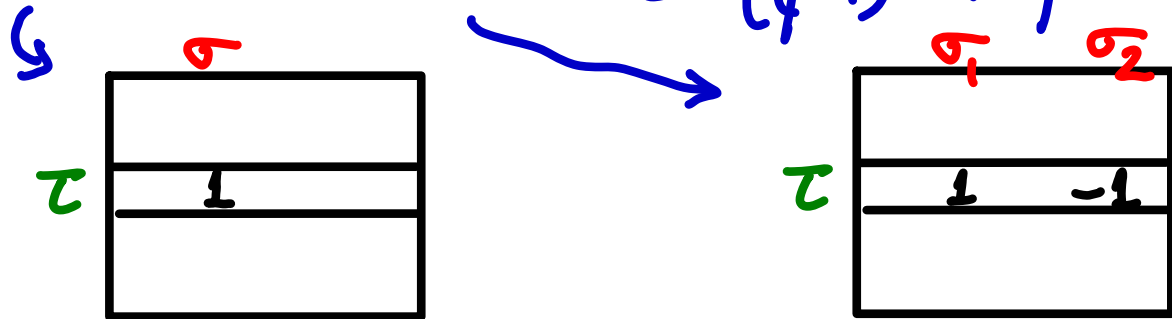
Proof.  $\tau$  ( $p$ -simplex): face of one or two  $\sigma$ 's ( $(p+1)$ -simplices)



$\Rightarrow [\partial_{p+1}]^T$  satisfies sufficient condition for TU.  
 (Heller & Tompkins, 1956)  $\Rightarrow [\partial_{p+1}]$  is TU.

# ORIENTABLE MANIFOLDS

Proof.  $\tau$  ( $p$ -simplex): face of one or two  $\sigma$ 's ( $(p+1)$ -simplices)

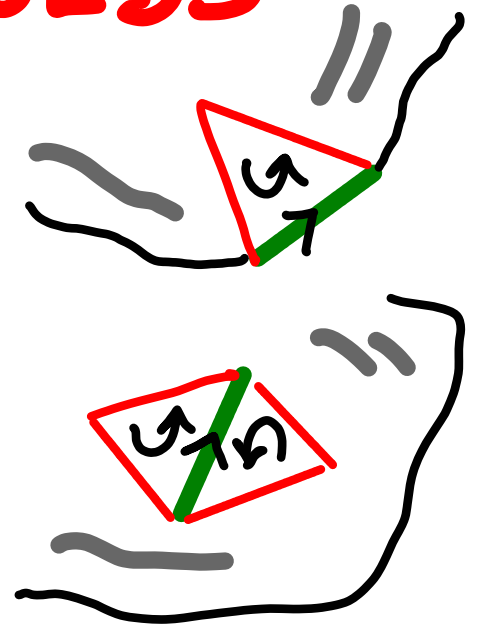
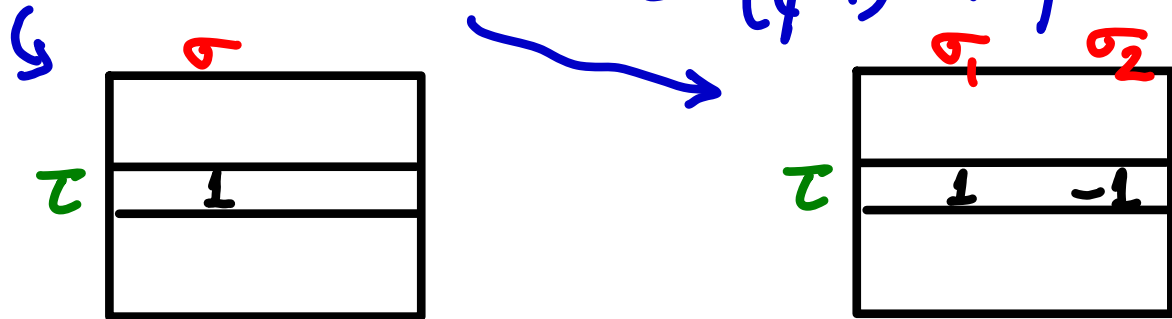


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 (Heller & Tompkins, 1956)  $\Rightarrow [\partial_{p+1}]$  is TU.

Arbitrary orientations  $\equiv$  scale rows/columns of  $[\partial_{p+1}]$  by  $-1 \Rightarrow$  preserves TU.

# ORIENTABLE MANIFOLDS

Proof.  $\tau$  ( $p$ -simplex): face of one or two  $\sigma$ 's ( $(p+1)$ -simplices)



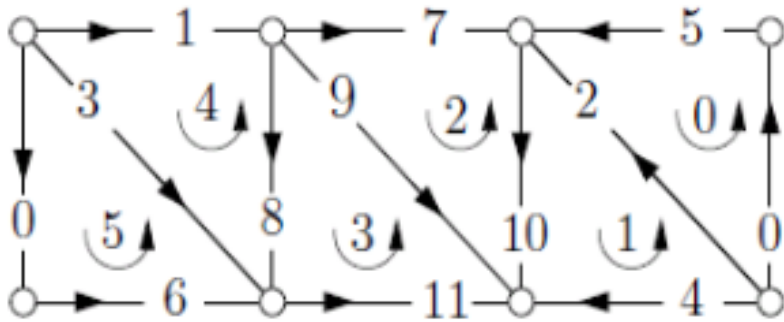
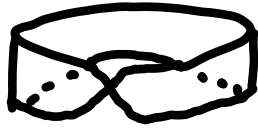
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Also observed by John Sullivan (1992)

# NON-ORIENTABLE MANIFOLDS

Möbius strip:

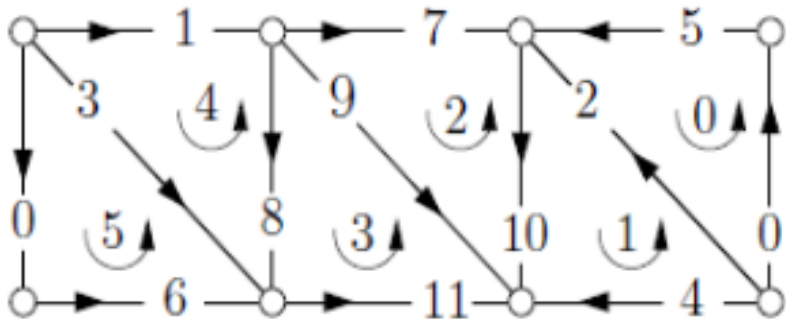
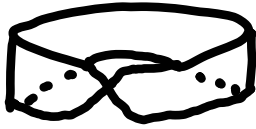


$[\partial_2]$  for Möbius strip:

	0:	1:	2:	3:	4:	5:
0:	1	0	0	0	0	1
1:	0	0	0	0	-1	0
2:	-1	1	0	0	0	0
3:	0	0	0	0	1	-1
4:	0	-1	0	0	0	0
5:	1	0	0	0	0	0
6:	0	0	0	0	0	1
7:	0	0	-1	0	0	0
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# NON-ORIENTABLE MANIFOLDS

Möbius strip:



$$S = \begin{matrix} & \begin{matrix} 5 & 4 & 3 & 2 & 1 & 0 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \end{matrix} & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} \end{matrix} \begin{matrix} 0 \\ 3 \\ 8 \\ 9 \\ 10 \\ 2 \end{matrix}$$

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$\det S = -2. \Rightarrow [\partial_2]$  is not TU.

# MAIN RESULT

Theorem 2:  $[\partial_{p+1}]$  is TU iff  $H_p(L, L_0)$  is torsion-free for all pure subcomplexes  $L, L_0$  of  $K$  of dimensions  $(p+1)$  and  $p$ , respectively, where  $L_0 \subset L$ .

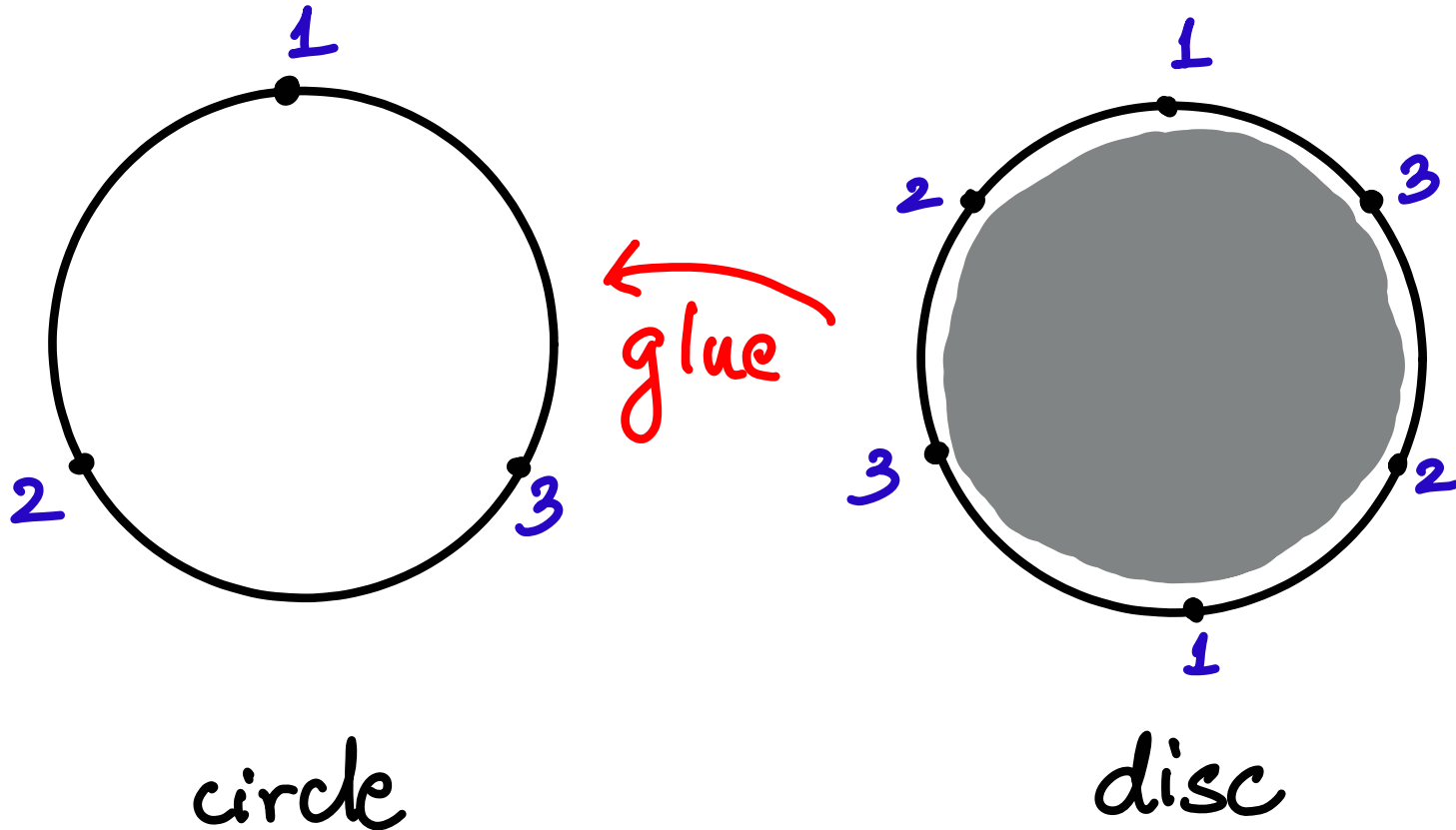


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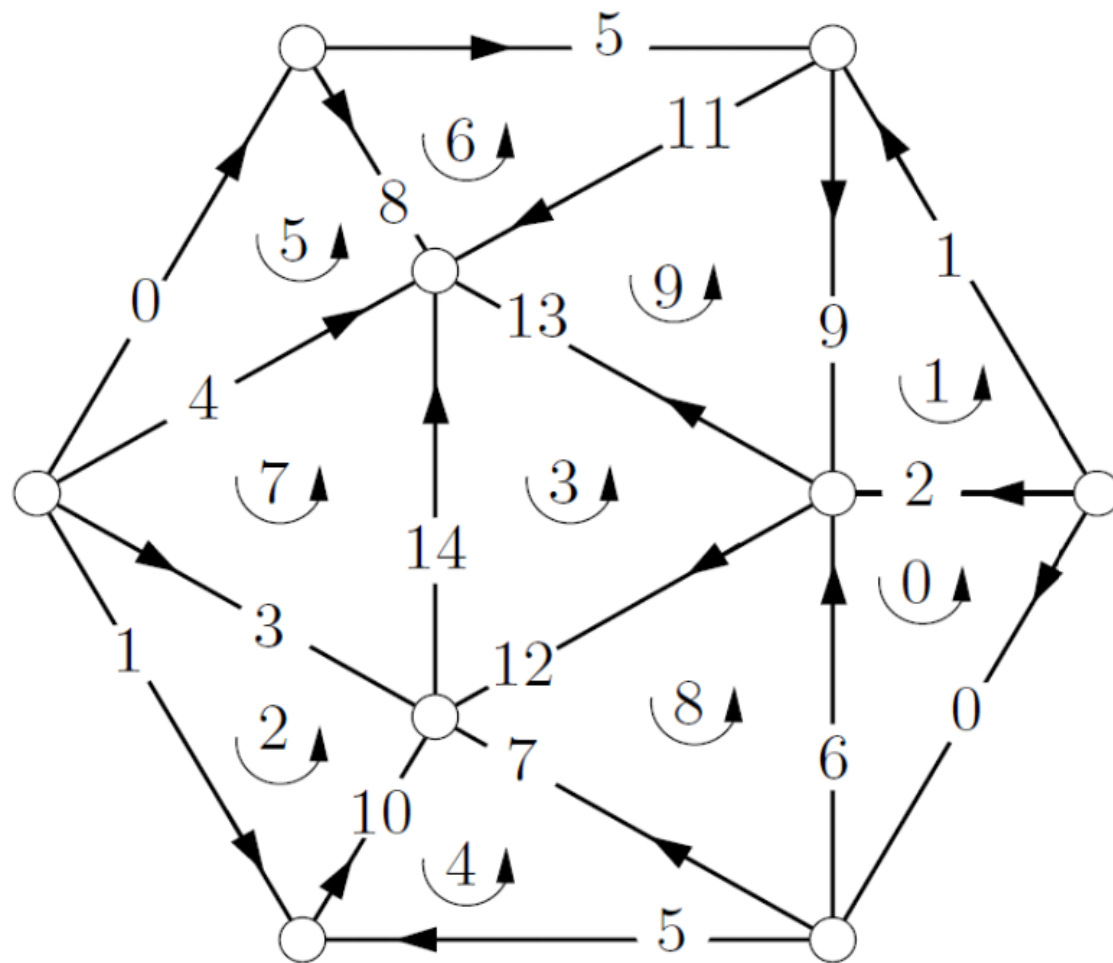
\* topological characterization of TU.

# VISUALIZE TORSION

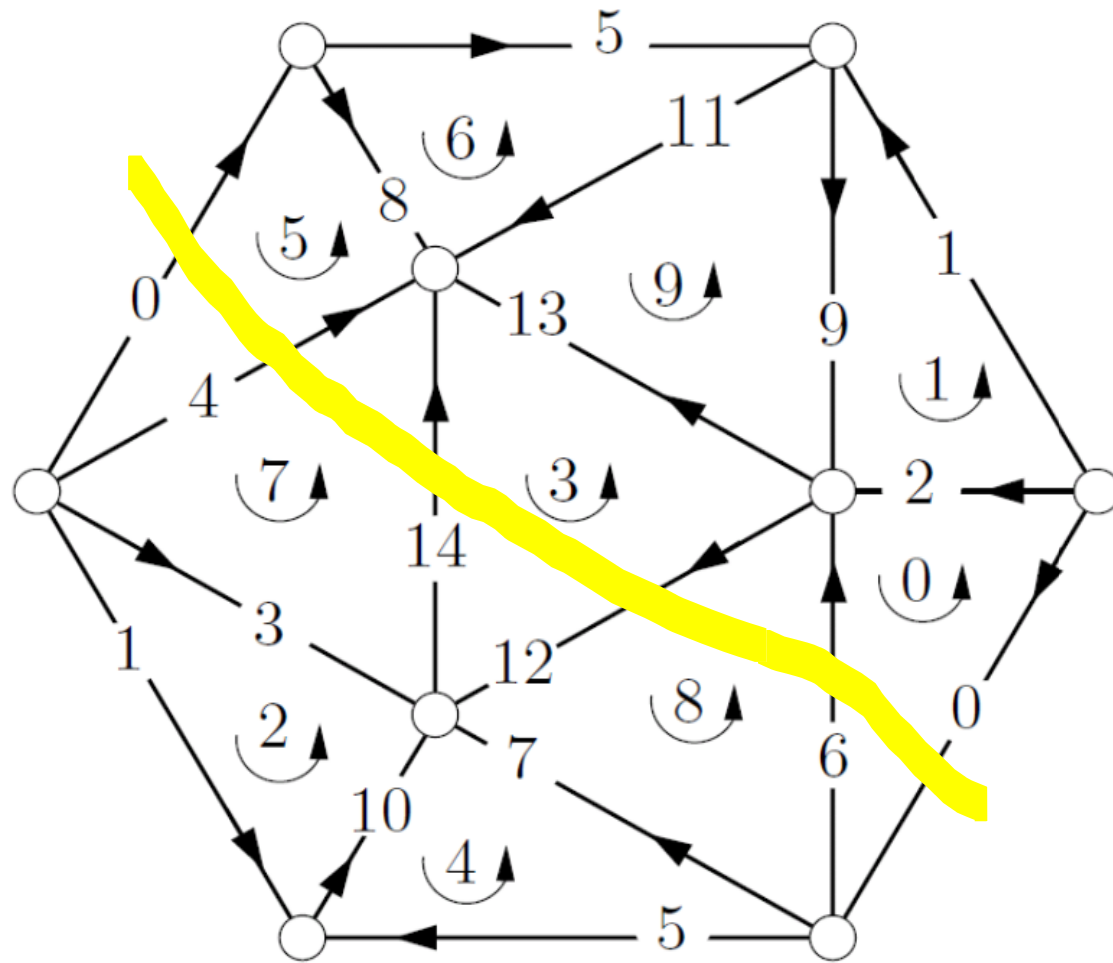


Poincaré (1899): projective plane  
(or Dunce hat)

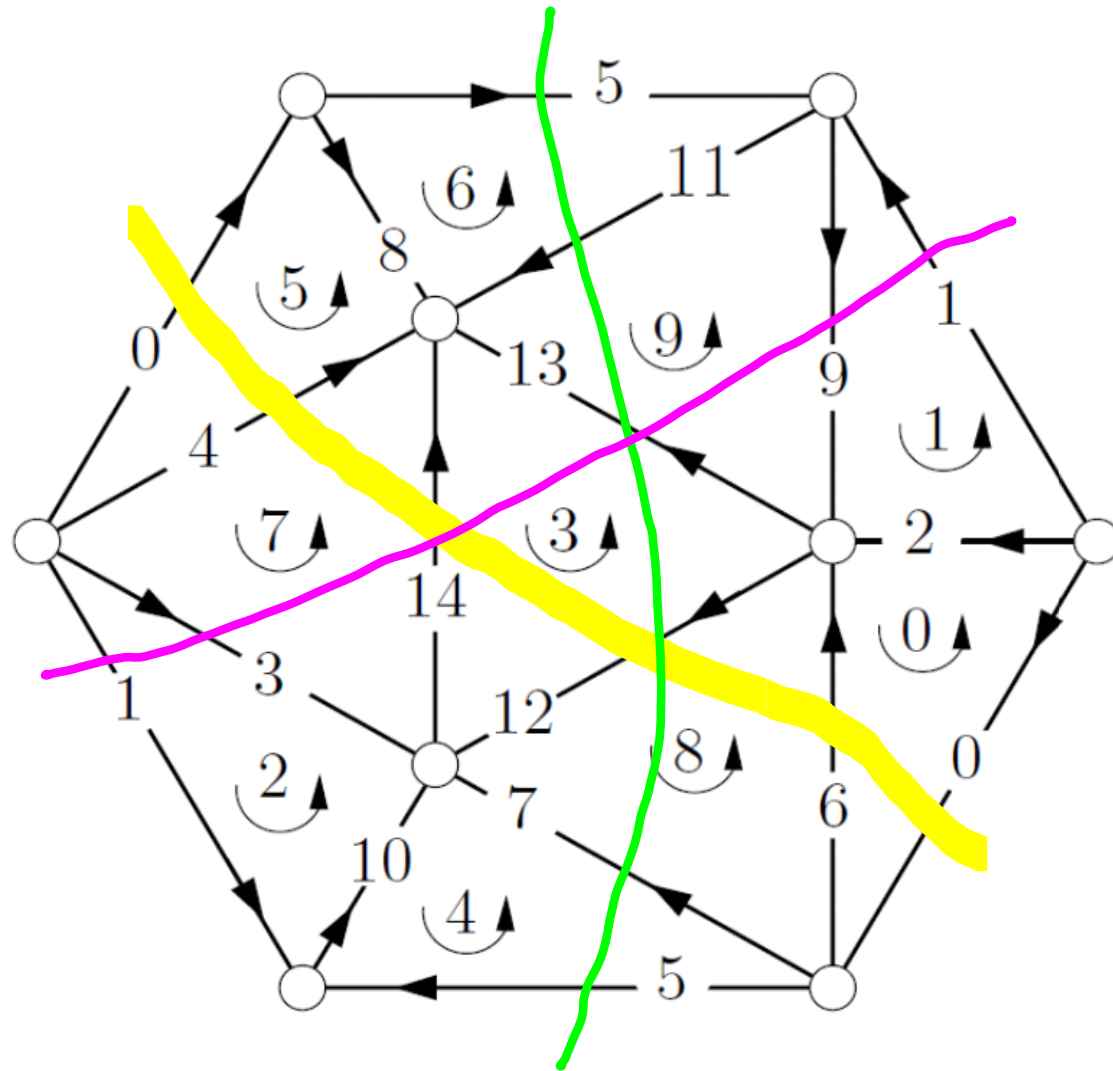
# PROJECTIVE PLANE



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→  $[\partial_d]$  is TU  $\iff K$  embedded in  $\mathbb{R}^d$

e.g., tetrahedra-triangles  $[\partial_3]$  in  $\mathbb{R}^3$



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$T$ :  $d$ -current  
 $S$ :  $(d+1)$ -current

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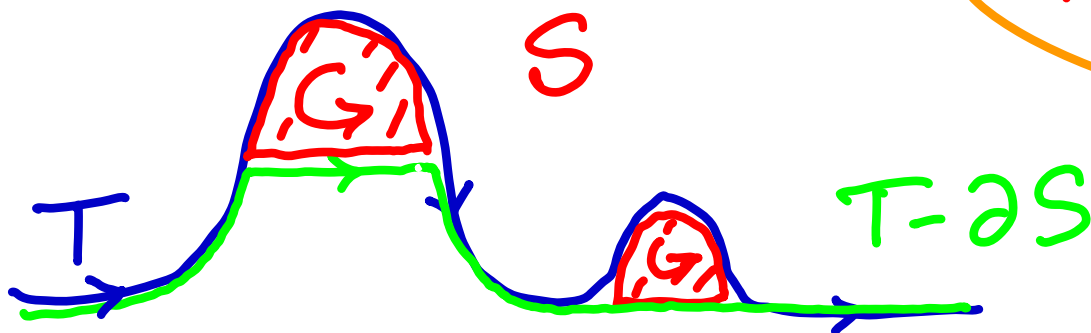
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Integer Optimization model:

$$\min \sum_{i=1}^m w_i |x_i| + \lambda \left( \sum_{j=1}^n v_j |s_j| \right)$$

$$\text{s.t. } x = t - [\partial_{d+1}]s \quad |x_i|, |s_j| \rightarrow \text{linearize}$$
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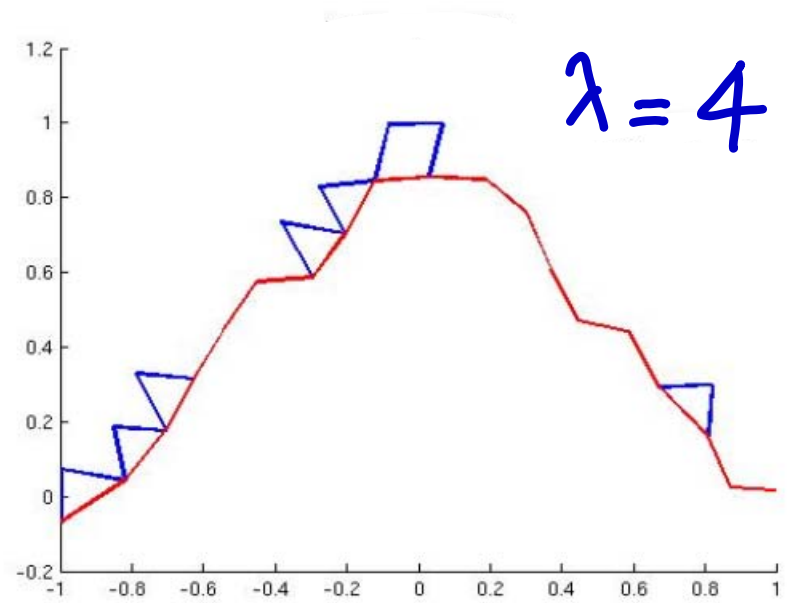
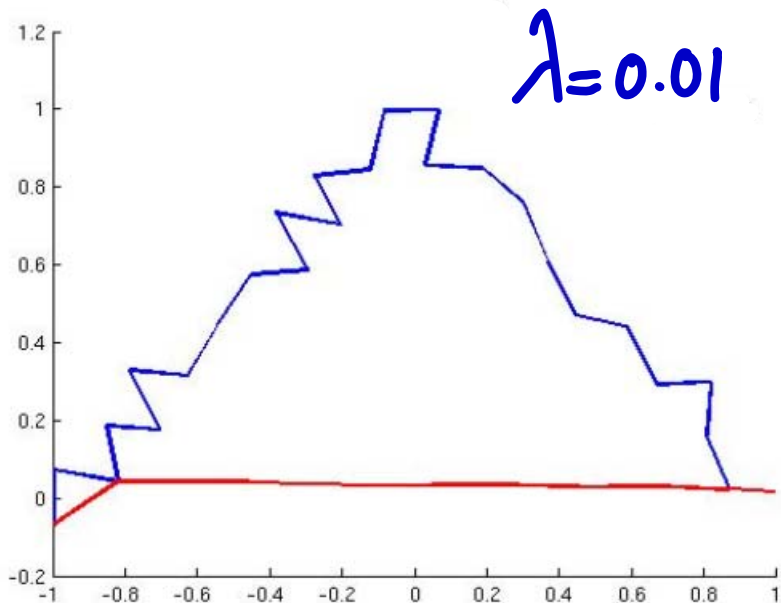
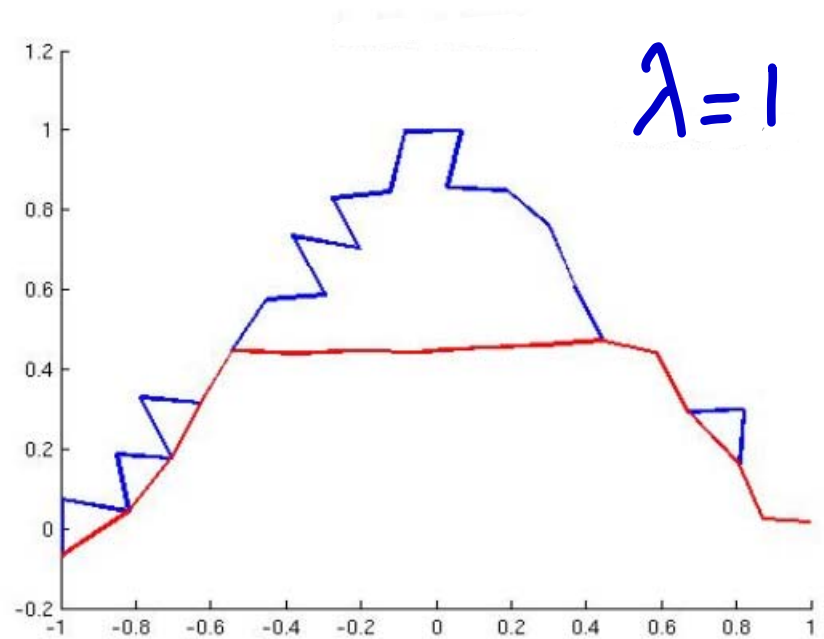
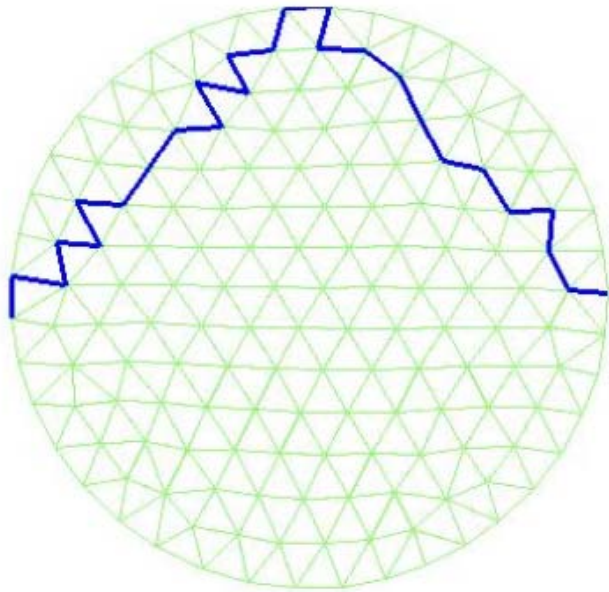
$w_i, v_j$ : volumes

Similar to OHCP LP

- Simplicial deformation theorem: can push any current onto simplicial complex in a controlled manner 28



# ILLUSTRATION



# OPEN QUESTIONS

- \* Can we still get integral solution in the presence of relative torsion?
- \* Faster algos to solve OHCP/MSFN LPs?
- \* LP for optimal homology basis?
- \* Shape signatures from flat norm with scale?