

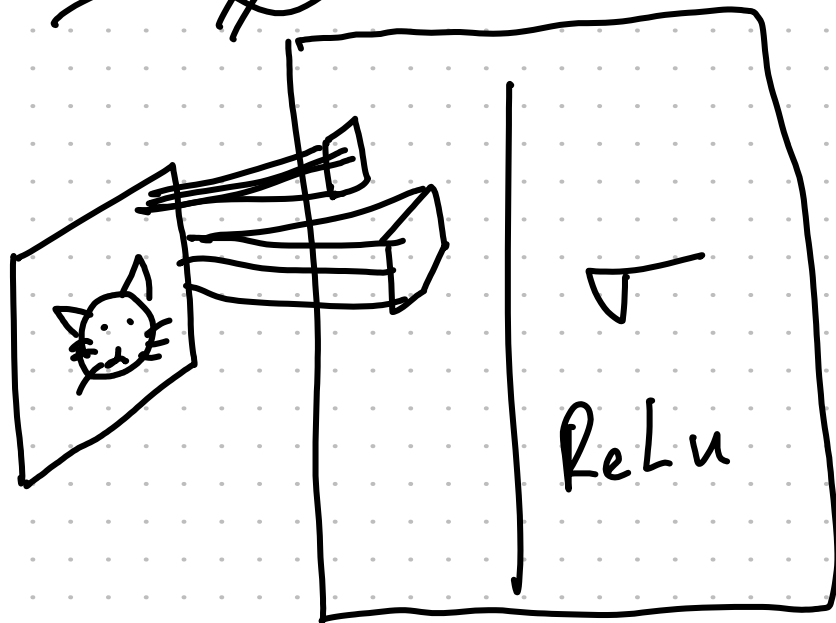
mitch.roddenberry.xyz

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Glaze, Segarra

icml 21

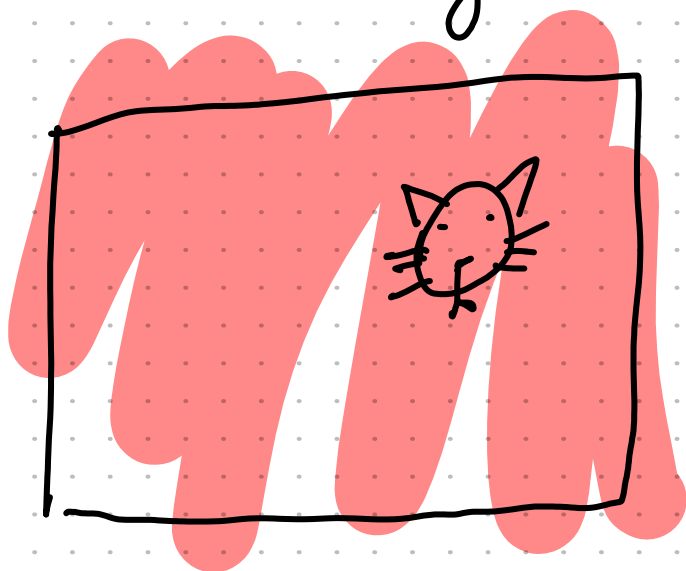
# CNNs



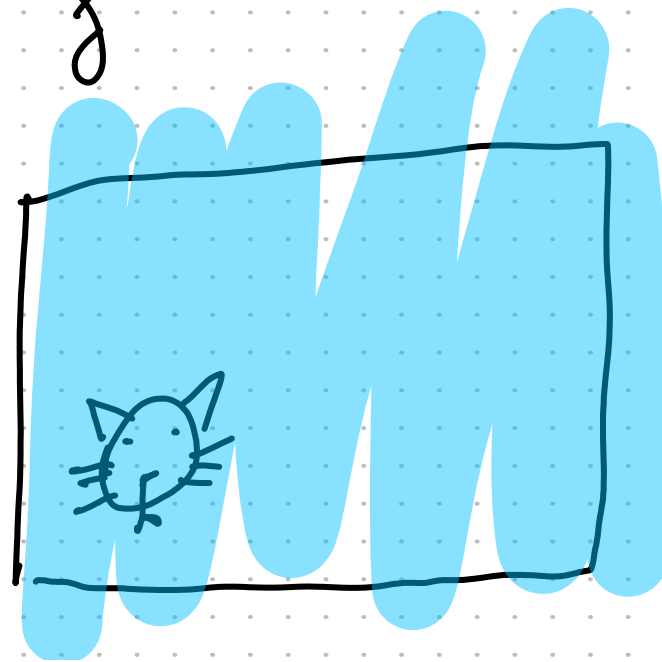
...



$g^{(1)}$



$g^{(L)}$

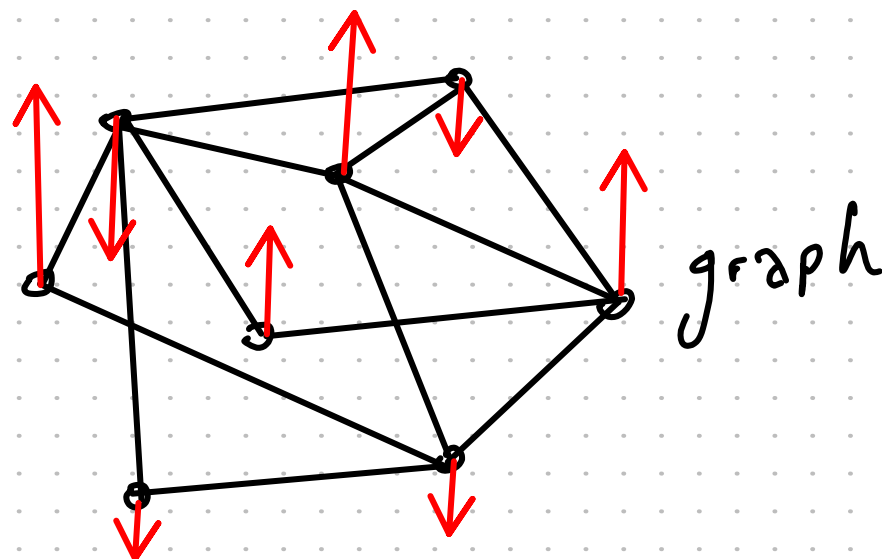
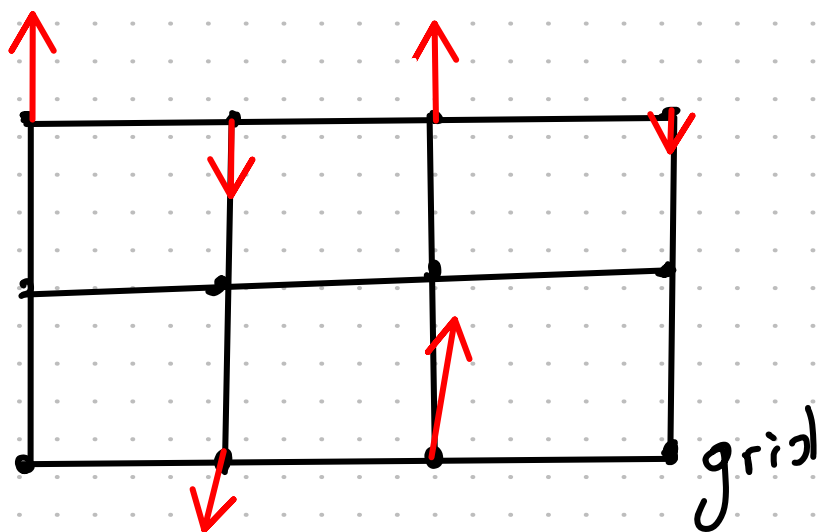


GNNs

vertices

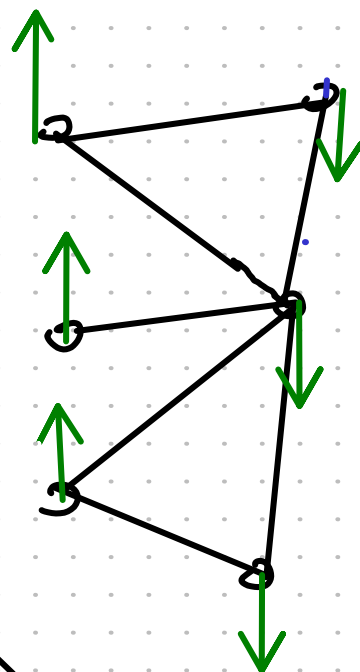
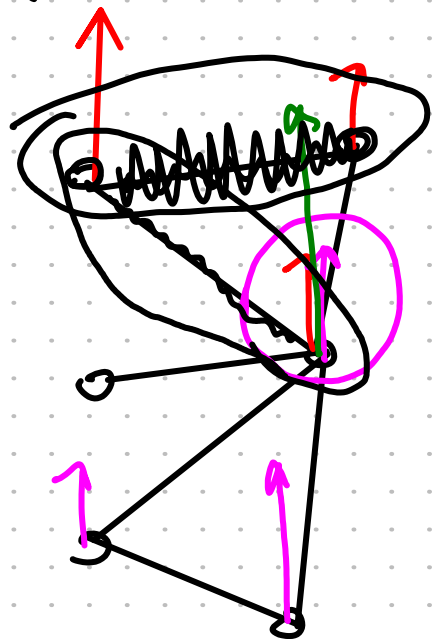
$$G = (V, E)$$

edges

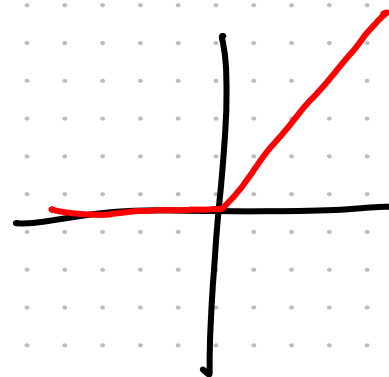
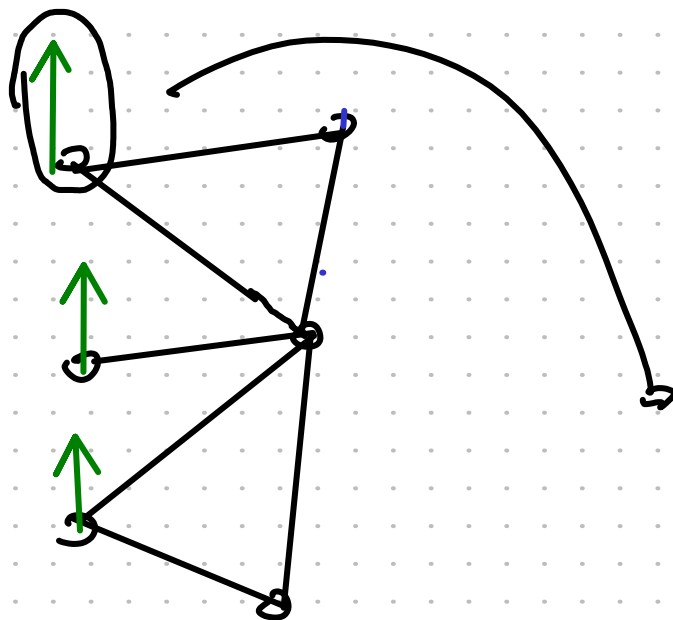


$$f: V \rightarrow \mathbb{R}^d$$

CNNs  $\rightarrow$  GNNs

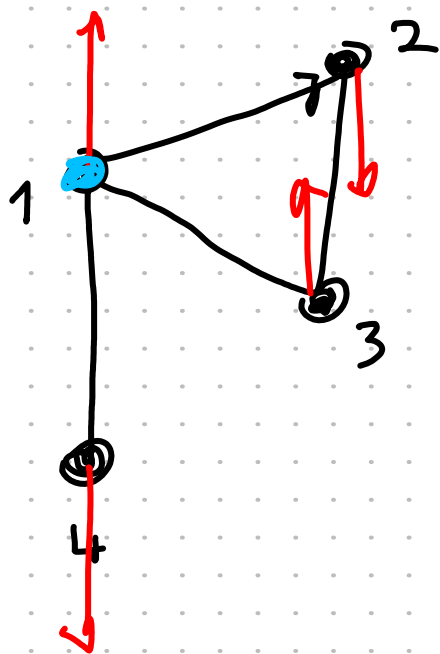


ReLU  
 $\rightarrow$



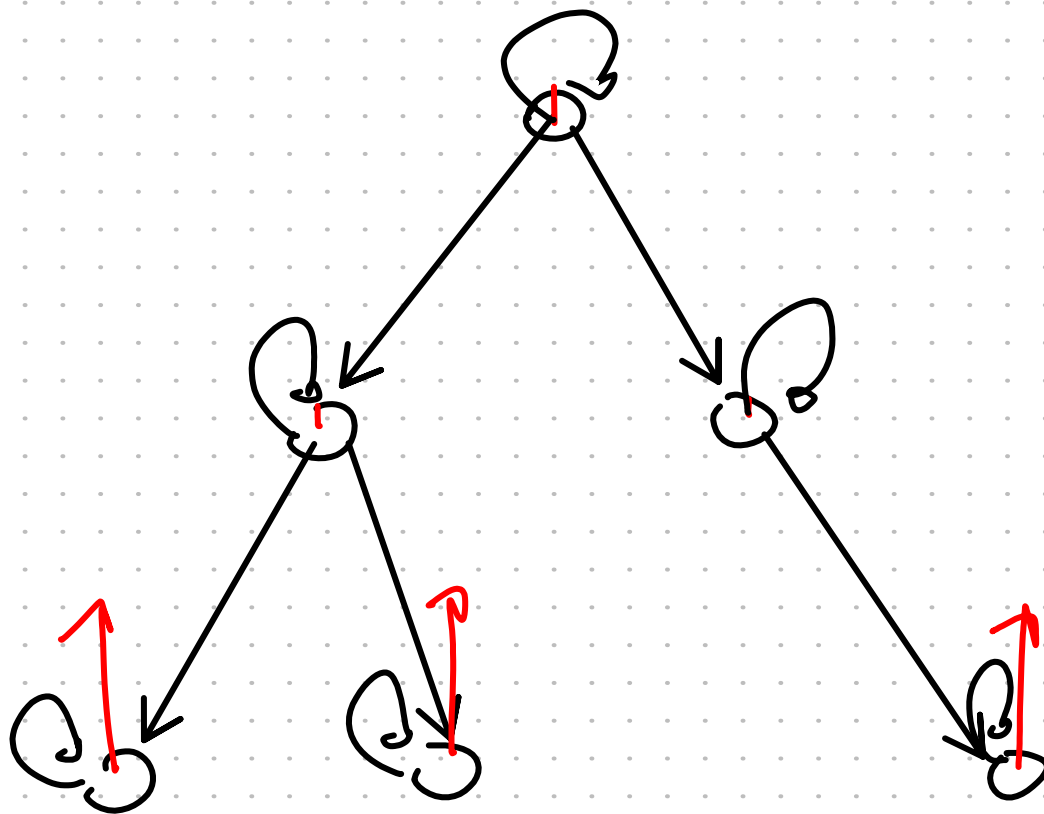
$$A = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \end{matrix}$$

$$L = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \end{matrix}$$



$$f = \begin{matrix} & \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{bmatrix} 0.7 \\ -0.1 \\ 0.5 \\ -0.9 \end{bmatrix} \end{matrix} \begin{matrix} - \\ + \\ + \\ + \end{matrix}$$

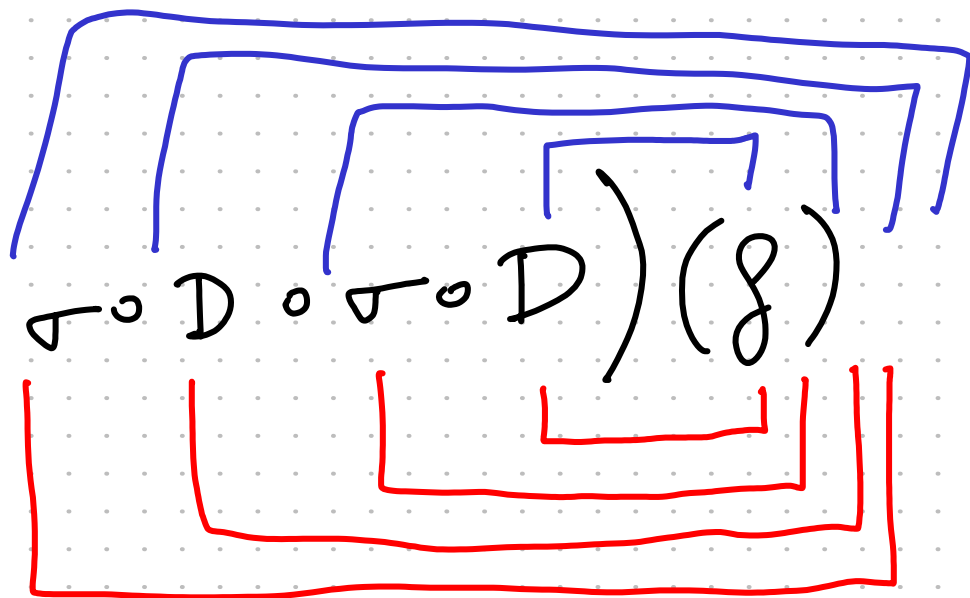
$$D(f) = [Lf]_1 = 3(0.7) - (-0.1) - 0.5 - (-0.9)$$



GNNs

$$\text{GNN}: f \mapsto g$$

$$\text{GNN}(f) = \left( \dots \sigma \circ D \circ \sigma \circ D \right) (f)$$



$$G = (V, E)$$

$$(v, f)$$

$$V_1 = V \setminus V_0 \rightarrow (v, f)$$

$$V_0 \subseteq V \rightarrow (v, f, \ell)$$

$$f = \begin{bmatrix} 1 \end{bmatrix}$$

$$F = \begin{bmatrix} \text{channel} \\ \bigcirc \\ \bigcirc \\ \bigcirc \\ \bigcirc \end{bmatrix}$$

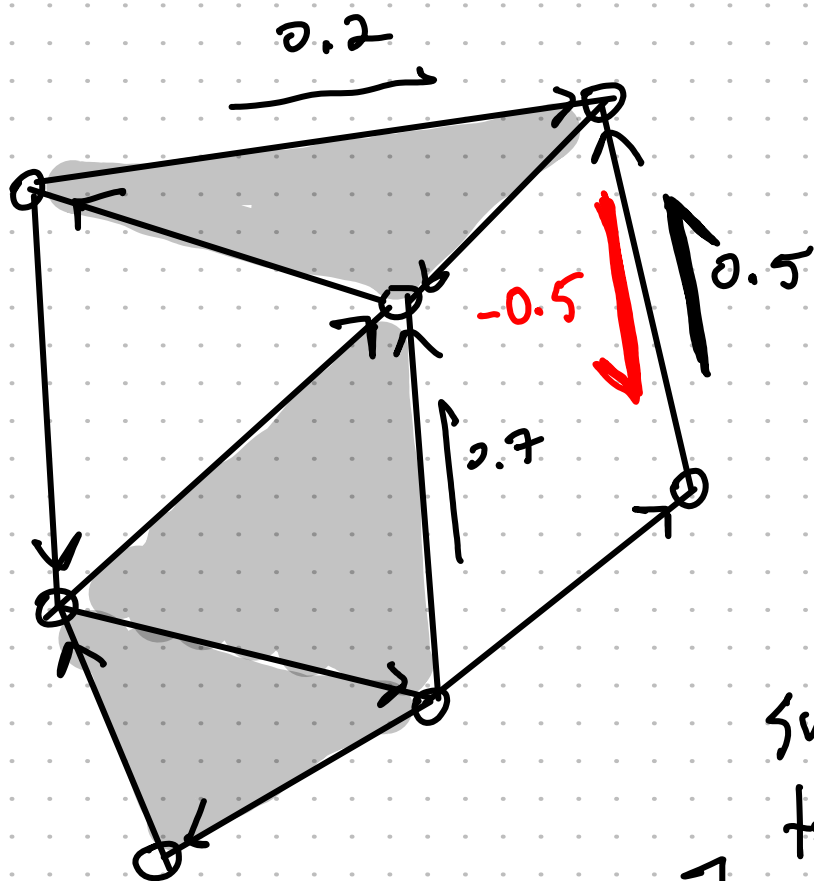
$$\underbrace{\begin{bmatrix} D & F^e \end{bmatrix}}_{e^{\text{th}} \text{ input data}} W^e$$

$$\rightarrow \begin{bmatrix} \bigcirc \\ \bigcirc \\ \bigcirc \end{bmatrix}$$

$$W = \begin{bmatrix} - & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

filter coeff.





nodes -  $X_0$

edges -  $X_1$

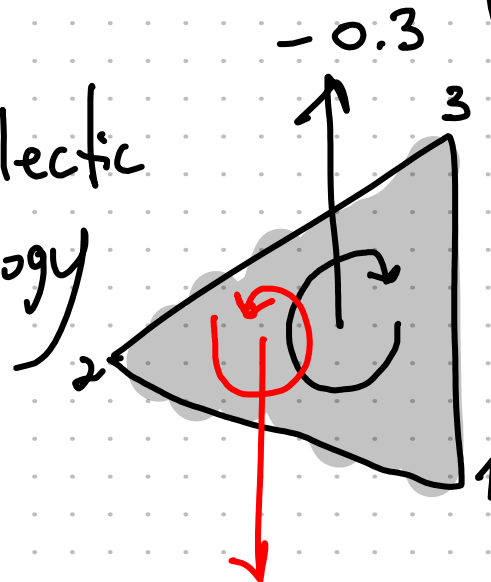
triangles -  $X_2$

0-chains:  $f: X_0 \rightarrow \mathbb{R}$

1-chains:  $\omega: X_1 \rightarrow \mathbb{R}$

2-chains:  $\Omega: X_2 \rightarrow \mathbb{R}$

symplectic  
topology



$[1, 2, 3]$

$[3, 1, 2]$

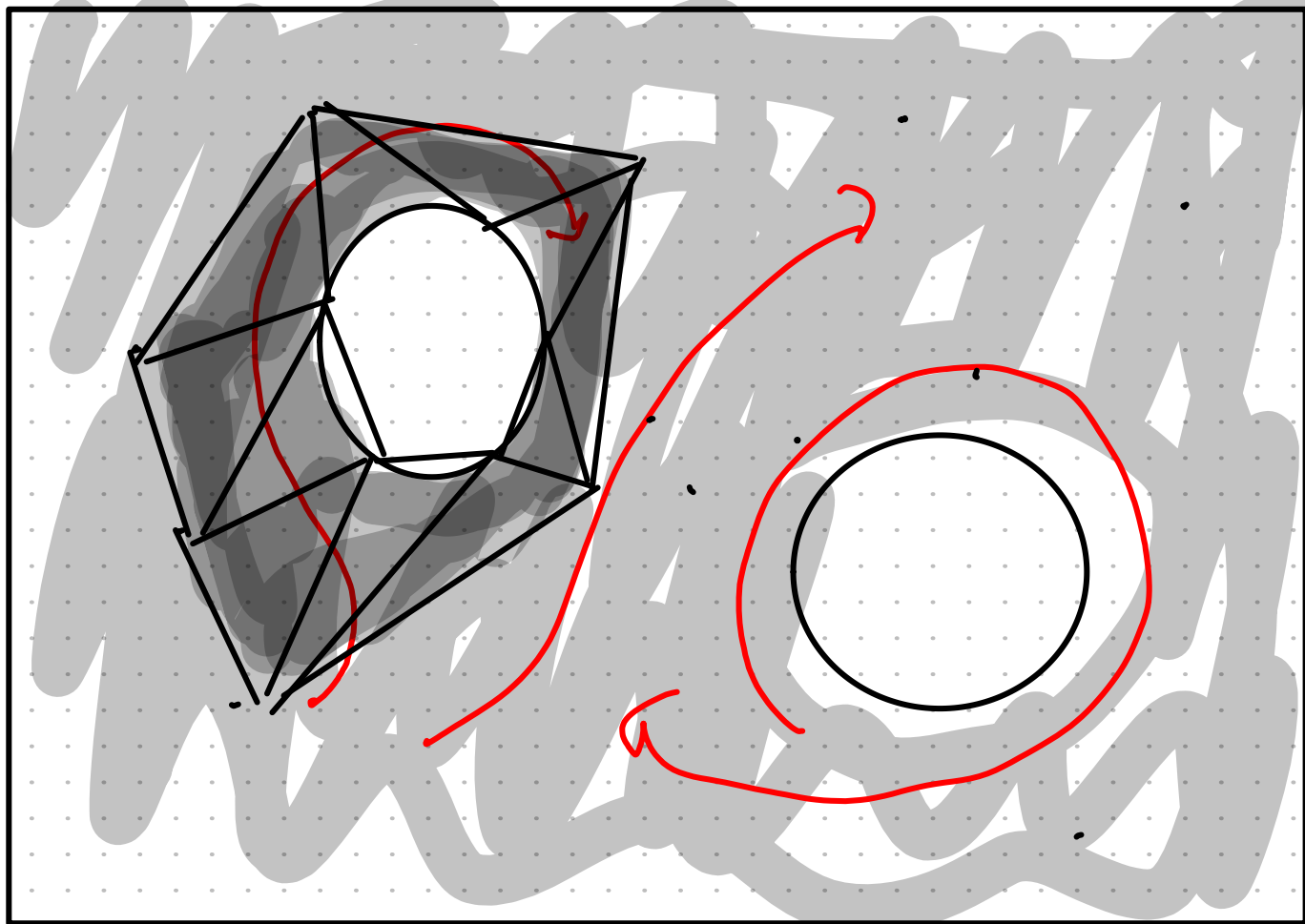
$[2, 3, 1]$

0.3

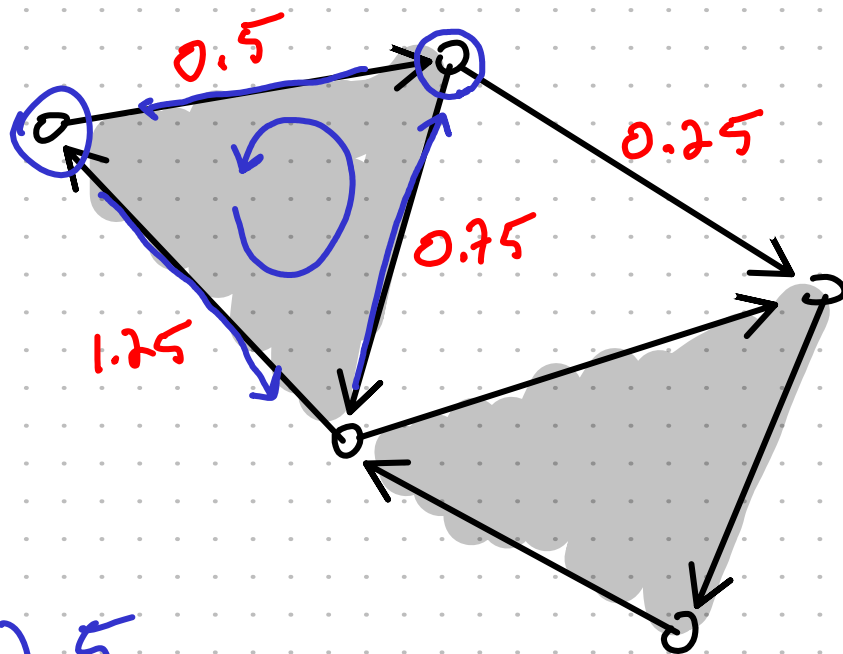
$[2, 1, 3]$

$[1, 3, 2]$

$[3, 2, 1]$



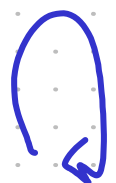
1-chains |  $\omega: X_1 \rightarrow \mathbb{R}$




• divergence

curl

harmonic

  $\rightarrow 2.5$

  $\rightarrow -2.5$

$B_1$   
 $B_2^T$

$\nabla \cdot$  : vec. fields  $\rightarrow$  scalar fields

1-chains  $\rightarrow$  0-chains

$\nabla \times$  : 1-chains  $\rightarrow$  2-chains

$B_1$ : div

$B_1^T$ : derivative

$B_2^T$ : curl

$B_2$ : boundary

$$B_1 B_2 = \bigcirc$$

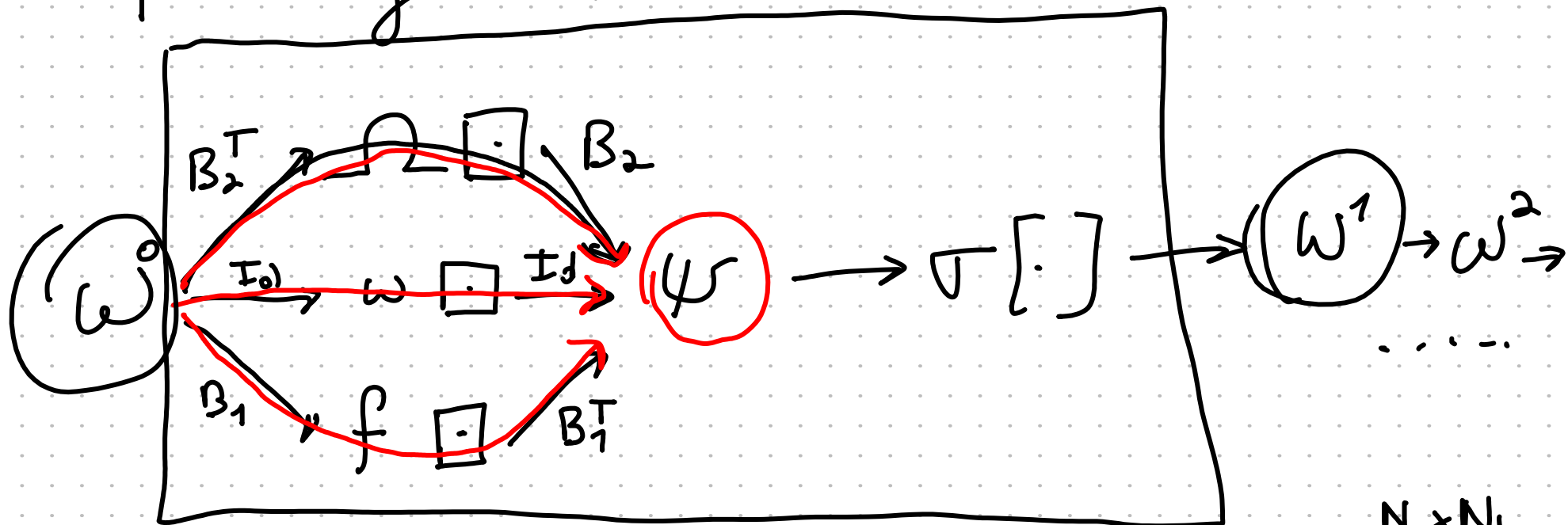
$\{B_1, B_2, B_3, \dots\}$

→ homology

$$B_k B_{k+1} = \bigcirc$$

$$\underline{B_{k+1}^T B_k^T = \bigcirc} \quad \text{mitch.rodtenberry.xyz/files/}$$

$$f \xrightarrow{D} g \xrightarrow{\Sigma} h$$



$$LF(\omega)$$

$$N_0 = |X_0|$$

$$N_1 = |X_1|$$

$$N_2 = |X_2|$$

$$B_1 \in \mathbb{R}^{N_0 \times N_1}$$

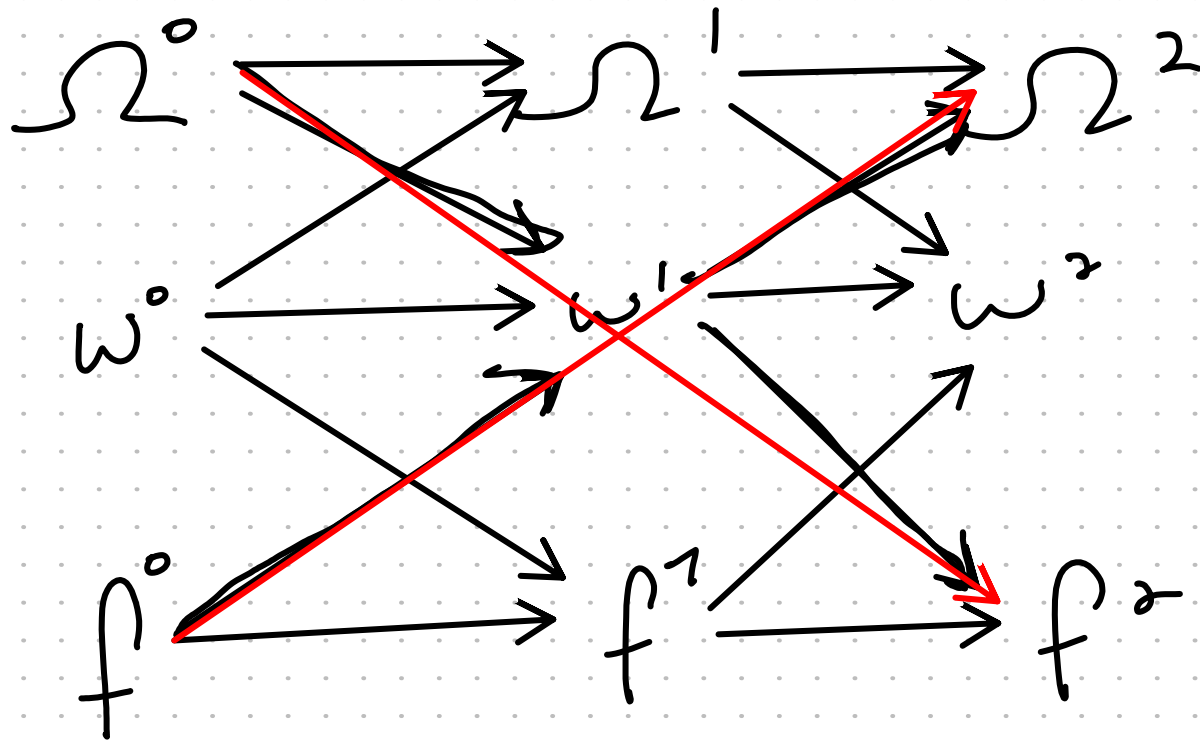
$$B_2 \in \mathbb{R}^{N_1 \times N_2}$$

$$Id \in \mathbb{R}^{N_1 \times N_1}$$

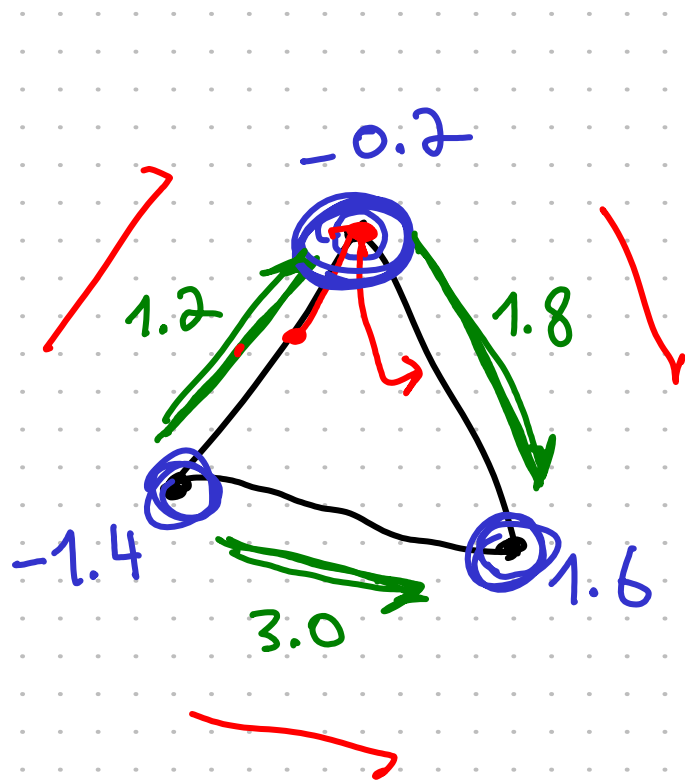
$\Omega$ : 2-chain ( $\Delta$ -signal)  
 $\omega$ : 1-chain ( $\nearrow$ -signal)  
 $f$ : 0-chain ( $\bullet$ -signal)

Eric Bunch et al

$$B_k B_{k+1} = 0$$



Claim nonlinearities are provably necessary  
for SNNs



$$\underline{B}_1 \underline{w} = \underline{f}$$

$$\underline{B}_1^T \underline{f} = \underline{\beta}$$

$$\underline{\Omega} = \underline{B}_2^T \underline{w}$$

$$\underline{\beta} = \underline{B}_2 \underline{\Omega}$$

