Integer Optimization and Computational Topology

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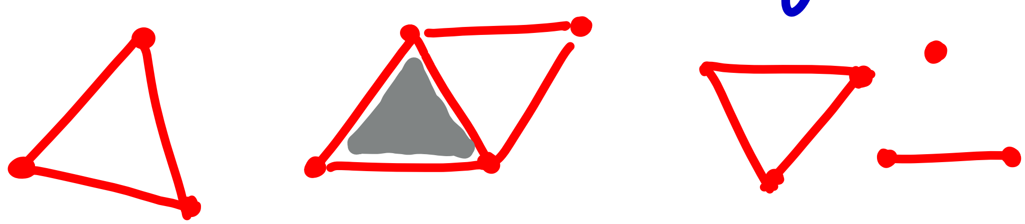
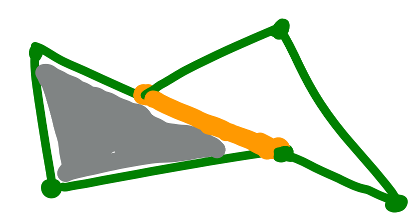
SIMPLICIAL COMPLEX

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.

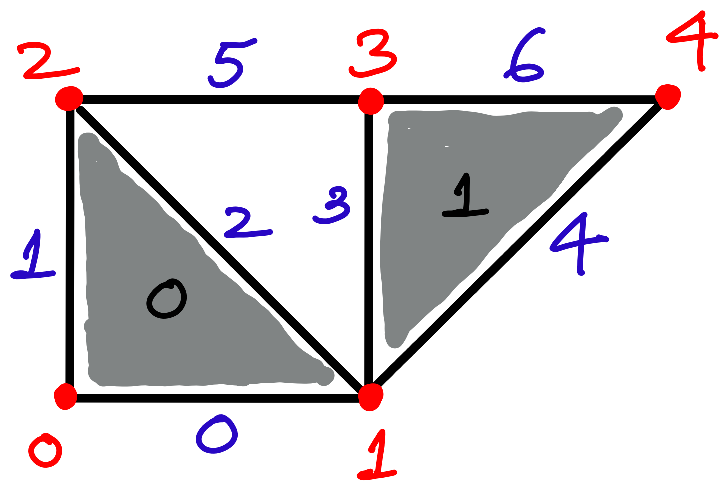




not a simplicial complex

AN EXAMPLE

K:



hole in the middle

AN EXAMPLE

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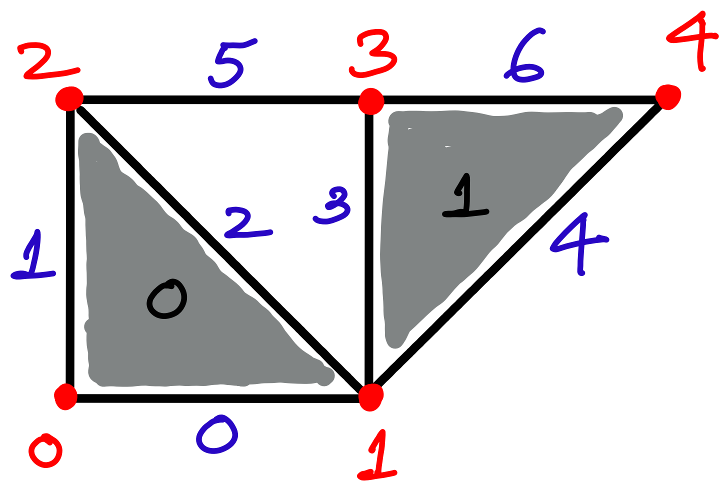

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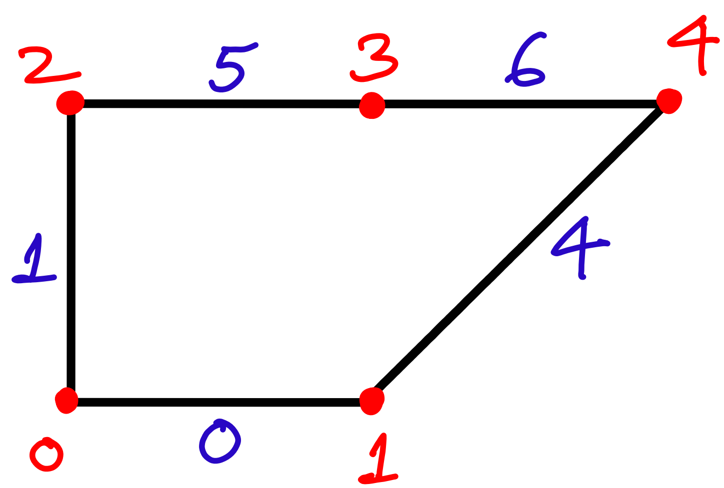
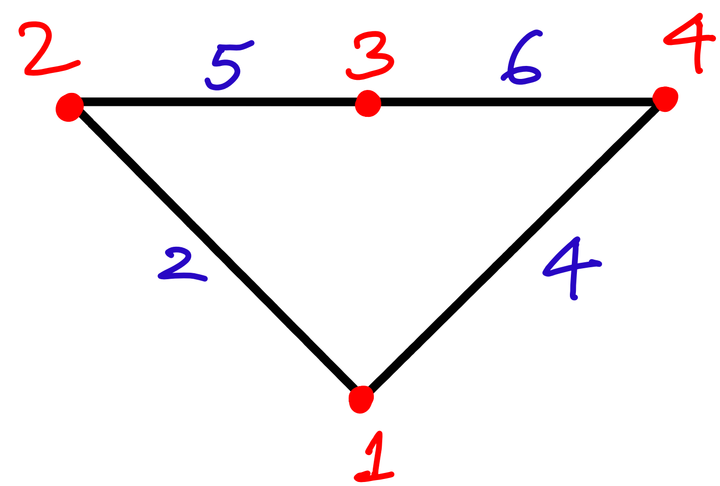
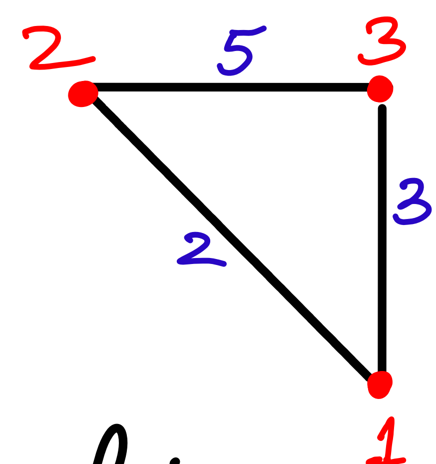
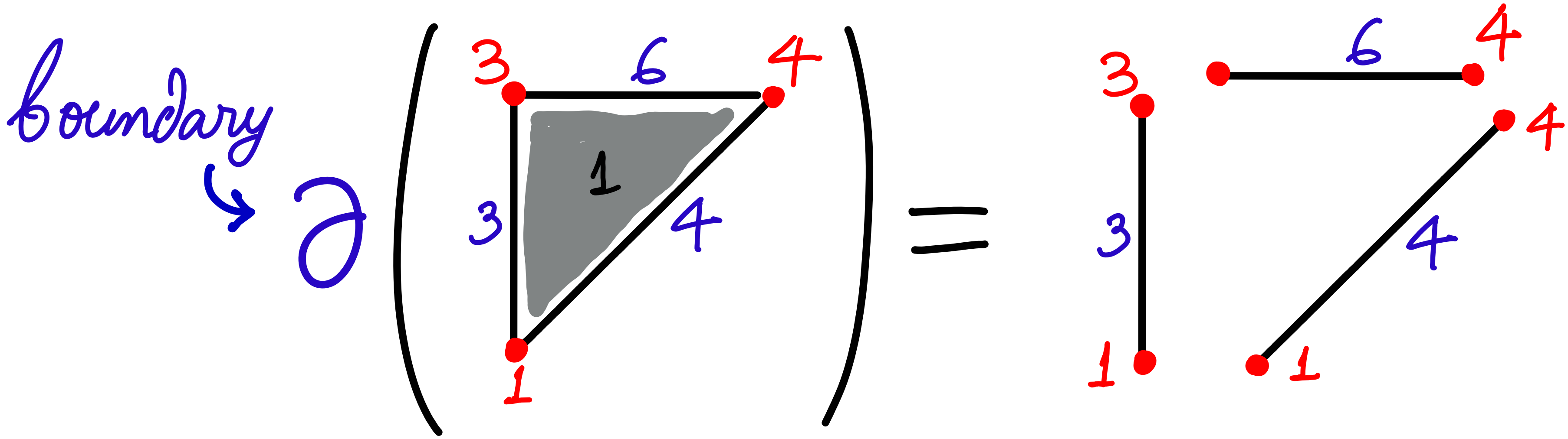






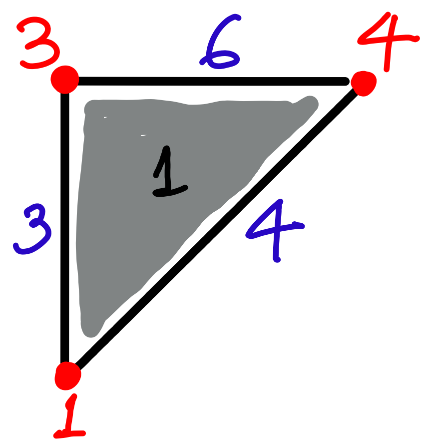
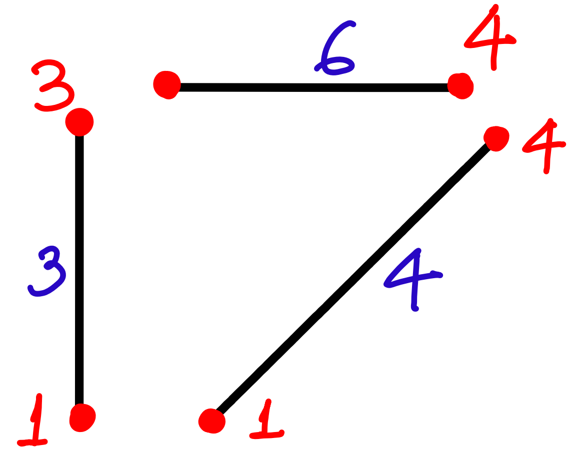
3 cycles representing the same hole

AN EXAMPLE

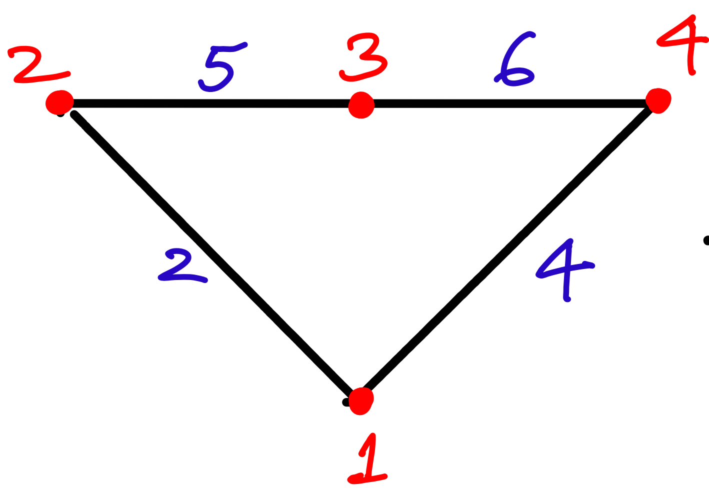
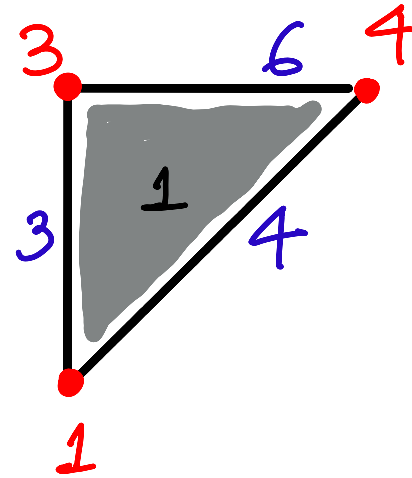
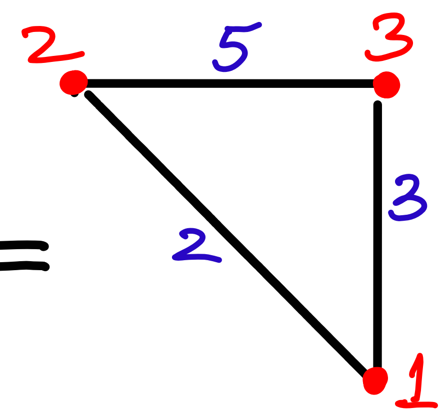


AN EXAMPLE

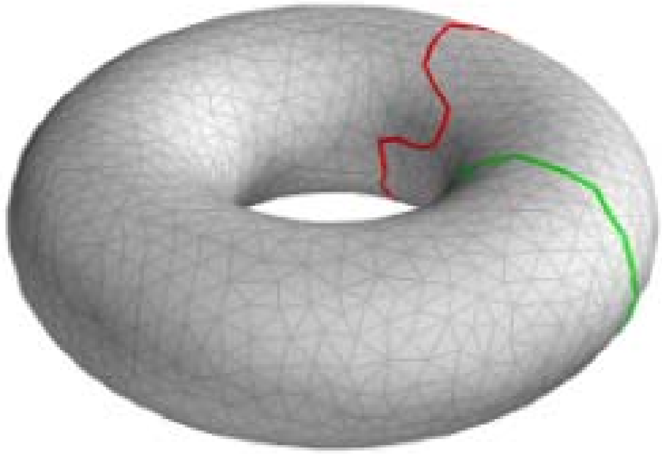
boundary

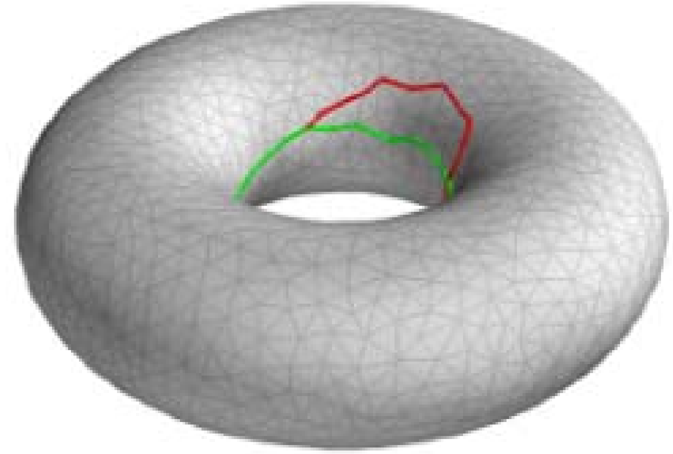
$\partial\Big($  $\Big) =$ 

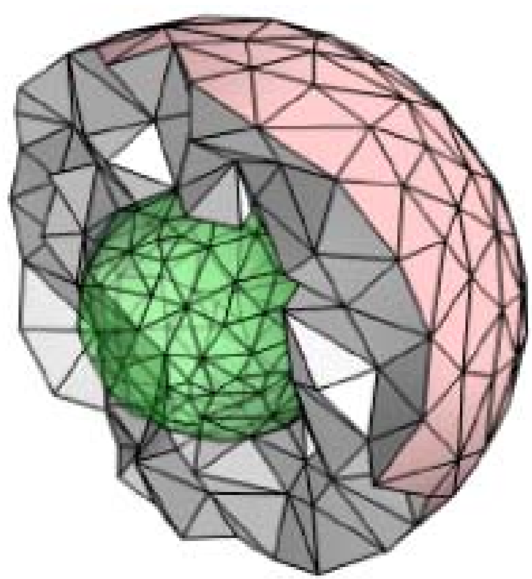
add edges in $\mathbb{Z}_2$ $(1+1=0)$

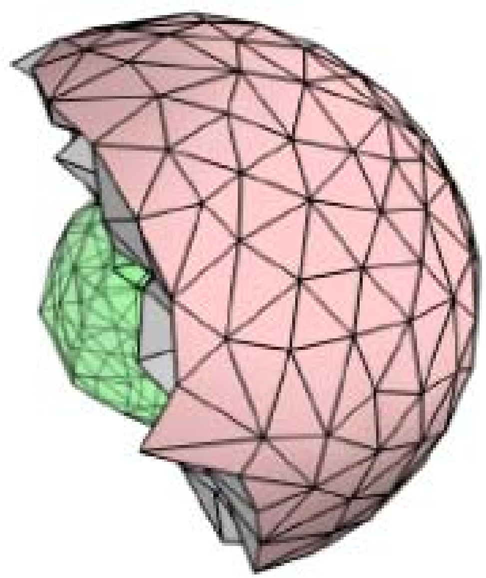
 $+\ \partial\Big($  $\Big) =$ 

Examples in 3D



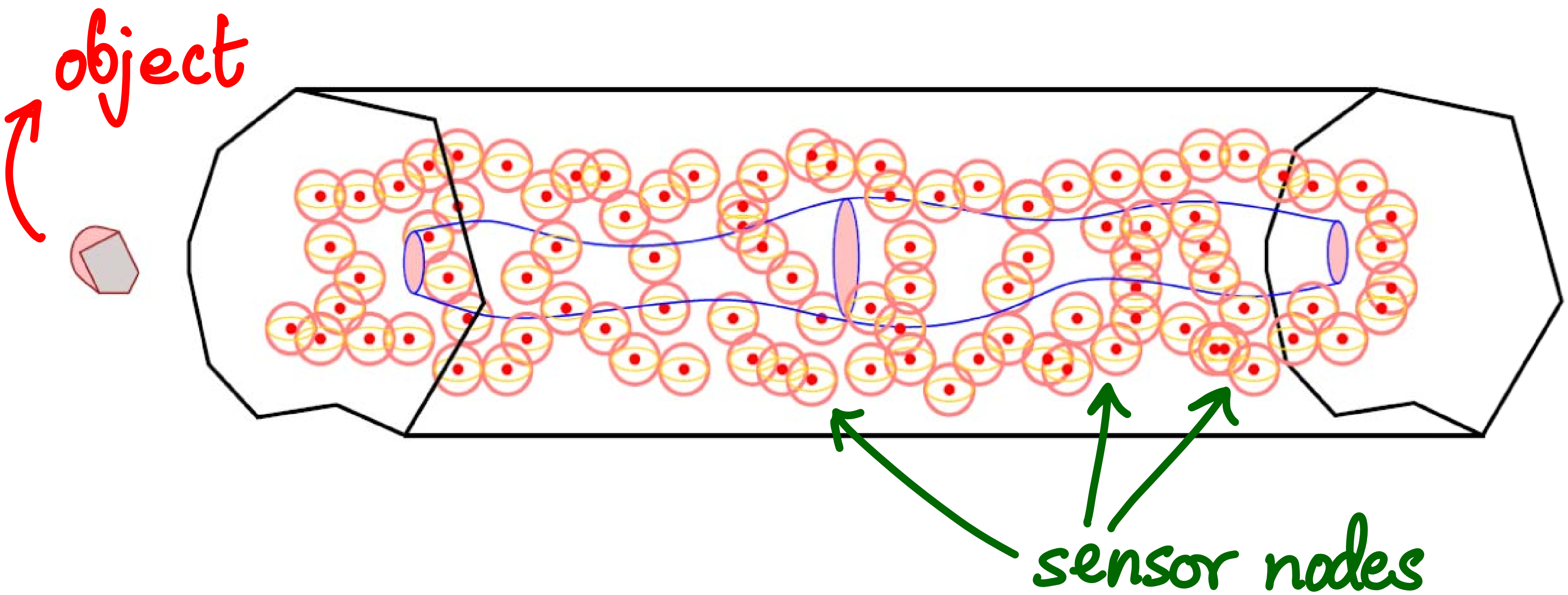






APPLICATIONS

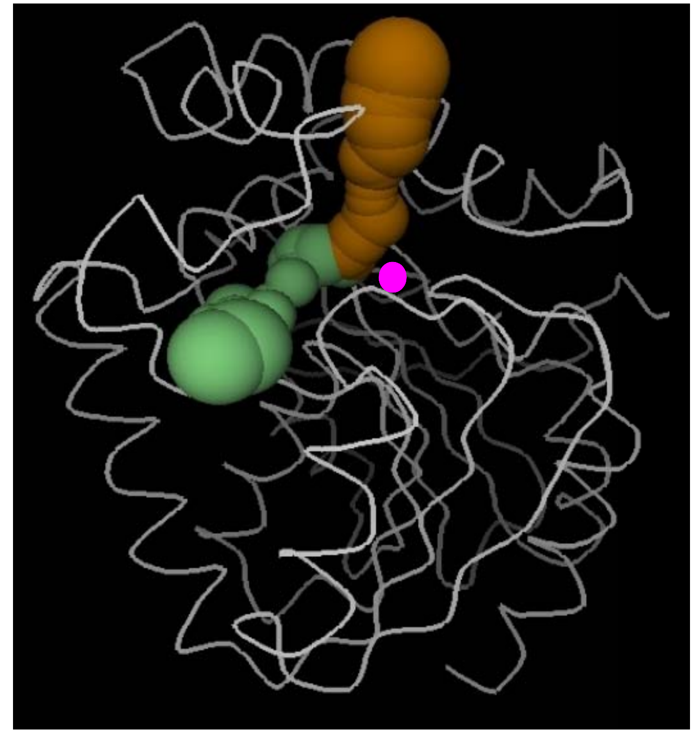
Sensor networks: object-specific coverage in 3D



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

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Tamal Dey (Ohio St.)
Anil Hirani (U. Illinois)
STOC '10
SICOMP 11

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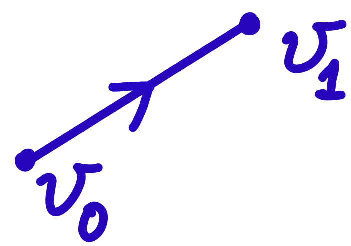
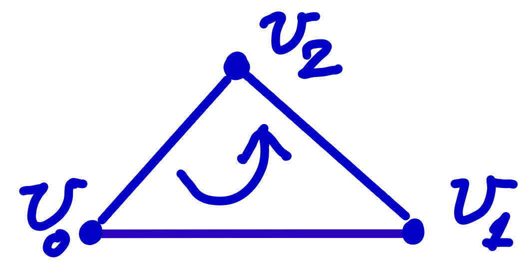
- ✓ flat norm of currents in simplicial complexes

Kevin Vixie, Sharif Ibrahim (WSU)

CHAINS

Orientation of a simplex:





$[v_0 v_1]$ or $[v_1 v_0]$ $\quad$ $[v_0 v_1 v_2]$ or $[v_0 v_2 v_1]$

1-chain:

collection of edges

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

$c(\sigma) = -c(\sigma')$ if σ and σ' 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 $\sigma \in K$:

$c(\sigma) = 1,$
$c(\sigma') = -1,$ if σ': opposite orientation of σ
$c(\tau) = 0 \quad \forall\ \tau \neq \sigma, \sigma'.$

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

BOUNDARY OPERATOR

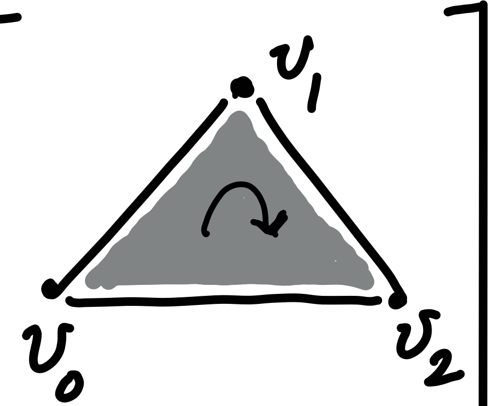
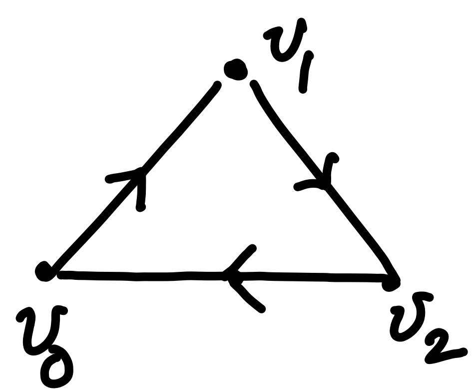
The homomorphism $\partial_p : C_p(K) \to C_{p-1}(K)$.

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

$$\partial_p \sigma = \partial_p [v_0, \dots, v_p] = \sum_{i=0}^{p} (-1)^i [v_0, \dots, \hat{v}_i, \dots v_p]$$

delete v_i

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

∂_2 [] = 

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

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

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

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

group of p-cycles that are NOT p-boundaries

p^{th} homology group of K.

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

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

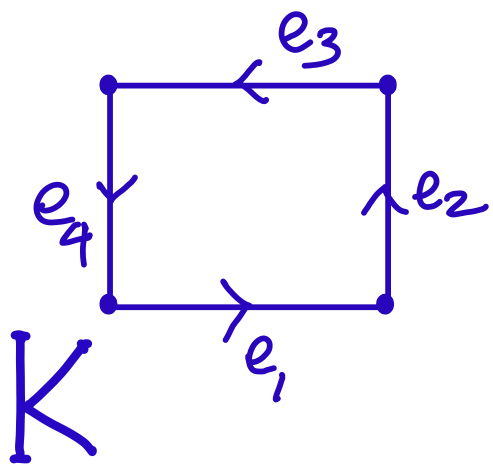
$\mathbb{Z}_2$: widely used for computation. field, simple, intuitive

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

group of p-cycles that are NOT p-boundaries

p^{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 $e_1 + e_2 + e_3 + e_4$

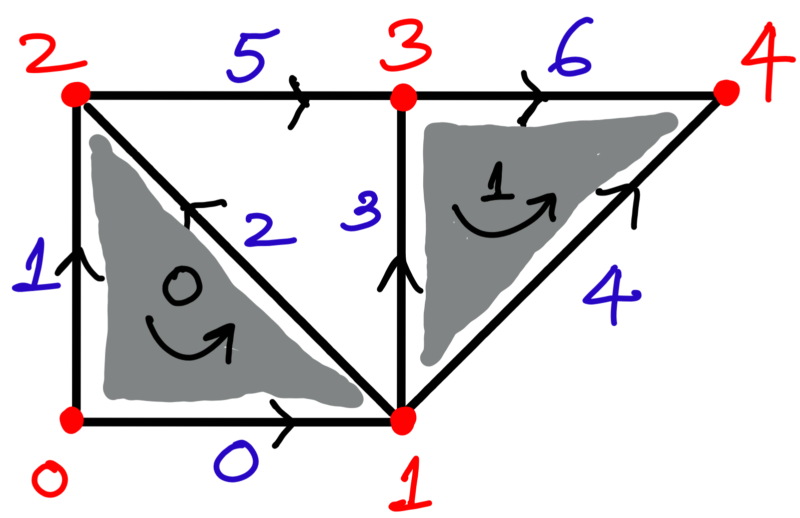
No 2-simplices in $K \Rightarrow B_1(K)$ is trivial.

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

Boundary Matrix $[\partial_p]$

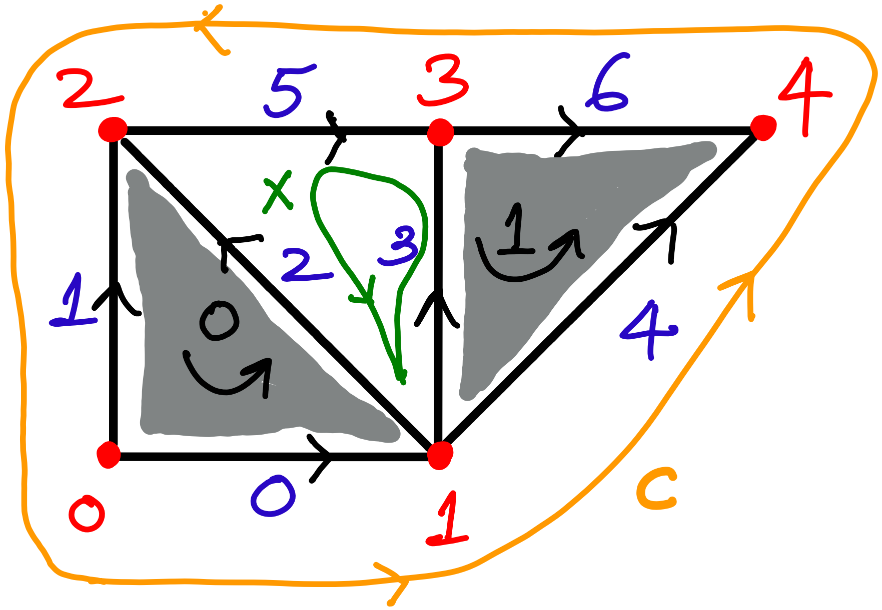
$\partial_p : C_p(K) \to C_{p-1}(K)$

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, $[\partial_p]_{ij} \in \{-1, 0, 1\}$.



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

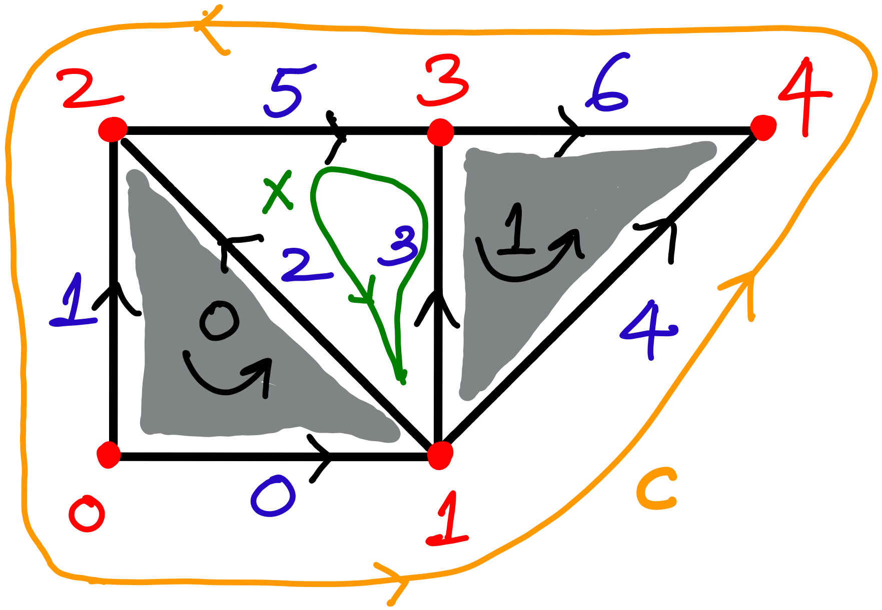
Short Homologous Cycles



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

represents hole in middle, but has 5 edges.

SHORT HOMOLOGOUS CYCLES

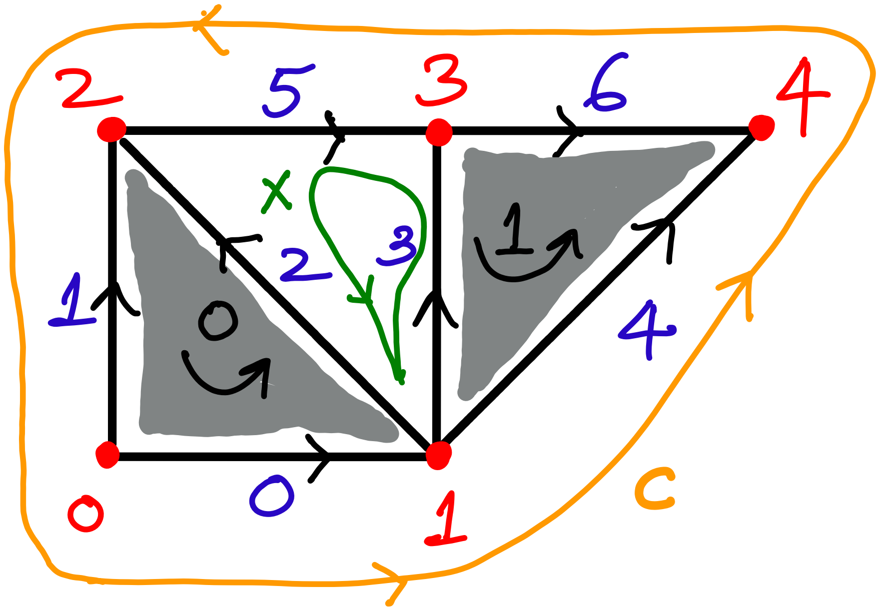


$$c = \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$ represents hole in middle, but has 5 edges.

$$x = \begin{bmatrix} 0 \\ 0 \\ -1 \\ 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}$$ is homologous to c, but is shorter (has only 3 edges)

x is "tightest" cycle around the hole

Short Homologous Cycles



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

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$$x = c + [\partial_2]\begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$x \sim c$ (x is homologous to c)

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

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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.

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

Optimal Homologous Cycle Problem

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

Optimal Homologous Chain Problem

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OHCP AS AN INTEGER PROGRAM

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

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

OHCP AS AN INTEGER PROGRAM

$$\min_{x,y} \|Wx\|_1 \quad = \sum_i |w_i||x_i| \quad \text{piecewise linear}$$

such that

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

OHCP as an Integer Program

$$\min_{x,y} \|Wx\|_1 \quad \text{such that} \qquad = \sum_i |w_i||x_i| \quad \text{piecewise linear}$$

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

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

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

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

OHCP AS AN INTEGER PROGRAM

$\min_{x,y} \|Wx\|_1$ such that $= \sum_i |w_i||x_i|$ piecewise linear

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ignore to get LP relaxation

IP and Total Unimodularity

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

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Result: (IP) can always be solved in polynomial time by solving (LP) iff A is totally unimodular.

IP and Total Unimodularity

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<u>Result:</u> (IP) can always be solved in polynomial time by solving (LP) iff A is totally unimodular.

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

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

IP and Total Unimodularity

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

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

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

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

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

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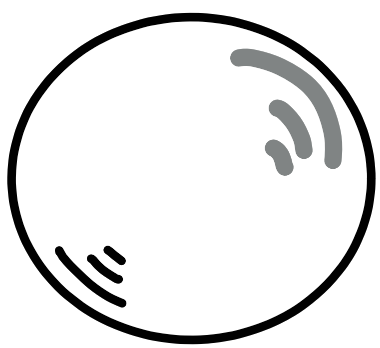
The constraint matrix of above LP is TU iff $[\partial_{p+1}]$ is TU.

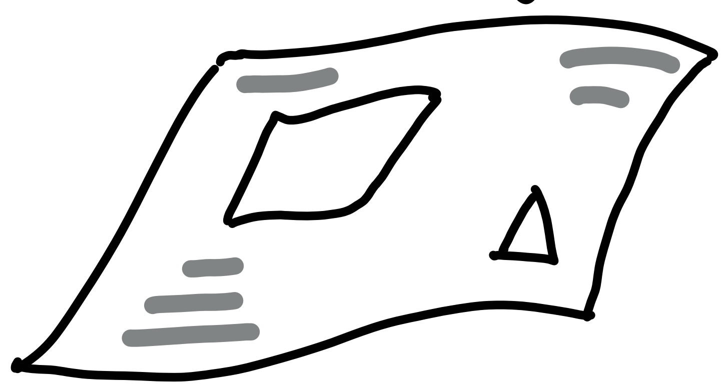
$\Rightarrow$ OHCP (with homology defined over $\mathbb{Z}$) is solvable in polynomial time iff $[\partial_{p+1}]$ is TU.

Orientable Manifolds

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

possibly empty





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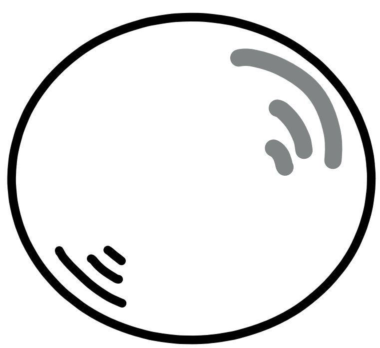
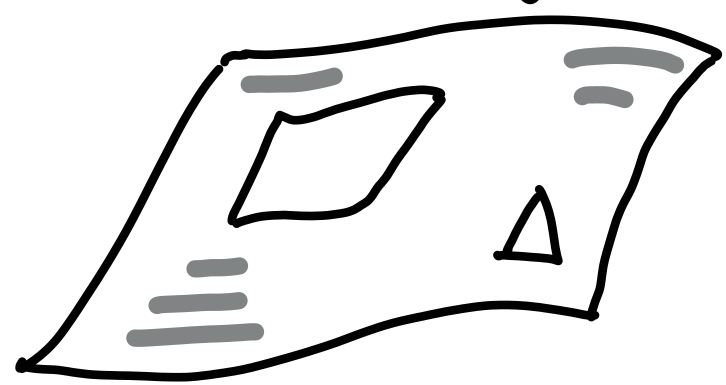
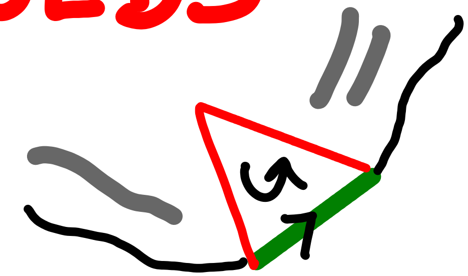


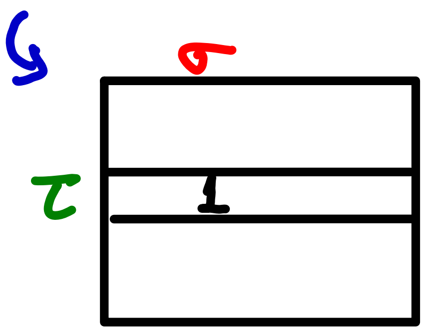


Theorem 1. For a finite simplicial complex triangulating a compact orientable manifold, $[\partial_{p+1}]$ is TU.

Orientable Manifolds



Proof. τ (p-simplex) : face of one σ ((p+1)-simplices)

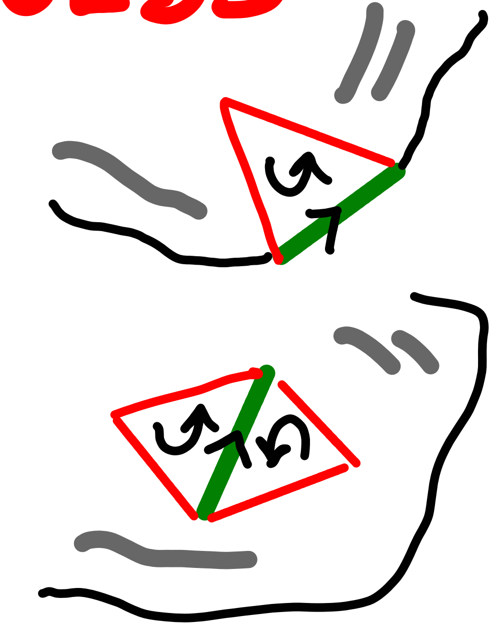


Orientable Manifolds

<u>Proof.</u> τ (p-simplex): face of one or two σ's ($(p+1)$-simplices)

	σ
τ	1

	σ_1	σ_2
τ	1	-1



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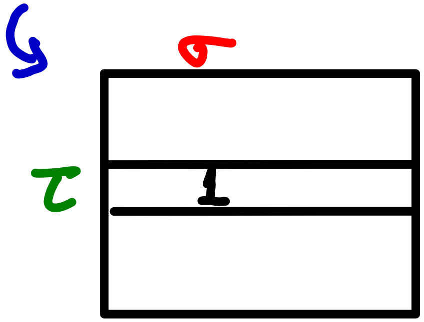

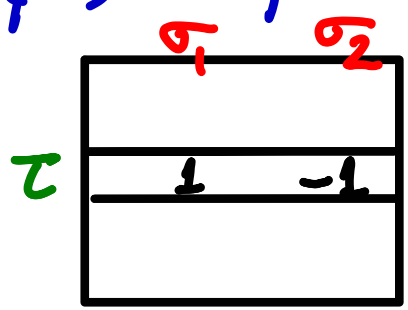

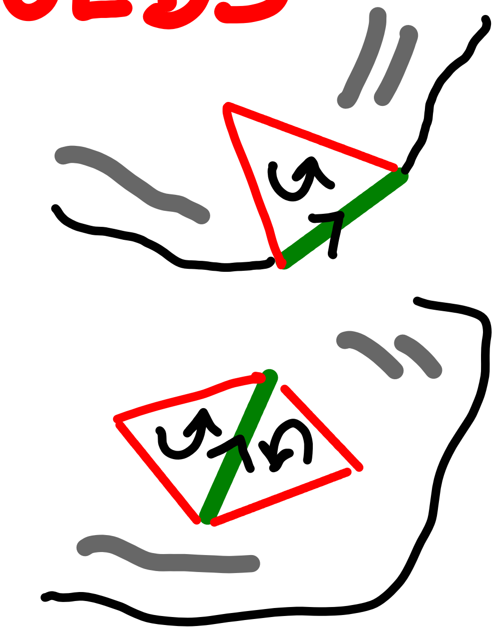

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(Heller & Tompkins, 1956) $\Rightarrow$ $[\partial_{p+1}]$ is TU.

ORIENTABLE MANIFOLDS

Proof. τ (p-simplex) : face of one or two σ's $(p+1)$-simplices)

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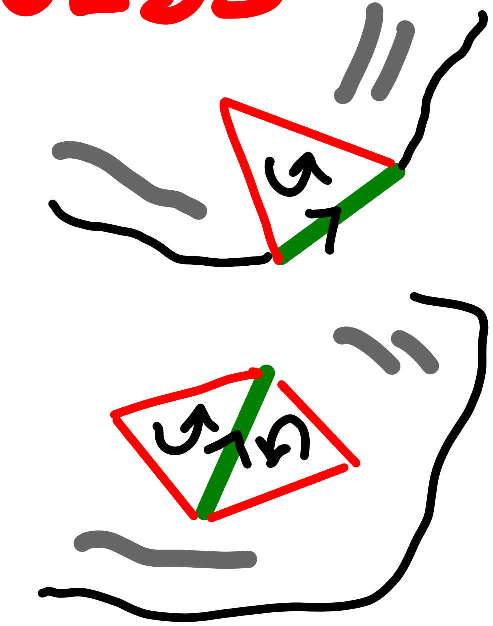

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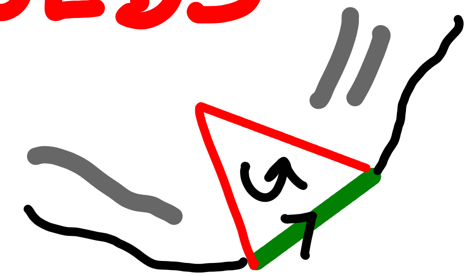

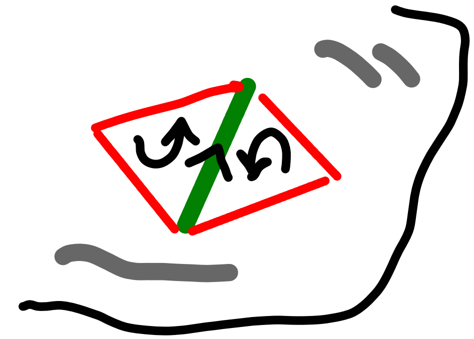

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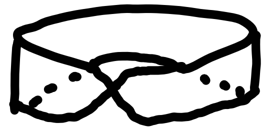
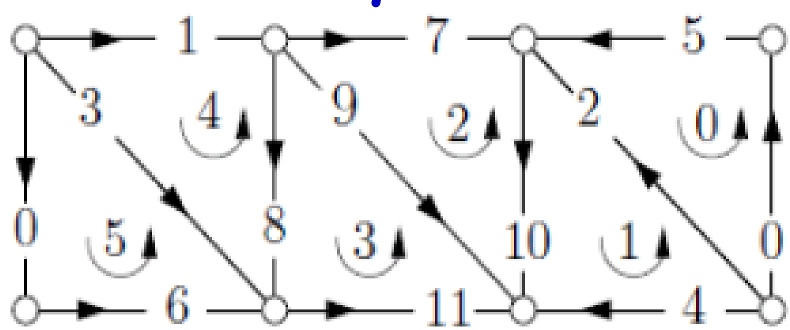
Also observed by John Sullivan (1992)

NON-ORIENTABLE MANIFOLDS

Möbius strip:





$[\partial_2]$ for Möbius strip :

$$\begin{array}{r|cccccc}
 & 0: & 1: & 2: & 3: & 4: & 5: \\
\hline
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 \\
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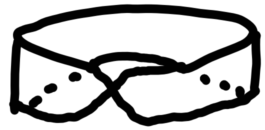

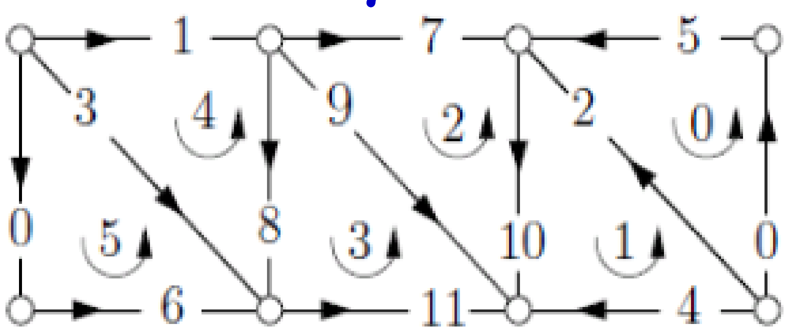

$$S = \begin{array}{cc} \begin{array}{cccccc} 5 & 4 & 3 & 2 & 1 & 0 \end{array} & \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} & \begin{array}{c} 0 \\ 3 \\ 8 \\ 9 \\ 10 \\ 2 \end{array} \end{array}$$

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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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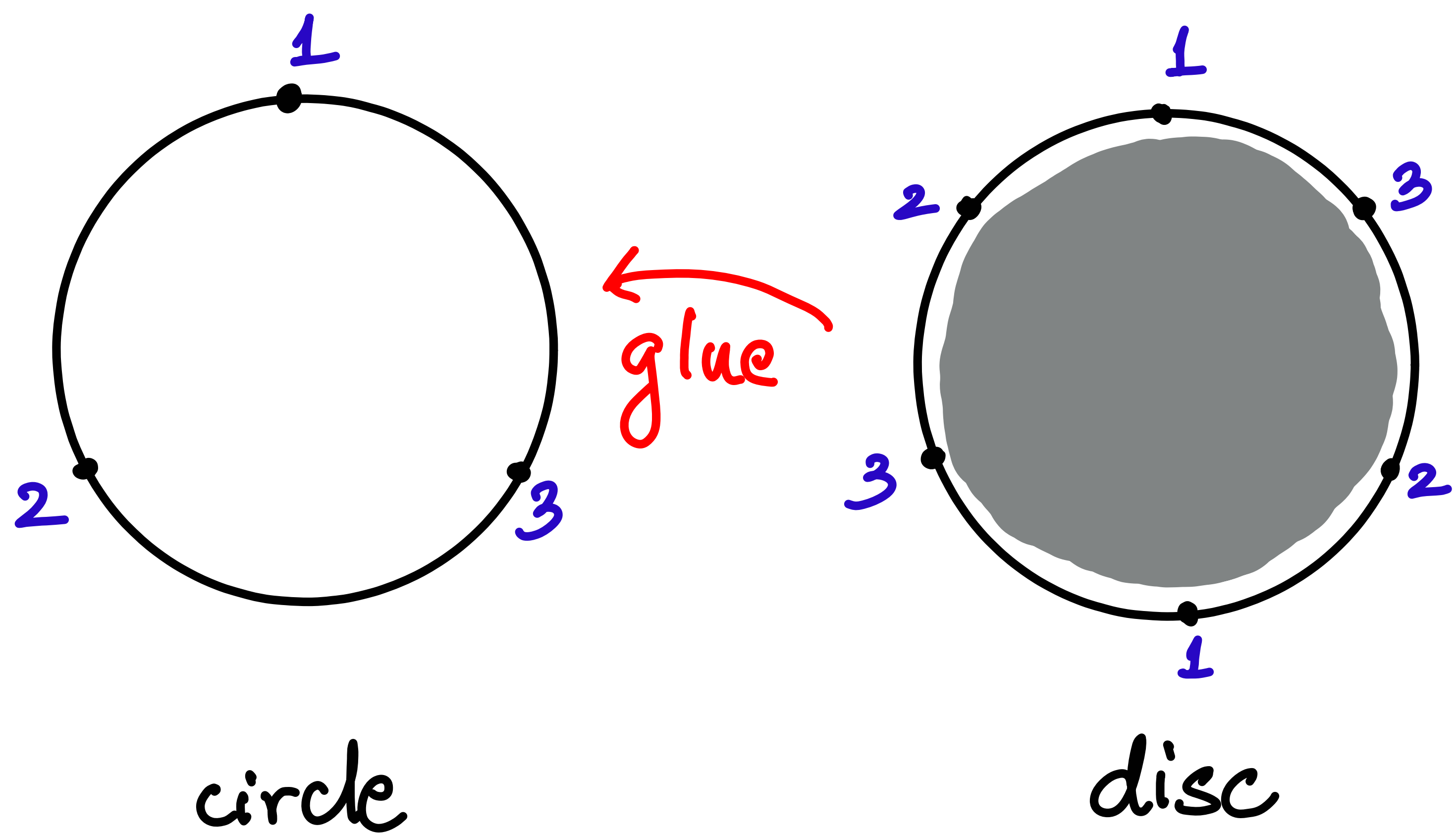
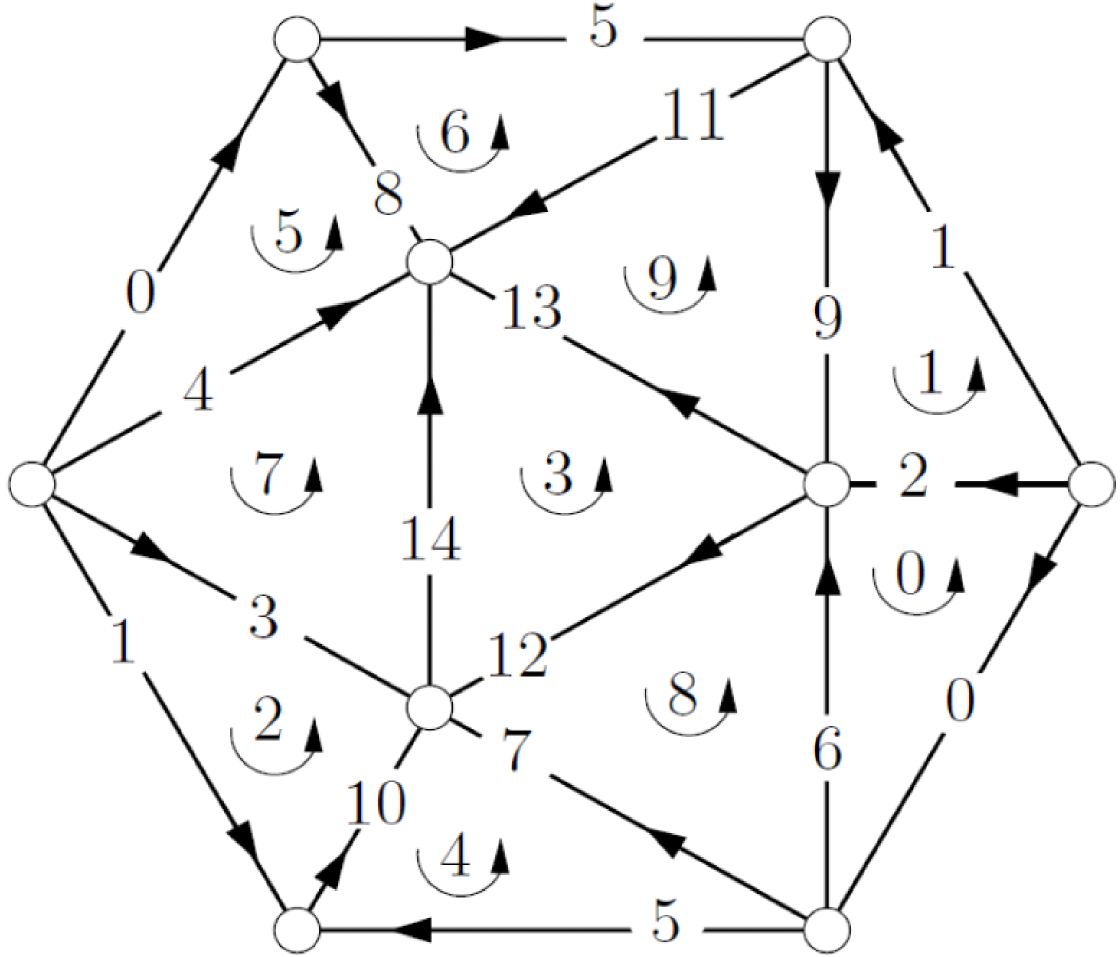
* topological characterization of TU.

VISUALIZE TORSION

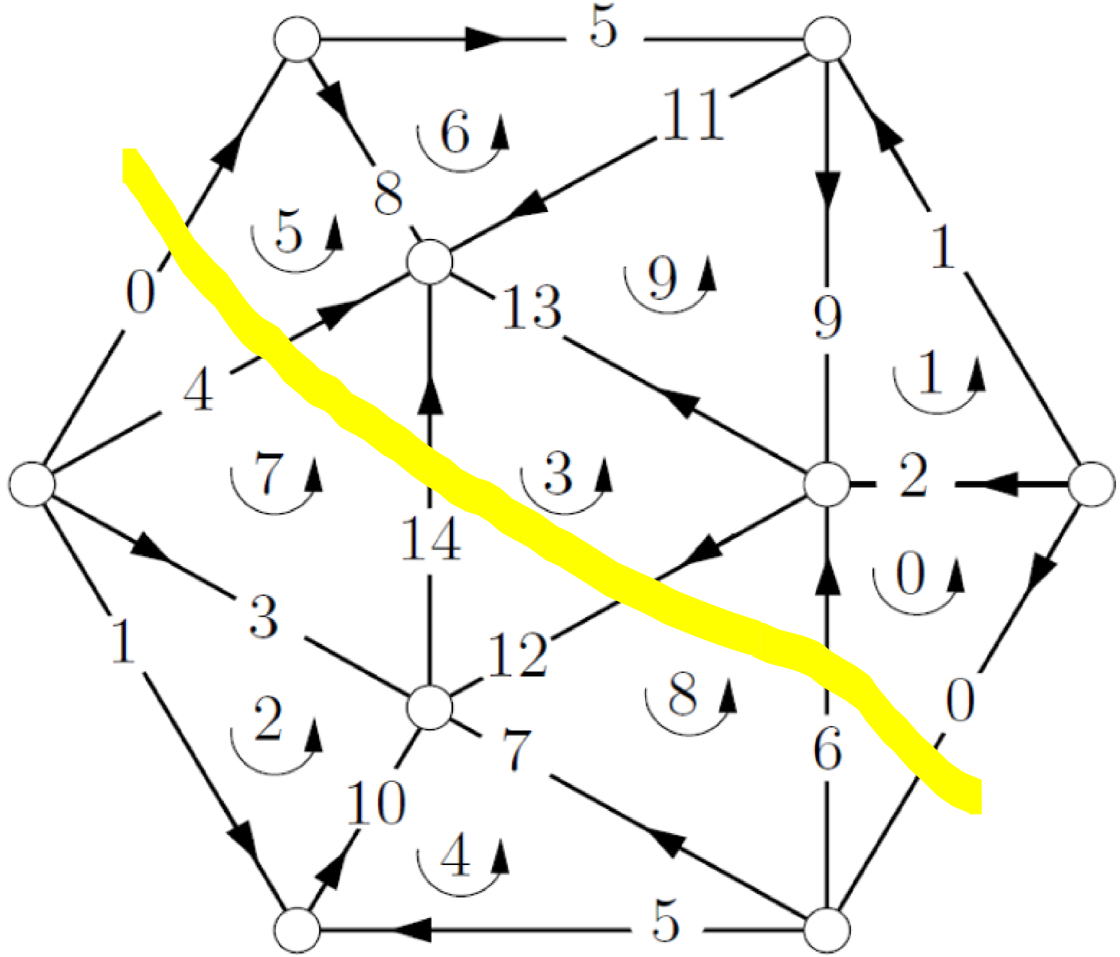


Poincaré (1899): projective plane
(or Dunce hat)

Projective Plane



Projective Plane



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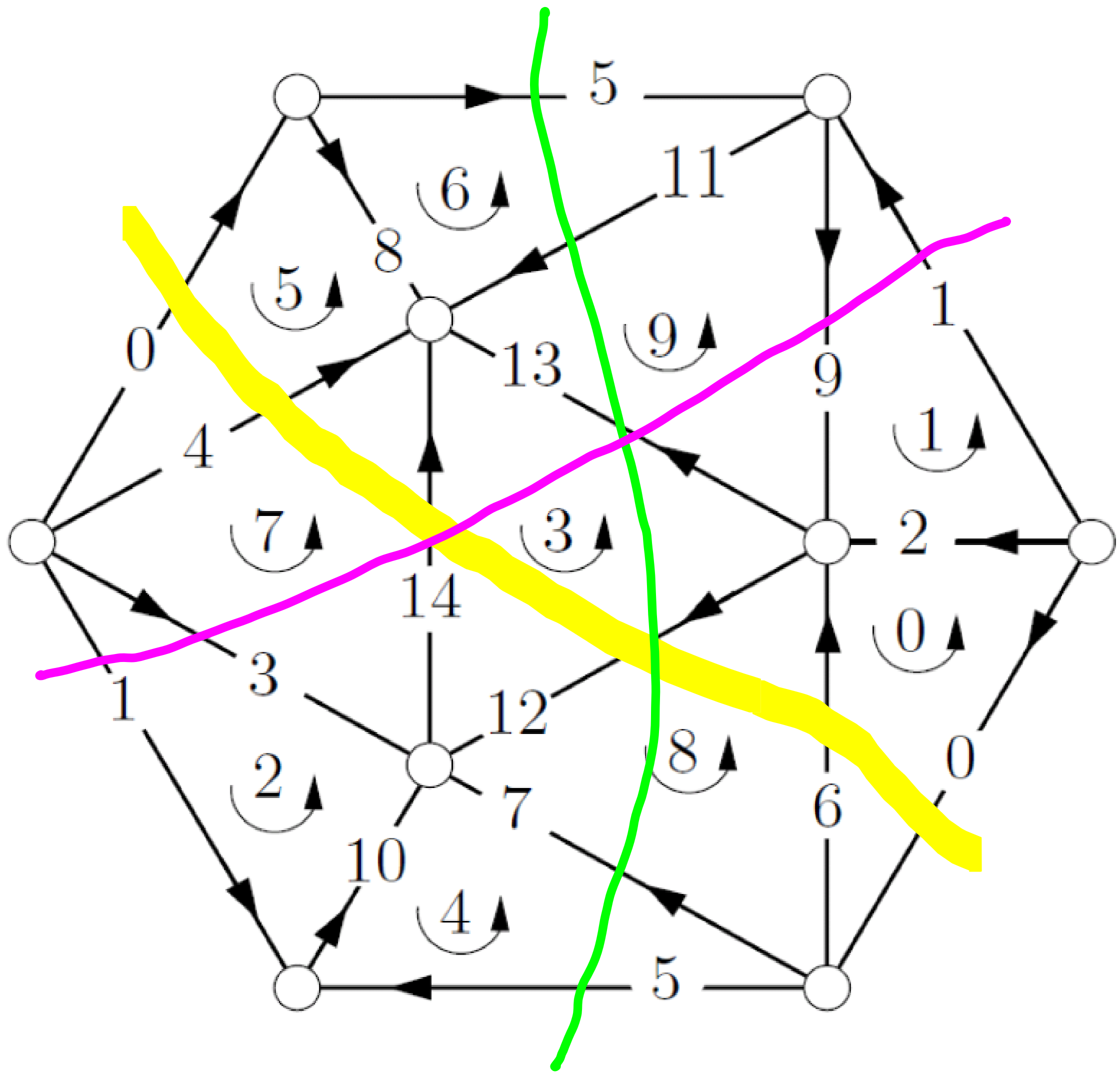

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- → $[\partial_p]$ is TU $\iff K$ is orientable manifold
- → $[\partial_d]$ is TU $\iff K$ embedded in $\mathbb{R}^d$

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

Currents and Flat Norm

- standard objects in geometric measure theory
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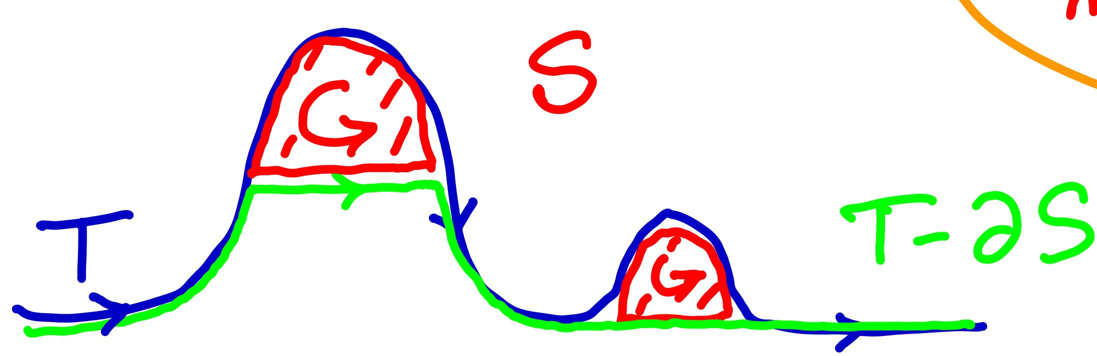

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$$\min \sum_{i=1}^{m} w_i |x_i| + \lambda \left(\sum_{j=1}^{n} v_j |s_j| \right)$$

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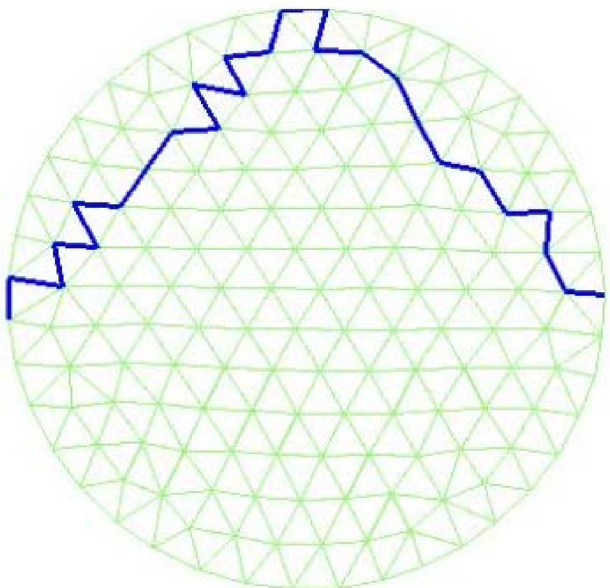
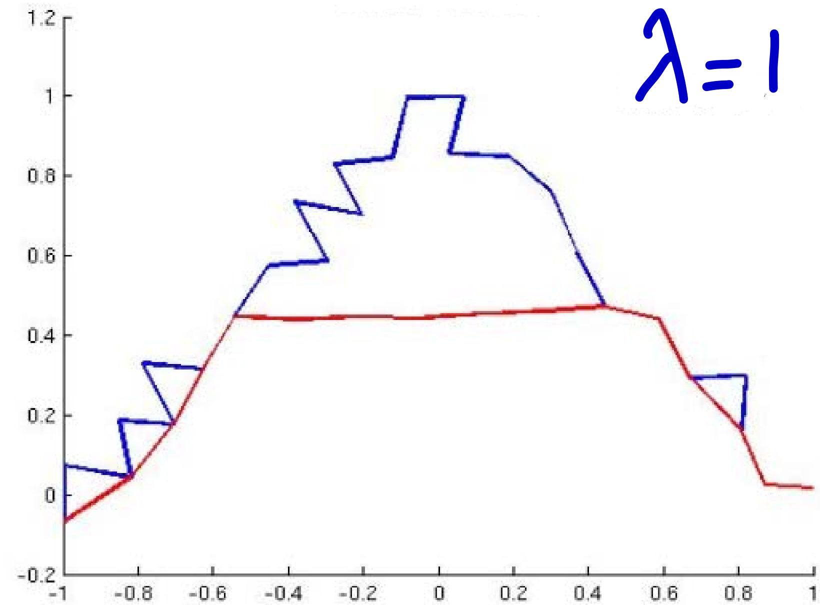
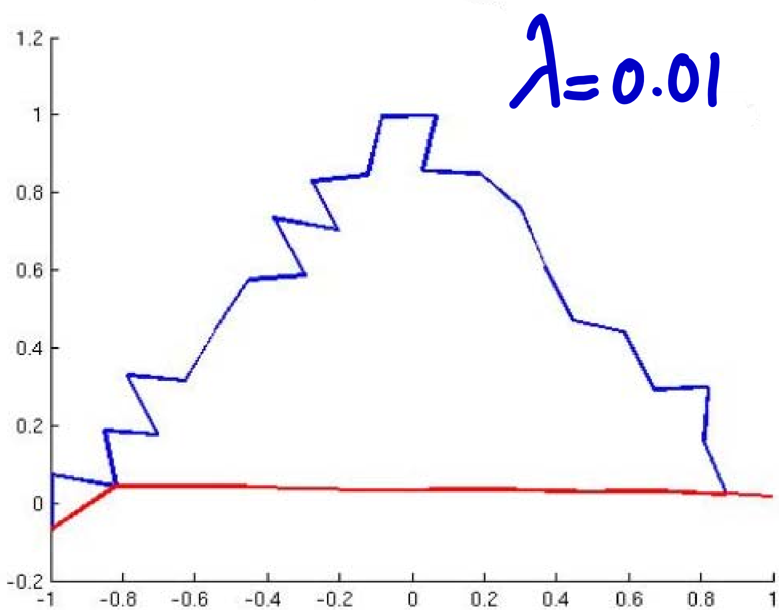
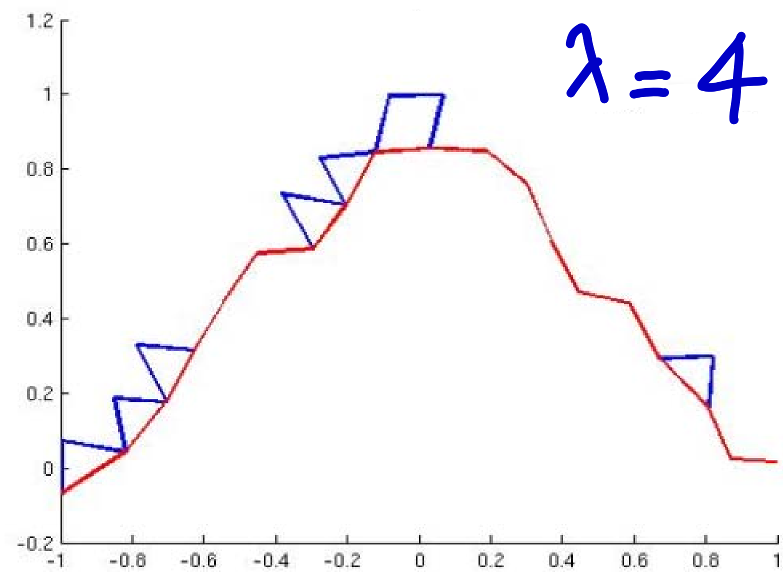
- Simplicial deformation theorem: can push any current onto simplicial complex in a controlled manner

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?