Cochains are all you need

LOGML 2024

11 July 2024

A summary of work from the thesis of

Kelly Maggs

Structure of the talk

1) What are cochains and what do they encode?
2) Cochains in signal processing
3) Cochains in machine learning
4) Cochains in computational biology

What are cochains?

And what do they encode?

Chain complexes of $\mathbb{R}$-vector spaces

$\mathbb{R}$-linear transformation

$$C_* = C_0 \xleftarrow{d_1} C_1 \xleftarrow{d_2} C_2 \leftarrow \cdots \leftarrow C_n \xleftarrow{d_{n+1}} C_{n+1} \leftarrow \cdots$$

$$d_n \circ d_{n+1} = 0 \quad \forall n$$

Chain complexes of $\mathbb{R}$-vector spaces

$\mathbb{R}$-linear transformation

$$
\begin{tikzcd}
C_* \arrow[d, "f_*"'] & = & C_0 \arrow[d, "f_0"'] & C_1 \arrow[l, "d_1"'] \arrow[d, "f_1"] \arrow[dl, phantom, "\circlearrowleft"] & C_2 \arrow[l, "d_2"'] \arrow[d, "f_2"] \arrow[dl, phantom, "\circlearrowleft"] & \cdots \arrow[l] & C_n \arrow[l] \arrow[d, "f_n"] & C_{n+1} \arrow[l, "d_{n+1}"'] \arrow[d, "f_{n+1}"] \arrow[dl, phantom, "\circlearrowleft"] & \cdots \arrow[l] \\
C'_* & = & C'_0 & C'_1 \arrow[l, "d'_1"'] & C'_2 \arrow[l, "d'_2"'] & \cdots \arrow[l] & C'_n \arrow[l] & C'_{n+1} \arrow[l, "d'_{n+1}"'] & \cdots \arrow[l]
\end{tikzcd}
$$

Chain complexes of $\mathbb{R}$-vector spaces

$$
\begin{tikzcd}
C_* = C_0 \arrow[d, "f_0"'] & C_1 \arrow[l, "d_1"'] \arrow[d, "f_1"] \arrow[dl, phantom, "\circlearrowleft"] & C_2 \arrow[l, "d_2"'] \arrow[d, "f_2"] \arrow[dl, phantom, "\circlearrowleft"] & \cdots \arrow[l] & \cdots & C_n \arrow[l] \arrow[d, "f_n"] & C_{n+1} \arrow[l, "d_{n+1}"'] \arrow[d, "f_{n+1}"] \arrow[dl, phantom, "\circlearrowleft"] & \cdots \arrow[l] \\
C'_* = C'_0 & C'_1 \arrow[l, "d'_1"'] & C'_2 \arrow[l, "d'_2"'] & \cdots \arrow[l] & \cdots & C'_n \arrow[l] & C'_{n+1} \arrow[l, "d'_{n+1}"'] & \cdots \arrow[l]
\end{tikzcd}
$$

$f_* : C_* \to C'_*$

$$\operatorname{Im} d_{n+1} \subseteq \ker d_n \quad \forall n$$

$$H_n(C_*) = \ker d_n / \operatorname{Im} d_{n+1}$$

Chain complexes of $\mathbb{R}$-vector spaces

$$\begin{tikzcd}
C_* \arrow[r, phantom, "="] \arrow[d, "f_*"'] & C_0 \arrow[d, "f_0"'] \arrow[dr, phantom, "\circlearrowleft"] & C_1 \arrow[l, "d_1"'] \arrow[d, "f_1"] \arrow[dr, phantom, "\circlearrowleft"] & C_2 \arrow[l, "d_2"'] \arrow[d, "f_2"] & \cdots \arrow[l] & C_n \arrow[l] \arrow[d, "f_n"] \arrow[dr, phantom, "\circlearrowleft"] & C_{n+1} \arrow[l, "d_{n+1}"'] \arrow[d, "f_{n+1}"] & \cdots \arrow[l] \\
C'_* \arrow[r, phantom, "="] & C'_0 & C'_1 \arrow[l, "d'_1"'] & C'_2 \arrow[l, "d'_2"'] & \cdots \arrow[l] & C'_n \arrow[l] & C'_{n+1} \arrow[l, "d'_{n+1}"'] & \cdots \arrow[l]
\end{tikzcd}$$

$$H_n(C_*) = \ker d_n / \operatorname{Im} d_{n+1}$$

$$f_* : C_* \longrightarrow C'_*$$

$$\Downarrow$$

$$H_n(f_*) : H_n(C_*) \to H_n(C'_*)$$

Cochain complexes of $\mathbb{R}$-vector spaces

$$\begin{tikzcd}
C^* = C^0 \arrow[r, "d^1"] \arrow[d, "f^0"'] \arrow[dr, phantom, "\circlearrowleft"] & C^1 \arrow[r, "d^2"] \arrow[d, "f^1"] \arrow[dr, phantom, "\circlearrowleft"] & C^2 \arrow[r] \arrow[d, "f^2"] & \cdots \arrow[r] & C^n \arrow[r, "d^{n+1}"] \arrow[d, "f^n"] \arrow[dr, phantom, "\circlearrowleft"] & C^{n+1} \arrow[r] \arrow[d, "f^{n+1}"] & \cdots \\
C^{0'} \arrow[r, "d^{1'}"] & C^{1'} \arrow[r, "d^{2'}"] & C^{2'} \arrow[r] & \cdots \arrow[r] & C^{n'} \arrow[r, "d^{n+1'}"] & C^{n+1'} \arrow[r] & \cdots
\end{tikzcd}$$

$$\operatorname{Im} d^n \subseteq \ker d^{n+1} \quad \forall n$$

$$f^* : C^* \longrightarrow C^{*'}$$

$$\Downarrow$$

$$H^n(f^*) : H^n(C^*) \to H^n(C^{*'})$$

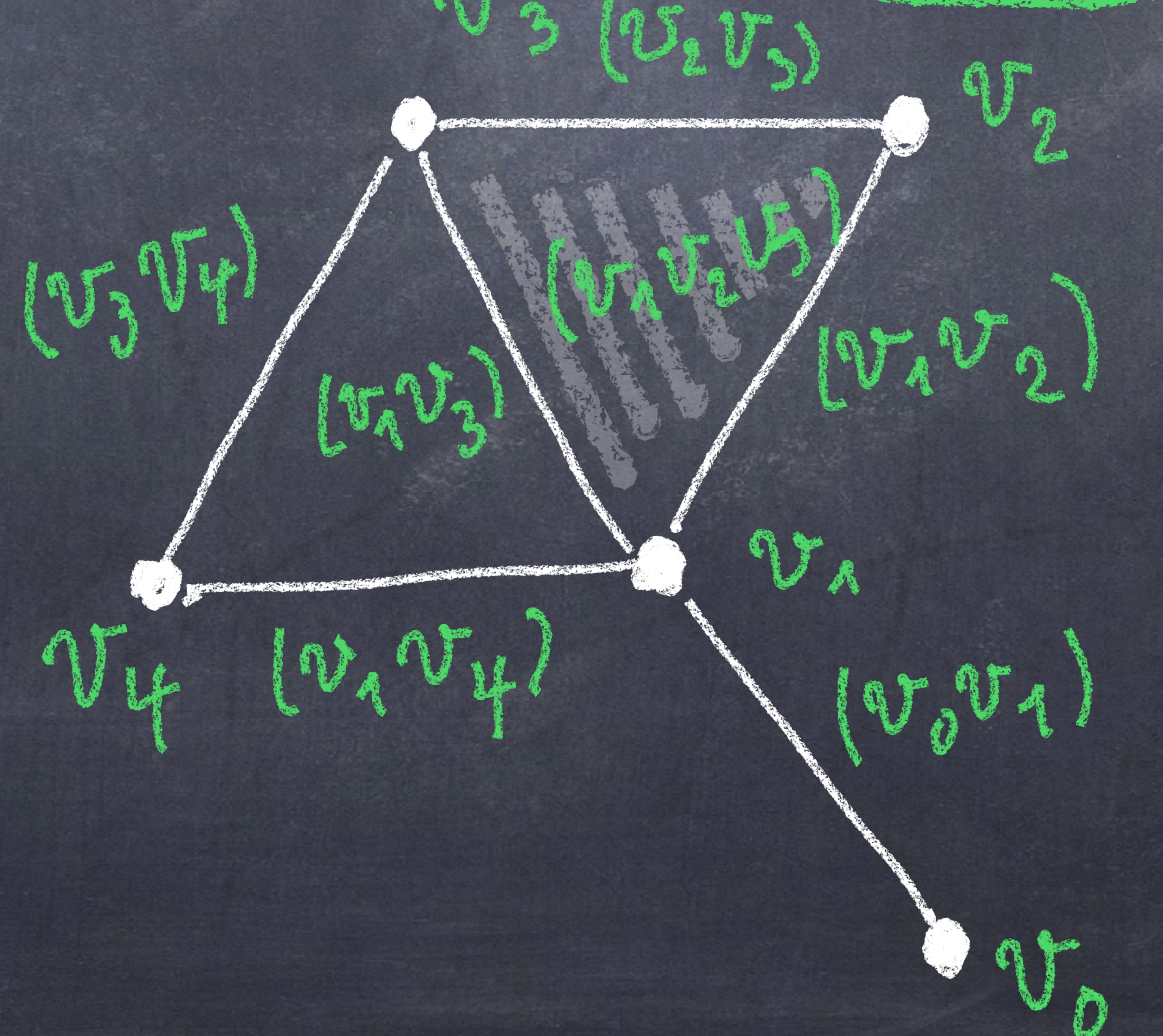
$$H^n(C^*) = \ker d^{n+1} / \operatorname{Im} d^n$$

Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V,
i.e., $\mathcal{K} \subseteq \mathcal{P}(V)$ satisfying

$$S \subseteq T \subseteq V \; + \; T \in \mathcal{K} \Rightarrow S \in \mathcal{K}.$$

Generalization of graphs.

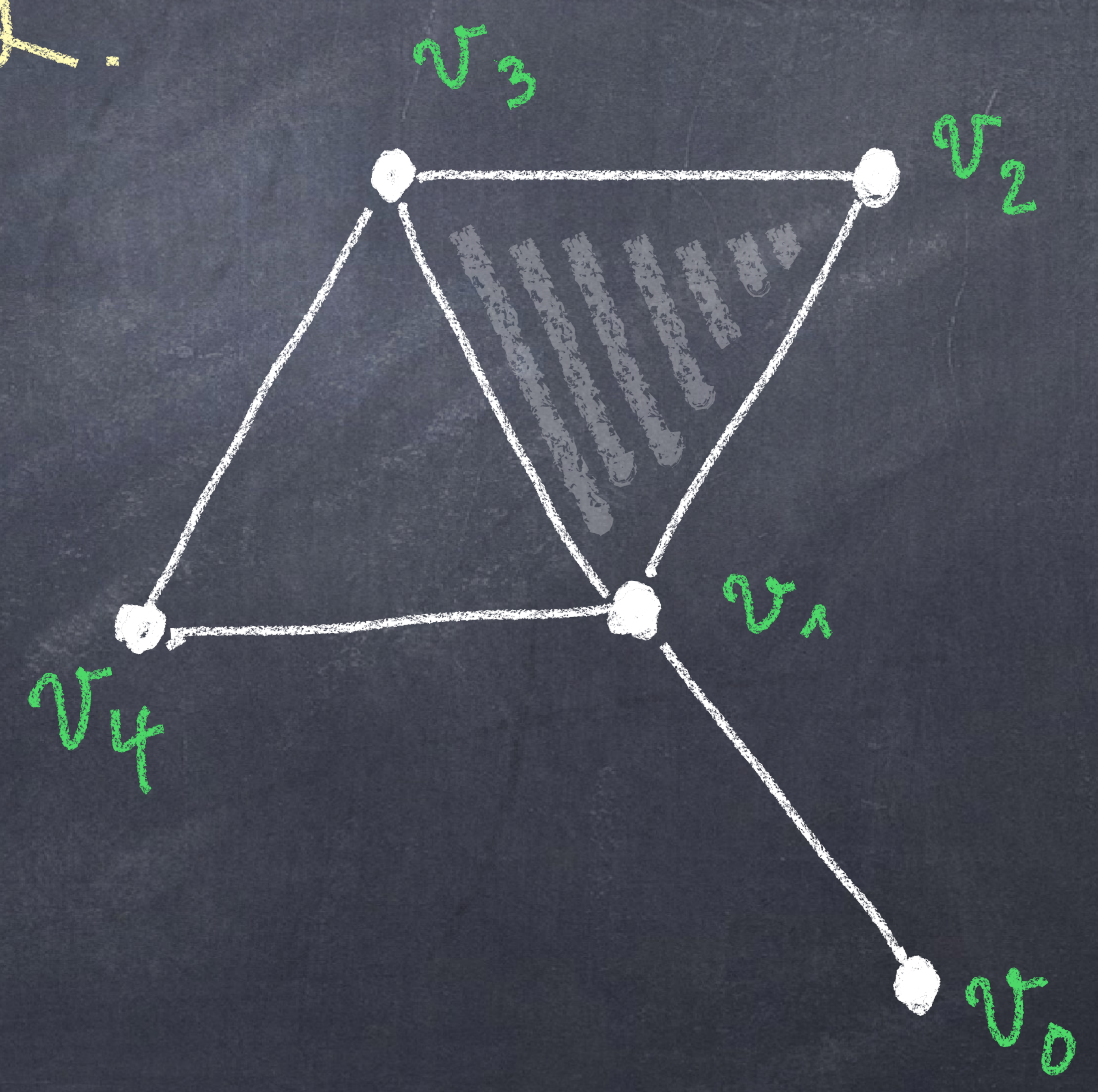


Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V, i.e., $\mathcal{K} \subseteq \mathcal{P}(V)$ satisfying

$$S \subseteq T \subseteq V \ + \ T \in \mathcal{K} \implies S \in \mathcal{K}.$$

$$\mathcal{K}_n = \{ T \in \mathcal{K} \mid \# T = n+1 \}$$



Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V, i.e., $\mathcal{K} \subseteq \wp(V)$ satisfying

$$S \subseteq T \subseteq V \;+\; T \in \mathcal{K} \implies S \in \mathcal{K}.$$

$$\mathcal{K}_n = \{ T \in \mathcal{K} \mid \# T = n+1 \}$$

Choose a total order $<$ on V.

Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V.

The chain complex $C_*(\mathcal{K}, <)$:

- $C_n(\mathcal{K}, <) = \mathrm{Span}_{\mathbb{R}}(\mathcal{K}_n)$

Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V.

The chain complex $C_*(\mathcal{K}, <)$:

- $C_n(\mathcal{K}, <) = \mathrm{Span}_{\mathbb{R}}(\mathcal{K}_n)$
- $d_n : C_n(\mathcal{K}, <) \longrightarrow C_{n-1}(\mathcal{K}, <)$

$$(v_0, \dots, v_n) \longmapsto \sum_{i=0}^{n} (-1)^i (v_0, \dots, \hat{v}_i, \dots, v_n)$$

Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V.

The chain complex $C_*(\mathcal{K}, <)$:

- $C_n(\mathcal{K}, <) = \mathrm{Span}_{\mathbb{R}}(\mathcal{K}_n)$
- $d_n : C_n(\mathcal{K}, <) \longrightarrow C_{n-1}(\mathcal{K}, <)$

$$(v_0, \ldots, v_n) \longmapsto \sum_{i=0}^{n} (-1)^i (v_0, \ldots, \hat{v}_i, \ldots, v_n)$$

$H_n(\mathcal{K}) = H_n(C_*(\mathcal{K}, <))$

<u>NB</u>: $<$ often dropped from the notation

Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V,

The cochain complex $C^*(\mathcal{K}, <)$:

- $C^n(\mathcal{K}, <) = \mathrm{Fun}(\mathcal{K}_n, \mathbb{R})$
- $d^n : C^{n-1}(\mathcal{K}, <) \longrightarrow C^n(\mathcal{K}, <)$

$$f \longmapsto d^n f : \mathcal{K}_n \longrightarrow \mathbb{R}$$

$$(v_0, .., v_n) \longmapsto \sum_{i=0}^{n} (-1)^i f((v_0, \dots, \hat{v}_i, .., v_n)).$$

NB: $<$ often dropped from the notation

$$H^n(\mathcal{K}) = H^n(C^*(\mathcal{K}, <)).$$

Example ①

Let $\mathcal{K}$ be a simplicial complex on a vertex set V,

The cochain complex $C^*(\mathcal{K}, <)$:

- $C^n(\mathcal{K}, <) = \mathrm{Fun}(\mathcal{K}_n, \mathbb{R})$
- $d^n : C^{n-1}(\mathcal{K}, <) \longrightarrow C^n(\mathcal{K}, <)$

$$f \mapsto d^n f : \mathcal{K}_n \longrightarrow \mathbb{R}$$

$H^n(\mathcal{K}) = H^n(C^*(\mathcal{K}, <))$. – detects non-trivial maps of $\mathcal{K}$ into spaces of interest

Example ①

Let $\mathcal{K}$ be a simplicial complex on a finite vertex set V.

- $C^n(\mathcal{K}, <) \cong C_n(\mathcal{K}, <) \quad \forall n$

- $H^n(\mathcal{K}) \cong H_n(\mathcal{K}) \quad \forall n$

Example ②

The de Rham complex of $\mathbb{R}^n$ is a cochain complex

$$\Omega^*(\mathbb{R}^n) = C^\infty(\mathbb{R}^n) \otimes \Lambda(dx_1, \ldots, dx_n)$$

Example ②

The de Rham complex of $\mathbb{R}^n$ is a cochain complex

$$\Omega^*(\mathbb{R}^n) = C^\infty(\mathbb{R}^n) \otimes \Lambda(dx_1, \dots, dx_n)$$

- $\Omega^k(\mathbb{R}^n) = \left\{ \sum_{t \in T} f_t \cdot dx_{i_{t,1}} \cdots dx_{i_{t,k}} \;\middle|\; \begin{array}{l} i_{t,1} < \dots < i_{t,k} \\ f_t \in C^\infty(\mathbb{R}^n) \end{array} \right\}$

Example ②

The de Rham complex of $\mathbb{R}^n$ is a cochain complex

$$\Omega^*(\mathbb{R}^n) = C^\infty(\mathbb{R}^n) \otimes \Lambda(dx_1, \dots, dx_n)$$

- $\Omega^k(\mathbb{R}^n) = \left\{ \sum_{t \in T} f_t \cdot dx_{i_{t,1}} \cdots dx_{i_{t,k}} \;\middle|\; \begin{matrix} i_{t,1} < \dots < i_{t,k} \\ f_t \in C^\infty(\mathbb{R}^n) \end{matrix} \right\}$

- $d^{k+1} : \Omega^k(\mathbb{R}^n) \longrightarrow \Omega^{k+1}(\mathbb{R}^n)$

$$f\, dx_{i_1} \cdots dx_{i_k} \longmapsto \sum_{j=1}^{n} \pm \frac{\partial f}{\partial x_j} dx_{i_1} \cdots dx_j \cdots dx_{i_k}$$

Example ②

Given $\varphi : \Delta^k \xrightarrow{\text{affine embedding}} \mathbb{R}^n$, $\omega = f\, dy_{i_1} \cdots dy_{i_k} \in \Omega^k(\mathbb{R}^n)$:

- $\varphi^*\omega = \sum (f \circ \varphi)\, d\varphi_{i_1} \cdots d\varphi_{i_k}$

  where $d\varphi_i = \sum_{j=1}^{k} \frac{\partial \varphi_i}{\partial x_j} dx_j$.

- Makes sense therefore to compute $\int_{\Delta^k} \varphi^*\omega \in \mathbb{R}$.

Relation between the examples

- The de Rham complex generalizes to $\Omega^*(M)$ for M a smooth n-manifold, by gluing together copies of $\Omega^*(\mathbb{R}^n)$ according to an atlas.

Relation between the examples

- The de Rham complex generalizes to $\Omega^*(M)$ for M a smooth n-manifold, by gluing together copies of $\Omega^*(\mathbb{R}^n)$ according to an atlas.
- If a simplicial complex $\mathcal{K}$ is a triangulation of M, then $H^*(\Omega^*(M)) \cong H^*(C^*(\mathcal{K}))$, mediated by integration.

Incorporating geometry

If M is a Riemannian manifold, each $\Omega^k(M)$ is equipped with an inner product $\langle -, - \rangle$.

Thus $\exists$:

$$\begin{tikzcd} \Omega^{k-1}(M) \arrow[r, shift left, "d^k"] & \Omega^k(M) \arrow[l, shift left, "(d^k)^\dagger"] \arrow[r, shift left, "d^{k+1}"] & \Omega^{k+1}(M) \arrow[l, shift left, "(d^{k+1})^\dagger"] \end{tikzcd}$$

Incorporating geometry

If M is a Riemannian manifold, each $\Omega^k(M)$ is equipped with an inner product $\langle -, - \rangle$.

Thus $\exists$:

$$\Omega^{k-1}(M) \underset{(d^k)^\dagger}{\overset{d^k}{\rightleftarrows}} \Omega^k(M) \underset{(d^{k+1})^\dagger}{\overset{d^{k+1}}{\rightleftarrows}} \Omega^{k+1}(M)$$

$$\Delta^k = d^k (d^k)^\dagger + (d^{k+1})^\dagger d^{k+1} : \Omega^k(M) \longrightarrow \Omega^k(M)$$

– the Hodge - Laplacian

Hodges' Theorem

If M is a compact Riemannian manifold, then

- $(\ker \Delta^*, 0) \hookrightarrow \Omega^*(M)$ is a map of cochain complexes inducing $\ker \Delta^* \cong H^*(M)$.

Hodges' Theorem

If M is a compact Riemannian manifold, then

- $(\ker \Delta^*, 0) \hookrightarrow \Omega^*(M)$ is a map of cochain complexes inducing $\ker \Delta^* \cong H^*(M)$.

- $\Omega^k(M) \cong \operatorname{Im} d^k \oplus \ker \Delta^k \oplus \operatorname{Im}(d^{k+1})^\dagger$ ← Harmonic classes

  – orthogonal decomposition

Each cohomology class has a unique harmonic representative.

Cochains in signal processing

Ebli - Hacker - Maggs

J. App Comp Top 2024

Goal

Generalize signal processing on graphs to simplicial complexes, in particular to better understand signal compression and reconstruction.

Signals on simplicial complexes

Informally: example of a signal on 2-simplices of $\mathcal{K}$

$\mathcal{K} =$ 

$s_i \in \mathbb{R} \ \forall\, 1 \leq i \leq 3$

Signals on simplicial complexes

Formally: for $\mathcal{K}$ a simplicial complex, a signal on the n-simplices of $\mathcal{K}$ can be viewed as either

$$s \in C_n(\mathcal{K}) \quad \text{or} \quad s \in C^n(\mathcal{K}).$$

$$s : \mathcal{K}_n \longrightarrow \mathbb{R}$$

Motivating question

How to compress or sparsify a signal on a simplicial complex while minimizing loss?

The approach of Ebli-Hacker-Maggs

Algebraic discrete Morse theory + Discrete Hodge theory $\Rightarrow$ algorithm for excellent compression of a given signal on a simplicial complex

The approach of Ebli - Hacker - Maggs

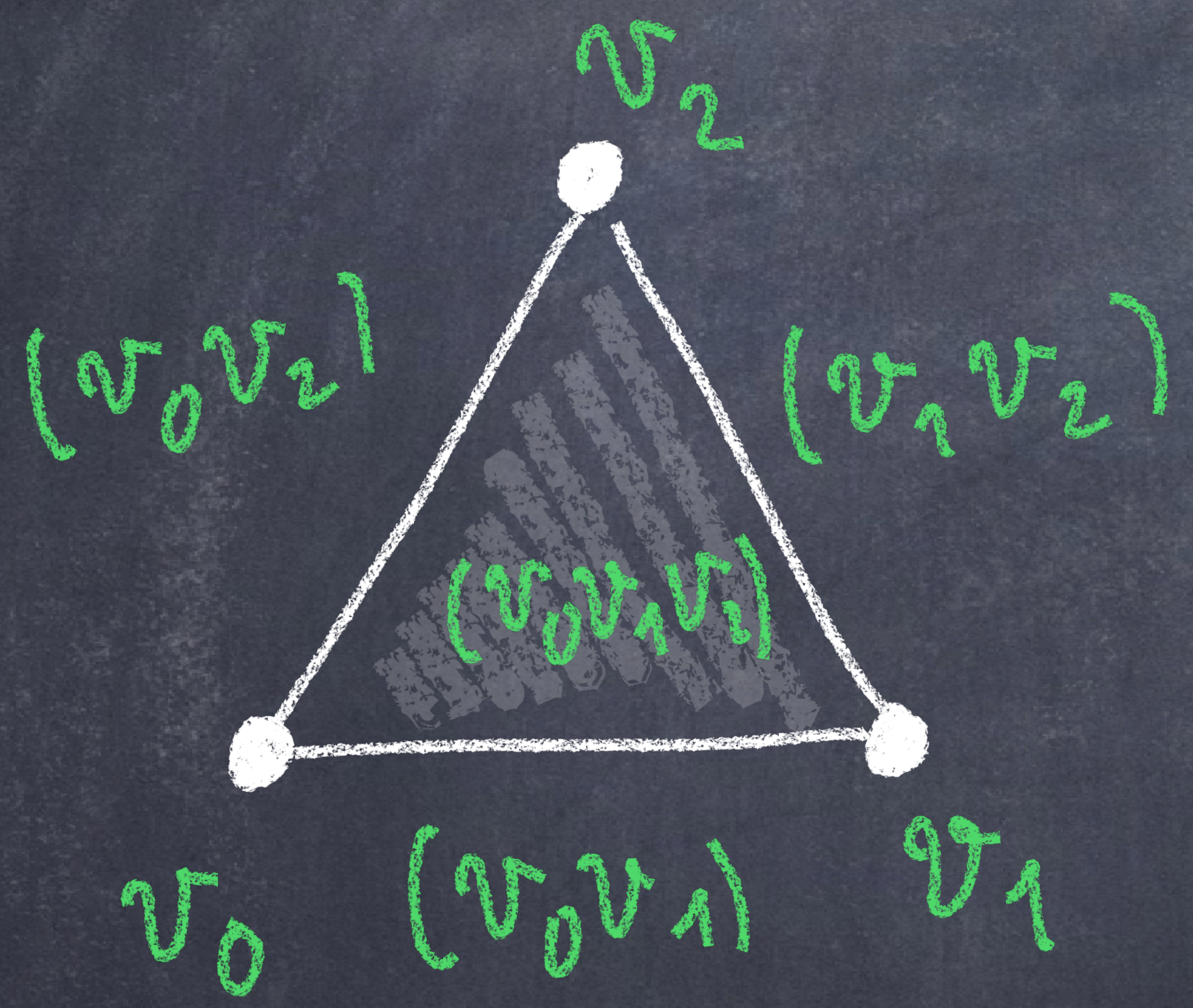
Algebraic discrete Morse theory

\+

Discrete Hodge theory

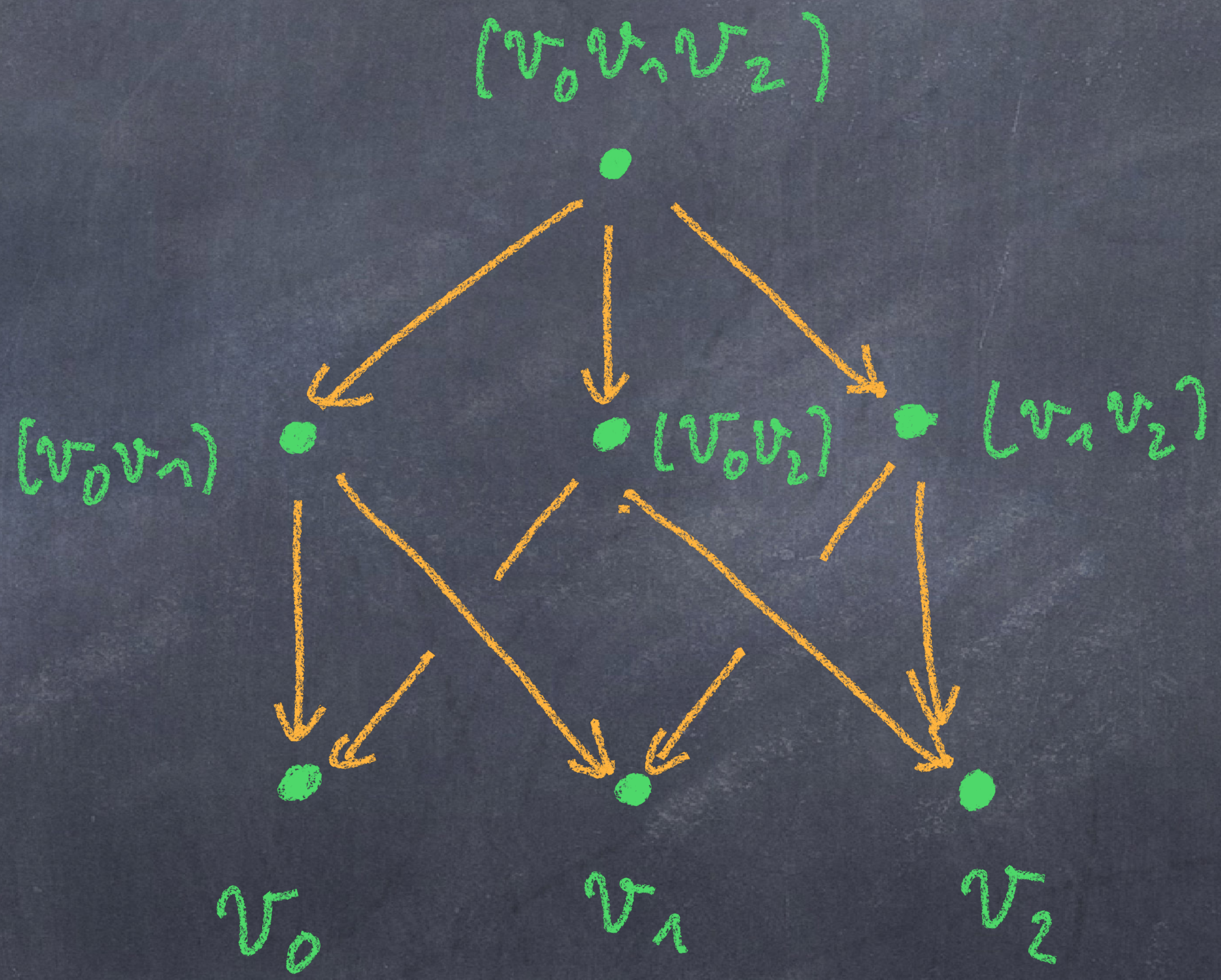
$\Rightarrow$ algorithm for excellent compression of a given signal on a simplicial complex

Essential mathematical notions



$\mathcal{K}$

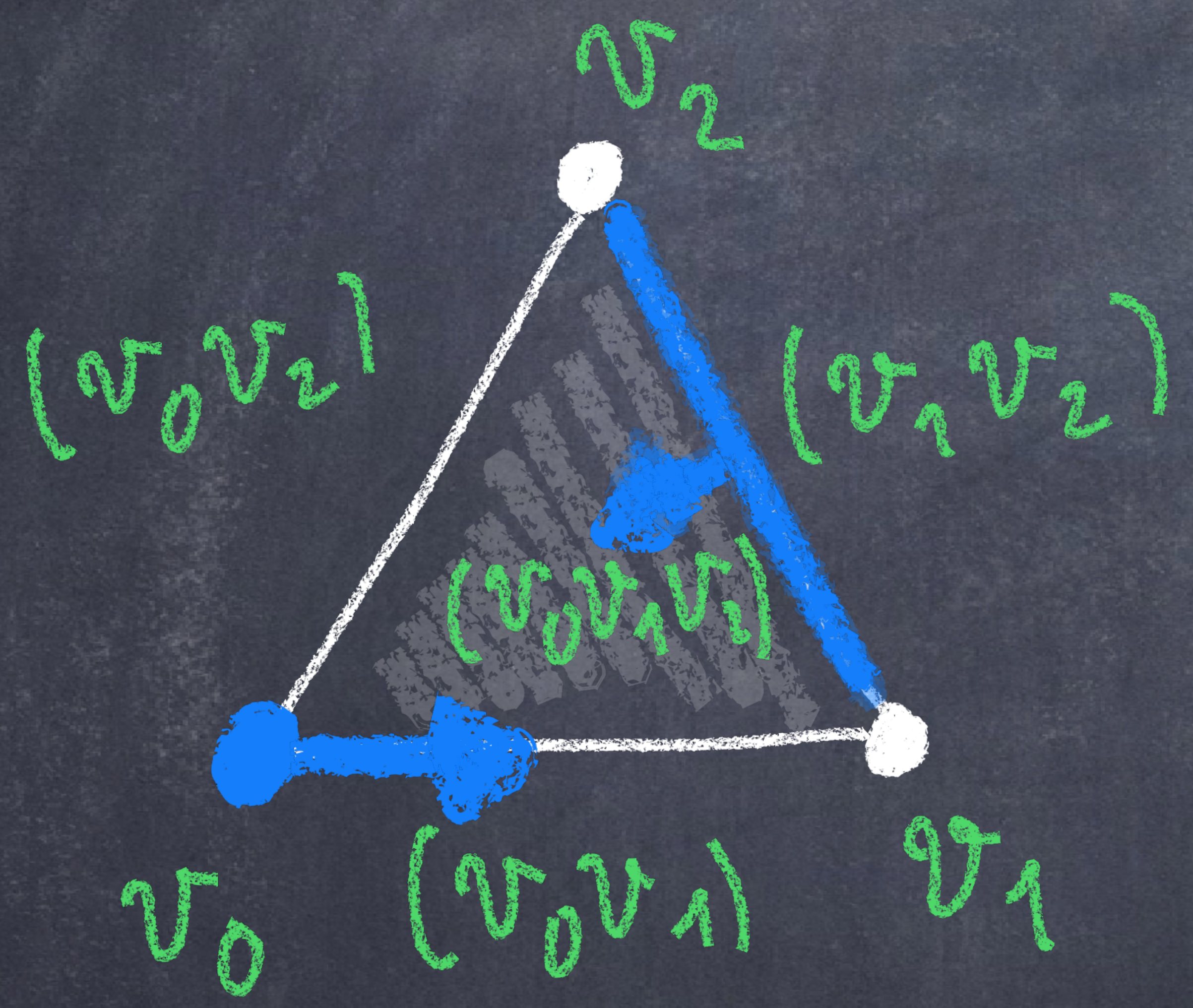
$\Longleftrightarrow$



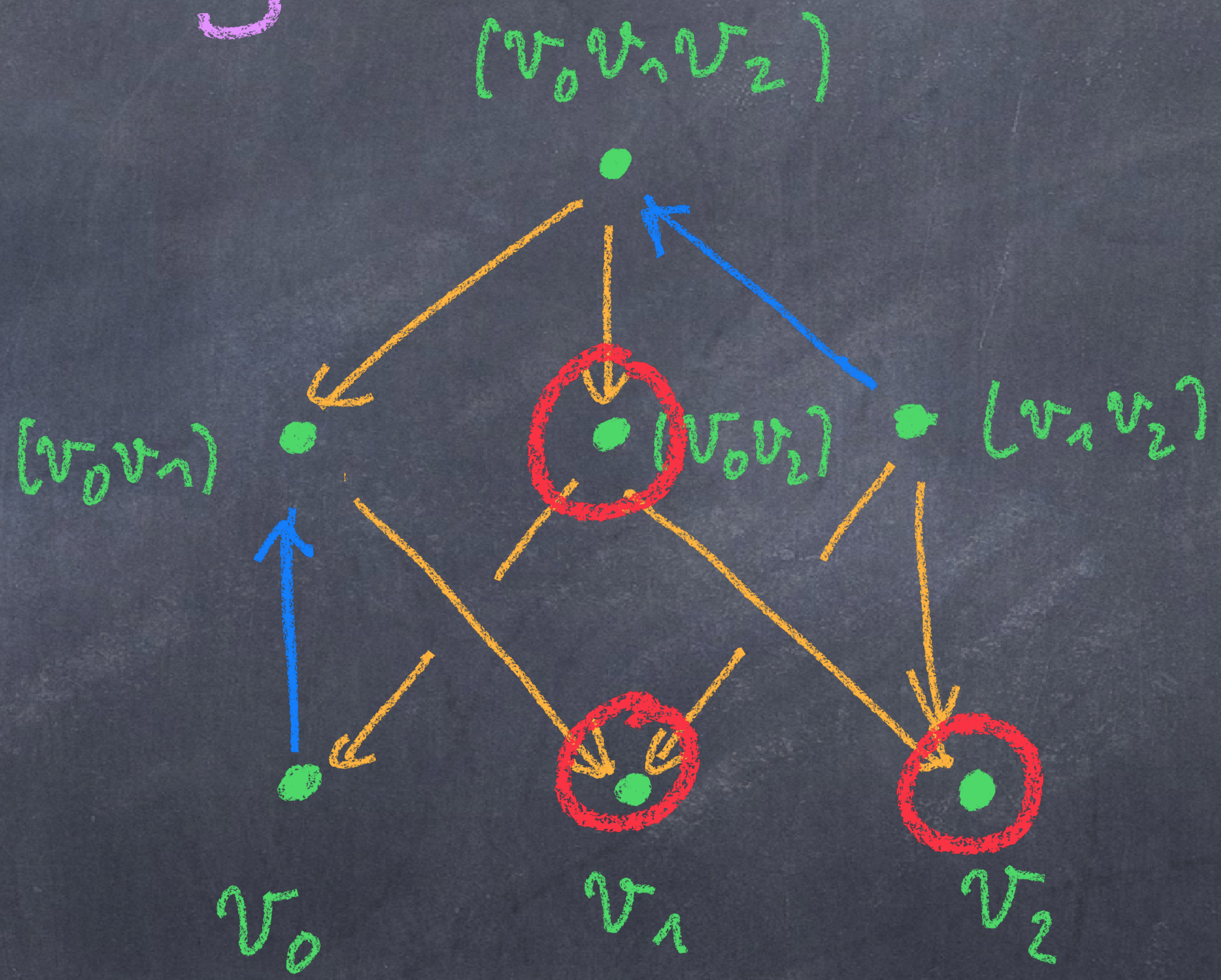
Hasse diagram of $\mathcal{K}$

Essential mathematical notions

Morse matching



$\Longleftrightarrow$



M - matching

$M \Longrightarrow M^0$ critical cells

Fundamental Thm of ADMT [Sköldberg]

For every Morse matching M on a chain complex C, $\exists$ deformation retract

$\rho^M \iota^M = \mathrm{Id}_{C'}$

$\iota^M \rho^M \simeq \mathrm{Id}_C$

$$C^M \underset{\rho^M}{\overset{\iota^M}{\rightleftarrows}} C \circlearrowright h^M$$

Explicit formulas!

where $C^M_n = \mathrm{Span}_R\{\text{critical } n\text{-cells}\}$.

Discrete Hodge theory

(C, ∂) = finite-type chain complex of real inner product spaces

$$\partial_n : C_n \longrightarrow C_{n-1} \implies \partial_n^\dagger : C_{n-1} \longrightarrow C_n$$

(adjoint)

$\forall n \geq 1$

Discrete Hodge theory

(C, ∂) = finite type chain complex of real inner product spaces

Up Laplacian

$\Delta_n^+ = \partial_{n+1}\partial_{n+1}^\dagger$

$$\begin{tikzcd} C_{n+1} \arrow[r, shift left, "\partial_{n+1}"] & C_n \arrow[l, shift left, "\partial_{n+1}^\dagger"] \arrow[r, shift left, "\partial_n"] & C_{n-1} \arrow[l, shift left, "\partial_n^\dagger"] \end{tikzcd}$$

Down Laplacian

$\Delta_n^- = \partial_n^\dagger \partial_n$

Discrete Hodge theory

(C,∂) = finite type chain complex of real inner product spaces

$$\Delta_n^+ = \partial_{n+1}\partial_{n+1}^\dagger \qquad
\begin{tikzcd}
C_{n+1} \arrow[r, shift left, "\partial_{n+1}"] & C_n \arrow[l, shift left, "\partial_{n+1}^\dagger"] \arrow[r, shift left, "\partial_n"] & C_{n-1} \arrow[l, shift left, "\partial_n^\dagger"]
\end{tikzcd}
\qquad \Delta_n^- = \partial_n^\dagger \partial_n$$

$$\Delta_n = \Delta_n^+ + \Delta_n^- : C_n \longrightarrow C_n$$ $\leftarrow$ The combinatorial Laplacian

Fundamental Thm of DHT [Eckmann]

For (C, ∂) any finite-type chain complex of real inner product spaces:

- $H_n(C, \partial) \cong \ker \Delta_n$

and

- $C_n \cong \mathrm{Im}\, \partial_{n+1} \oplus \ker \Delta_n \oplus \mathrm{Im}\, \partial_n^{+}$,

$\forall n \geq 0.$

Fundamental Thm of DHT [Eckmann]

For (C, ∂) any finite-type chain complex of real inner product spaces:

- $H_n(C, \partial) \cong \ker \Delta_n$

and

- $C_n \cong \operatorname{Im} \partial_{n+1} \oplus \ker \Delta_n \oplus \operatorname{Im} \partial_n^{+}$, $\forall n \geq 0$.

"curl-like" "harmonics" "gradient-like"

Fundamental Thm of DHT [Eckmann]

For (C, ∂) any finite-type chain complex of real inner product spaces:

$$C_n \cong \underset{\substack{\uparrow \\ \exists \text{ ON basis} \\ \text{of eigenvectors} \\ \text{of } \Delta_n^+}}{\operatorname{Im} \partial_{n+1}} \oplus \ker \Delta_n \oplus \underset{\substack{\uparrow \\ \exists \text{ ON basis} \\ \text{of eigenvectors} \\ \text{of } \Delta_n^-}}{\operatorname{Im} \partial_n^+},$$

∃ ON basis of eigenvectors of Δ_n^+ + ∃ ON basis of eigenvectors of Δ_n^- $\Longrightarrow$ Hodge basis of (C, ∂)

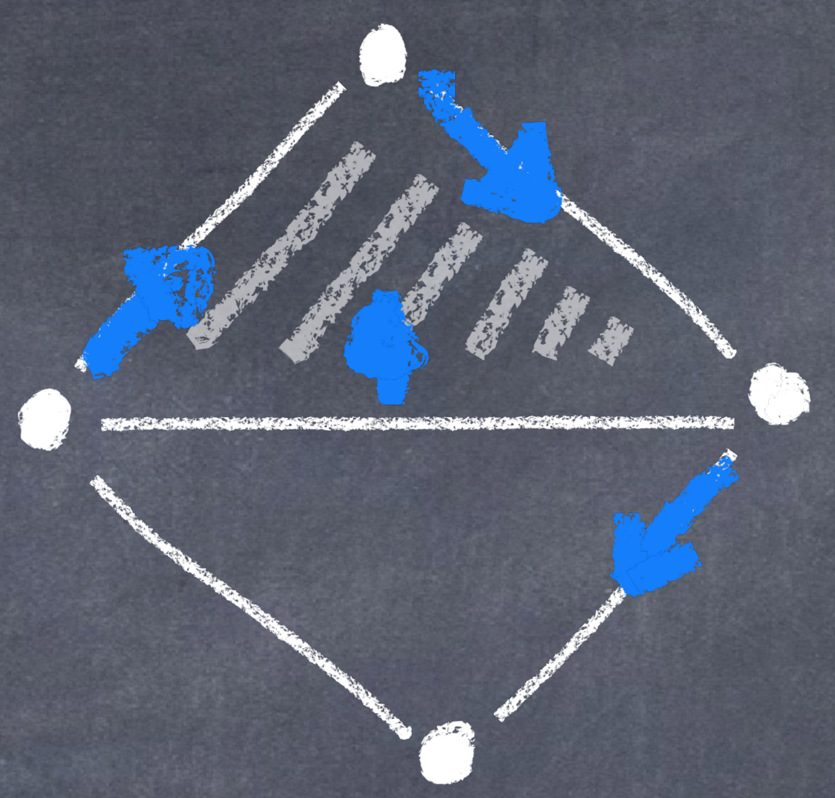
The Hodge Matching Thm [EHM '22]

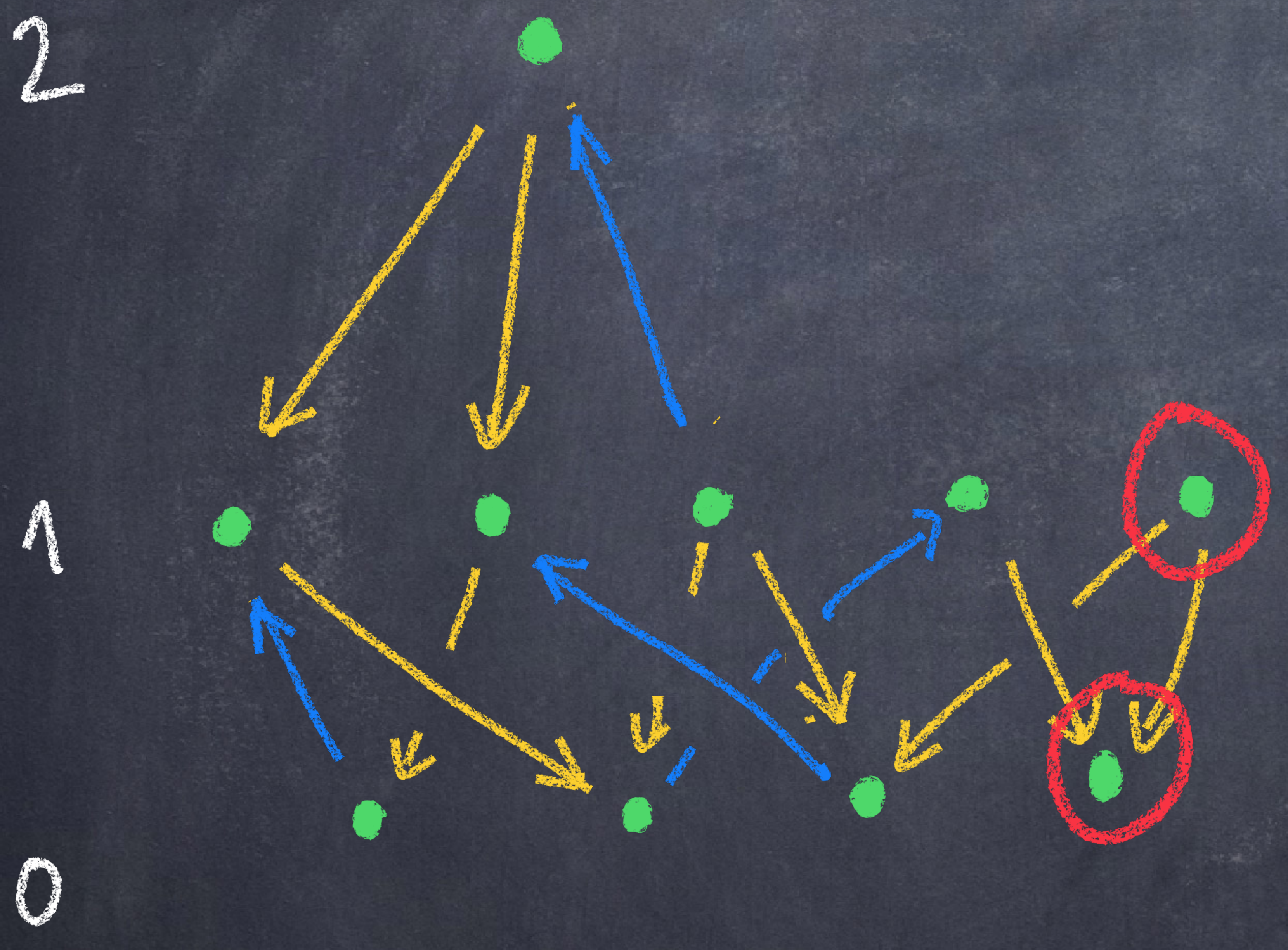
Given (C,∂) as above, the Hodge basis gives rise to a Moore matching with associated deformation retract

$$(\ker\Delta, 0) \rightleftarrows (C,\partial) \circlearrowleft h^{\Delta}.$$

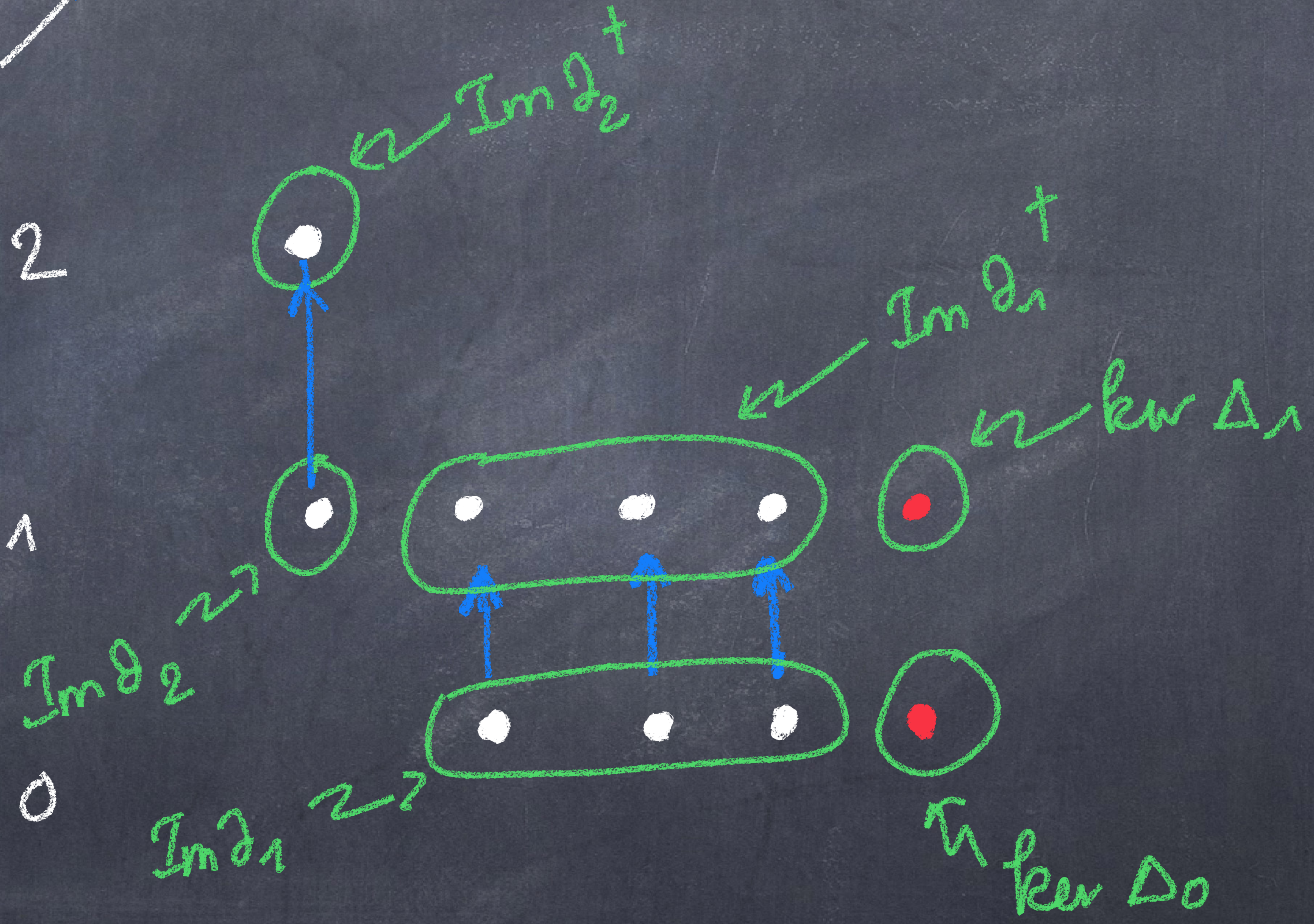
– the Hodge retraction

Example





Geometric Morse matching



Algebraic Morse matching

An autoencoder problem

Given a deformation retract

reconstruction

$$(C', \partial') \underset{\rho}{\overset{\iota}{\rightleftarrows}} (C, \partial) \circlearrowleft h$$

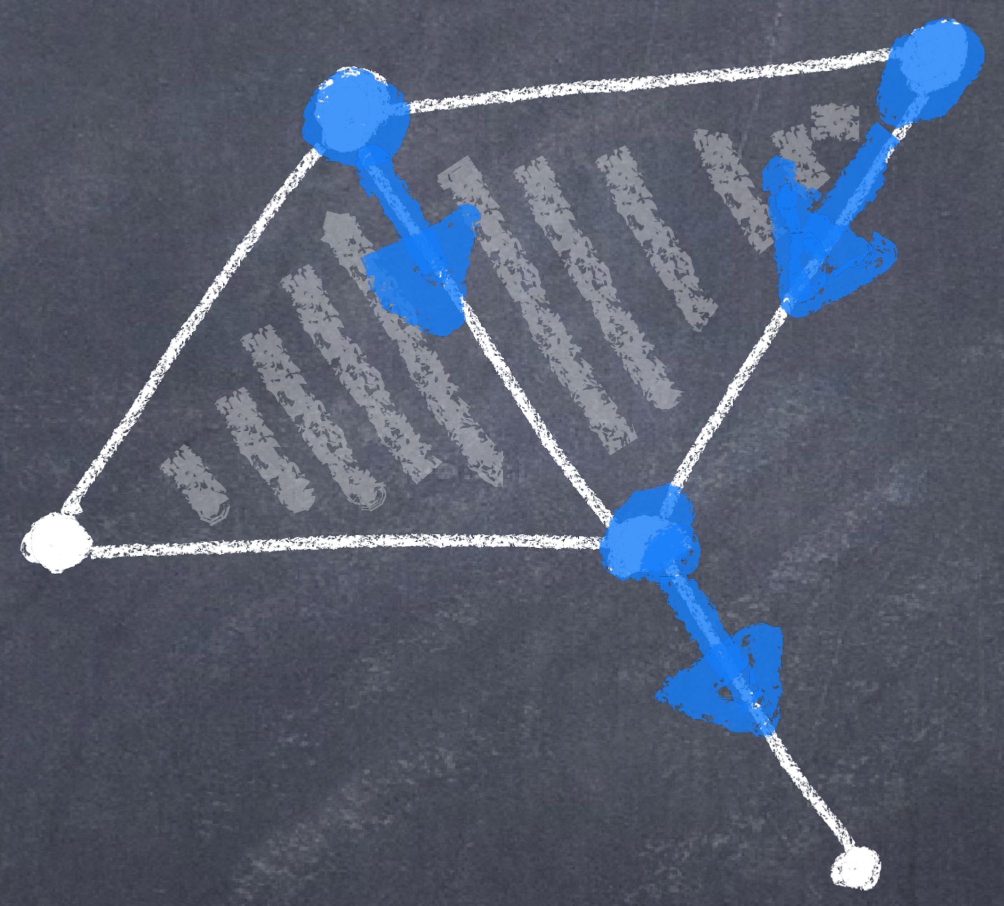
compression

and a "signal" $s \in C$, what can we say about $s - \iota\rho(s)$?

(n, n-1) free Morse matchings

No (n-1)-simplex matched to an n-simplex

(1,0)-free



(2,1)-free

Adjoint decompositions

Let (C, ∂) be a chain complex of f.dim'l real inner product spaces.

$$C_{n+1} \underset{\partial_{n+1}^{\dagger}}{\overset{\partial_{n+1}}{\rightleftarrows}} C_n \underset{\partial_n^{\dagger}}{\overset{\partial_n}{\rightleftarrows}} C_{n-1}$$

$$\Longrightarrow \ker \partial_n \oplus \operatorname{Im} \partial_n^{\dagger} \cong C_n \cong \operatorname{Im} \partial_{n+1} \oplus \ker \partial_{n+1}^{\dagger}$$

Reconstruction Theorem [EHM '22]

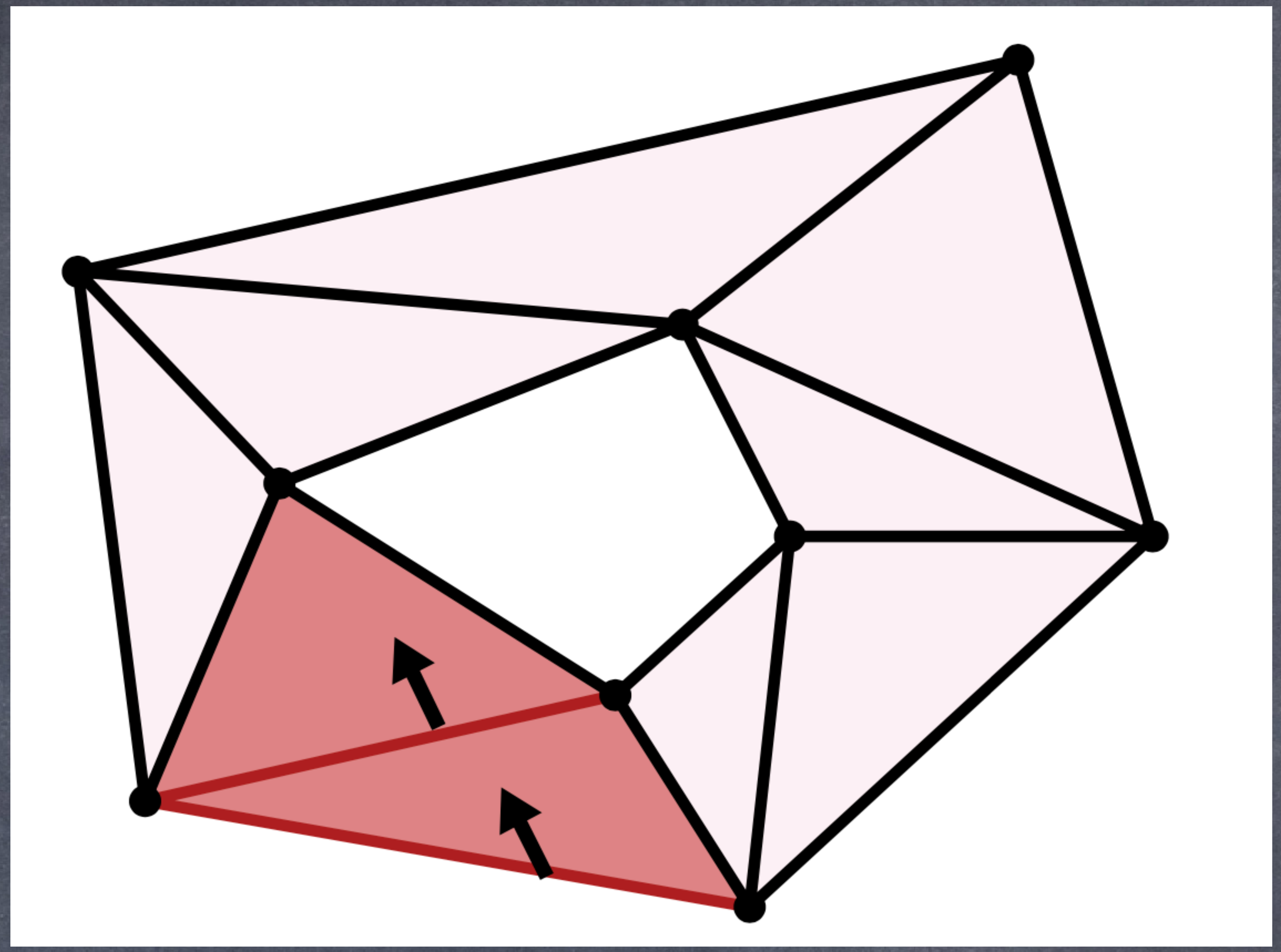
Let M be a $(n, n-1)$-free Morse matching on (C, ∂) chain complex of f.-dim'l inner product spaces.

Consider $(C,\partial)^M \underset{\rho^M}{\overset{\iota^M}{\rightleftarrows}} (C,\partial) \circlearrowleft h^M$.

Then: $\mathrm{Proj}_{\ker \partial_{n+1}^{\dagger}} \left(s - \iota^M \rho^M(s)\right) = 0 \quad \forall s \in C_n$

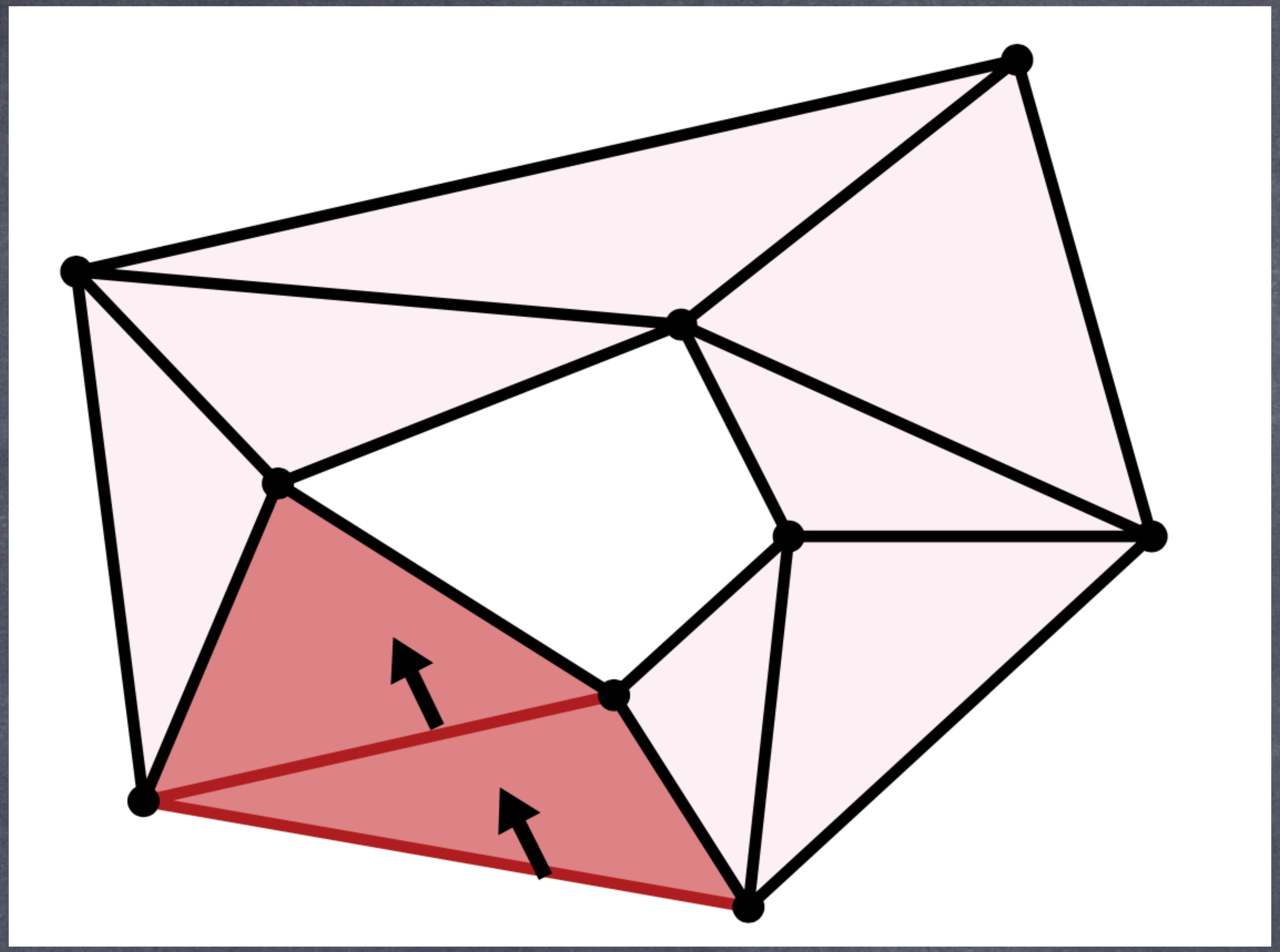
– the error lies uniquely in $\mathrm{Im}\, \partial_{n+1}$!

Example

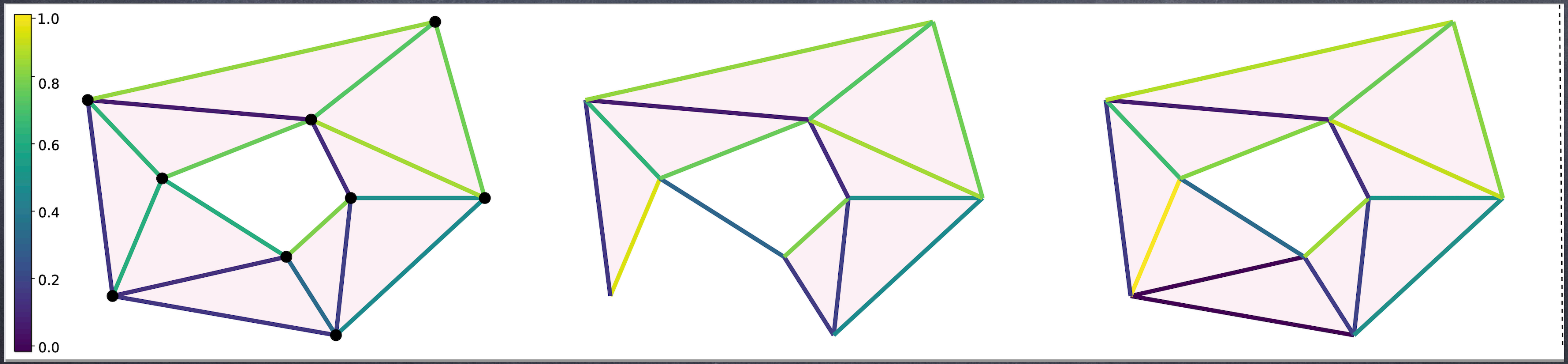


(1,0)- free
Morse matching

Example

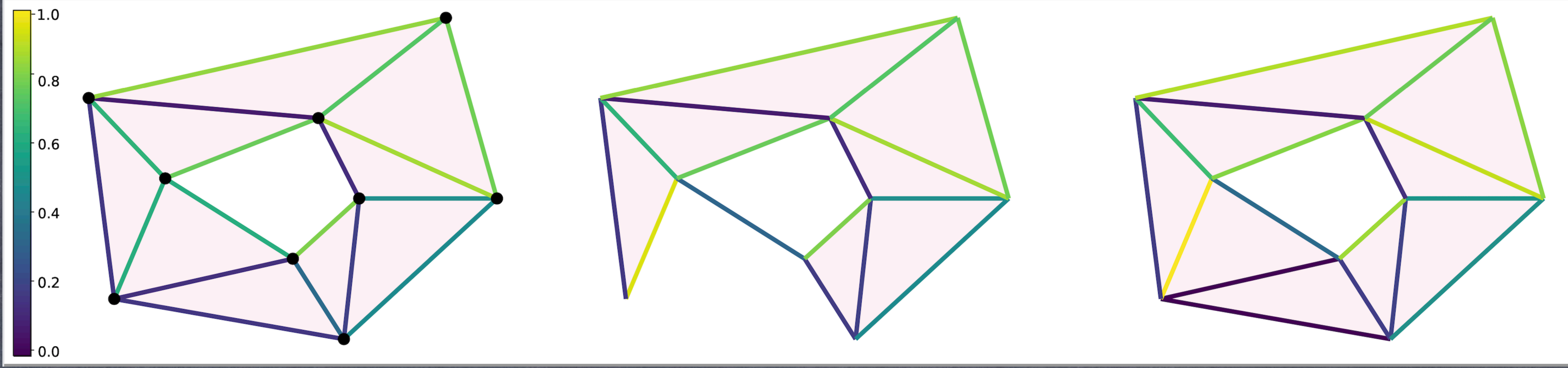


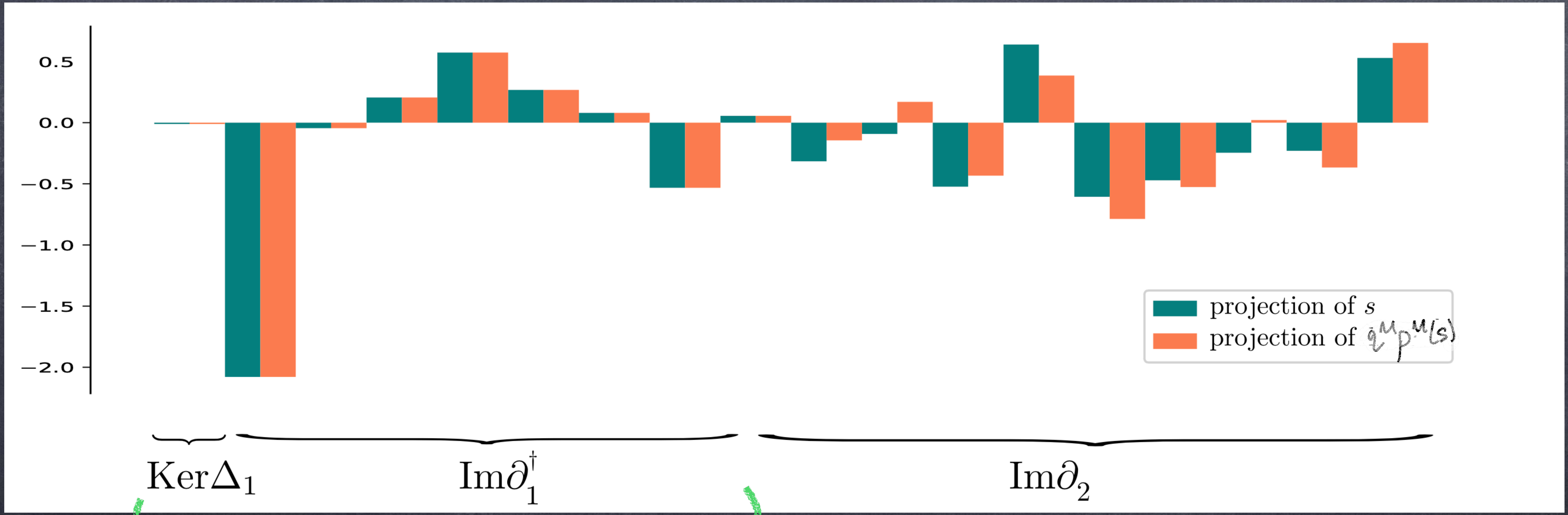
$(1,0)$-free Morse matching



$$s \in C_1(K) \longmapsto \rho^M(s) \in C_1(K)^M \mapsto \iota^M \rho^M(s) \in C_1(K)$$

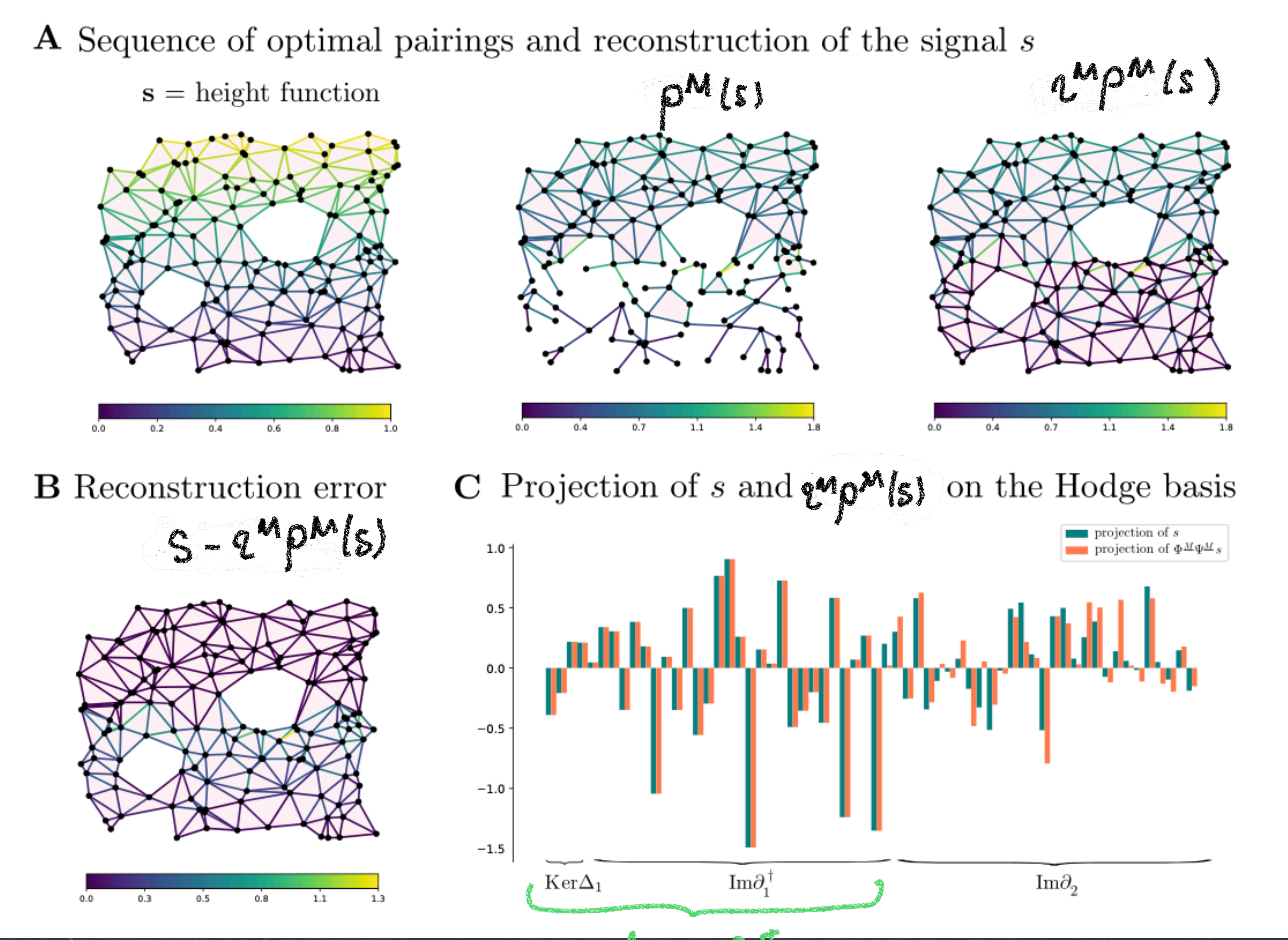
Example





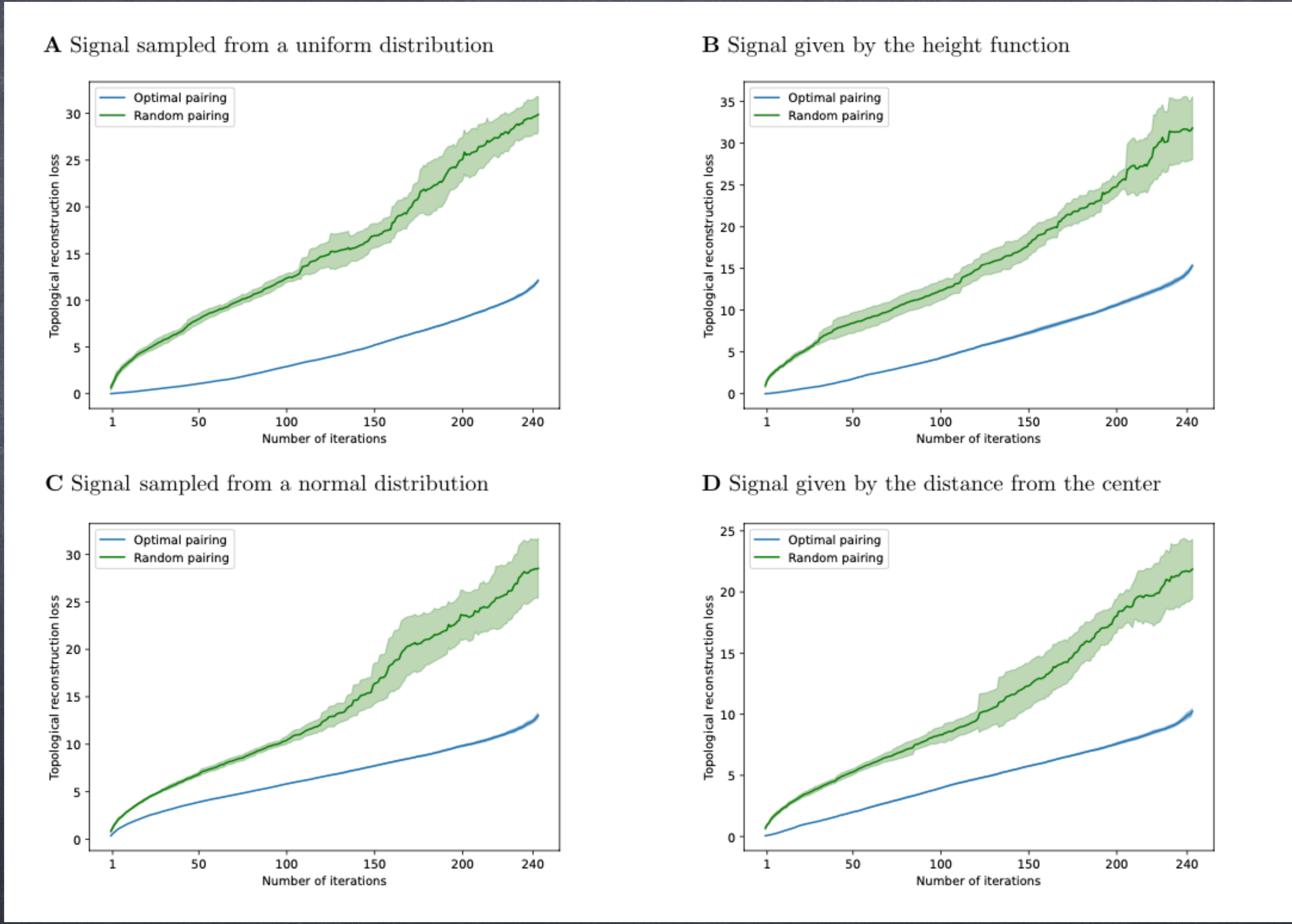
$= \ker \partial_2^\dagger$

Experiments



$\ker \partial_2^\dagger$

Experiments

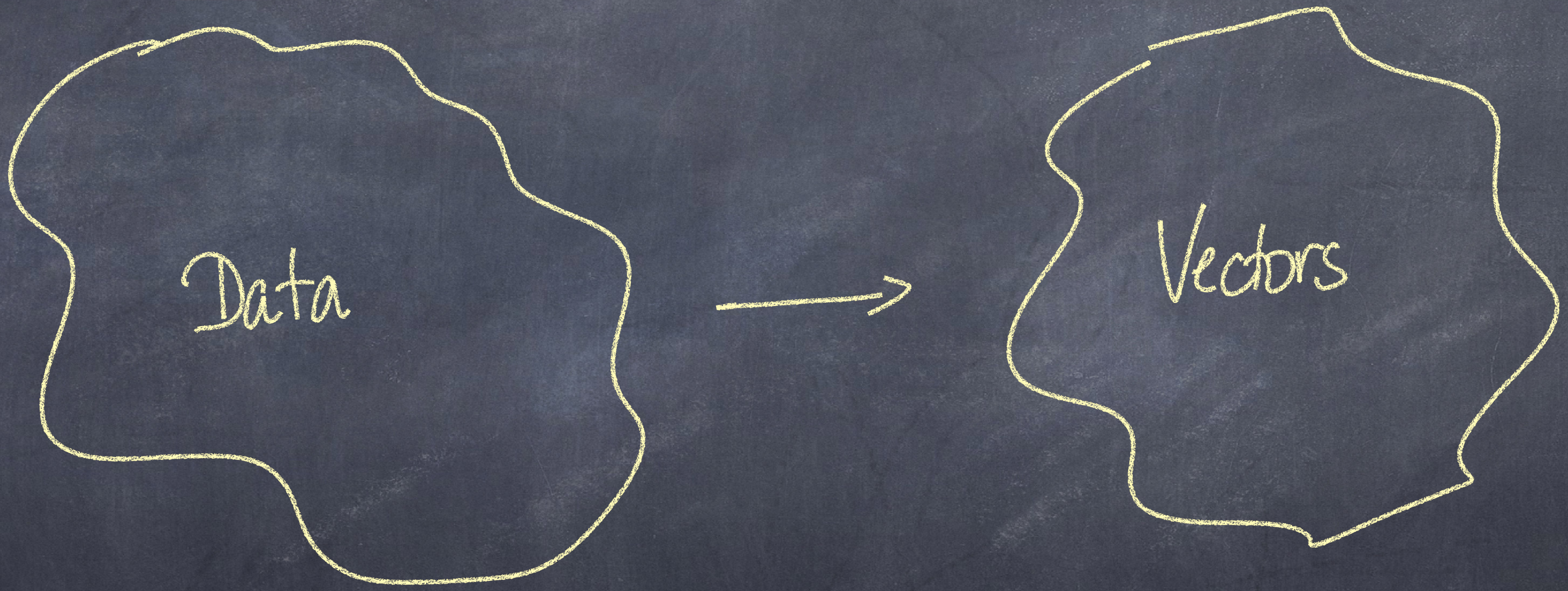


Cochains in machine learning

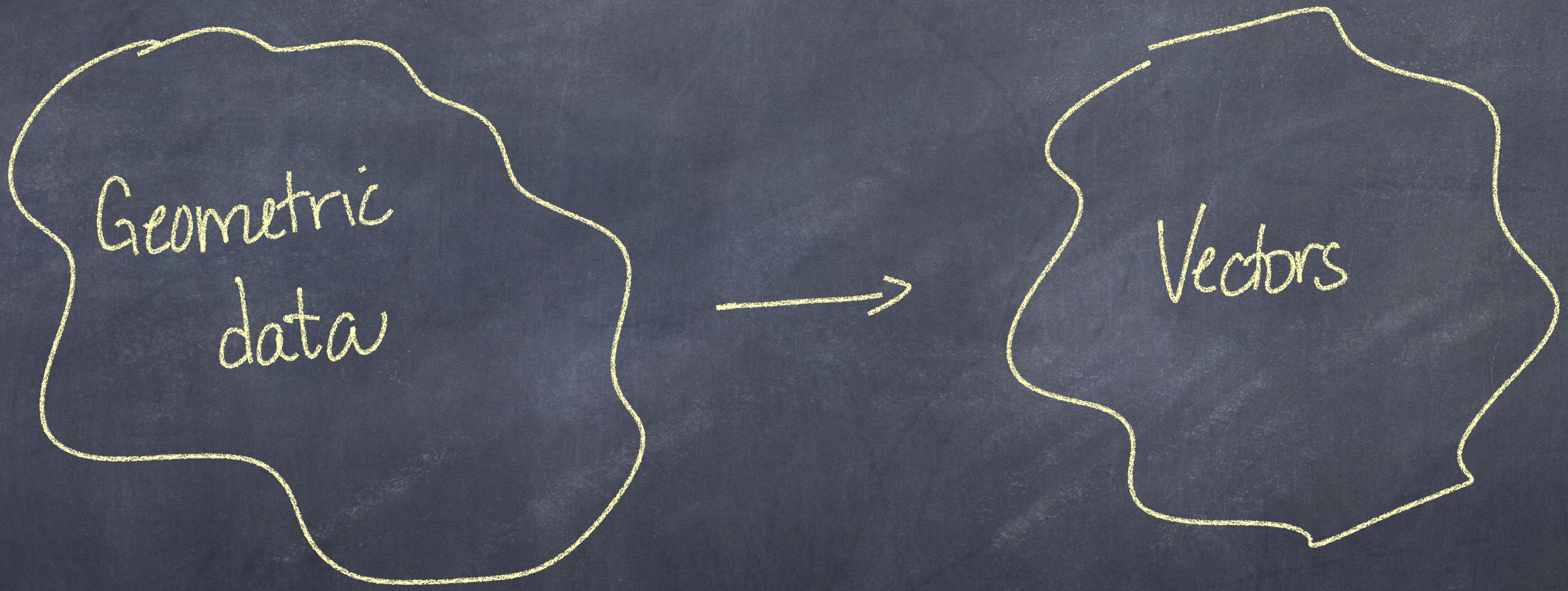
Maggs - Hacker - Rieck

ICLR 2024

Representation learning



Geometric representation learning



Simplicial representation learning

Embeddings of simplicial complexes into $\mathbb{R}^n$ $\longrightarrow$ Vectors in $\mathbb{R}^m$

From k-forms to simplicial representations

Let $\omega_1, \dots, \omega_m \in \Omega^k(\mathbb{R}^n)$.

Embeddings of simplicial complexes into $\mathbb{R}^n$ $\longrightarrow$ Vectors in $\mathbb{R}^m$

Slogan: k-forms are feature maps on the space of embedded k-simplices.

$$\Delta^k \xrightarrow{\varphi} \mathbb{R}^n \longmapsto \left(\int_{\Delta^k} \varphi^* \omega_1, \dots, \int_{\Delta^k} \varphi^* \omega_m \right)$$

Making it learnable

Recall: $\Omega^*(\mathbb{R}^n) = C^\infty(\mathbb{R}^n) \otimes \Lambda(dx_1, \dots, dx_n)$

- not appropriate for learning

Making it learnable

Recall: $\Omega^*(\mathbb{R}^n) = C^\infty(\mathbb{R}^n) \otimes \Lambda(dx_1, \dots, dx_n)$

- not appropriate for learning

The fix: $\Omega^*_{neu}(\mathbb{R}^n) = \mathrm{MLP}(\mathbb{R}^n) \otimes \Lambda(dx_1, \dots, dx_n)$

- neural k-forms

Neural k-forms generalize MLP's

Object	$f \in \mathrm{MLP}(\mathbb{R}^n)$	
Input	$* \xrightarrow{v} \mathbb{R}^n$	
Output	$f(v) \in \mathbb{R}$	

Neural k-forms generalize MLP's

Object	$f \in MLP(\mathbb{R}^n)$	$\omega \in \Omega^k_{neur}(\mathbb{R}^n)$
Input	$* \xrightarrow{v} \mathbb{R}^n$	$\Delta^k \xrightarrow{\varphi} \mathbb{R}^n$
Output	$f(v) \in \mathbb{R}$	$\int_{\Delta^k} \varphi^* \omega \in \mathbb{R}$

Universal Approximation Theorem [M-H-R, 24]

Compactly supported k-forms on $\mathbb{R}^n$ can be arbitrarily well approximated by neural k-forms with coefficients in MLP's with one hidden layer.

Architecture

simplicial complex

affine embedding

m_α - tuple of data k-chains

index set

- Input: $(\vec{\mathscr{I}}, \vec{\beta}) = \{ (\mathcal{K} \xrightarrow{\mathscr{I}_t} \mathbb{R}^n, \ \beta_t \in C_k(\mathcal{K}_\alpha)^{\oplus m_t}) \mid t \in T \}$

Architecture

- Input: $(\vec{\varphi}, \vec{\beta}) = \{ (\mathcal{K} \xrightarrow{\varphi_t} \mathbb{R}^n, \ \beta_t \in C_k(\mathcal{K}_\alpha)^{\oplus m_t}) \mid t \in T \}$

- Initiation: $\vec{\omega} = (\omega_1, \dots, \omega_\ell) \in \Omega^k_{\mathrm{nuur}}(\mathbb{R}^n)^{\oplus \ell}$

$\Rightarrow$ matrices $M^t_{\vec{\varphi}, \vec{\beta}}(\vec{\omega}) \in \mathbb{R}^{m_t, \ell}$

$$\left(M^t_{\vec{\varphi}, \vec{\beta}}(\vec{\omega}) \right)_{i,j} = \int_{\beta_{t,i}} \varphi_t^* (\omega_j)$$

admits finite approx., appropriatly differentiable

Architecture

- Input: $(\vec{\varphi},\vec{\beta}) = \{(\mathcal{K} \xrightarrow{\varphi_t} \mathbb{R}^n,\ \beta_t \in C_k(\mathcal{K}_\alpha)^{\oplus m_t}) \mid t \in T\}$

- Initiation: $\vec{\omega} = (\omega_1, \dots, \omega_\ell) \in \Omega^k_{\text{nuw}}(\mathbb{R}^n)^{\oplus \ell}$

  $\Rightarrow$ matrices $M^t_{\vec{\varphi},\vec{\beta}}(\vec{\omega}) \in \mathbb{R}^{m_t,\ell}$

- Readout: $\Psi : \mathbb{R}^{m_t,\ell} \longrightarrow \mathbb{R}^\ell$ (Ex: summing columns, taking norms of columns..)

Architecture

- **Input**: $(\vec{\varphi}, \vec{\beta}) = \{ (\mathcal{K} \xrightarrow{\varphi_t} \mathbb{R}^n,\ \beta_t \in C_k(\mathcal{K}_\alpha)^{\oplus m_t}) \mid t \in T \}$
- **Initiation**: $\vec{\omega} = (\omega_1, \ldots, \omega_\ell) \in \Omega^k_{\text{neur}}(\mathbb{R}^n)^{\oplus \ell}$

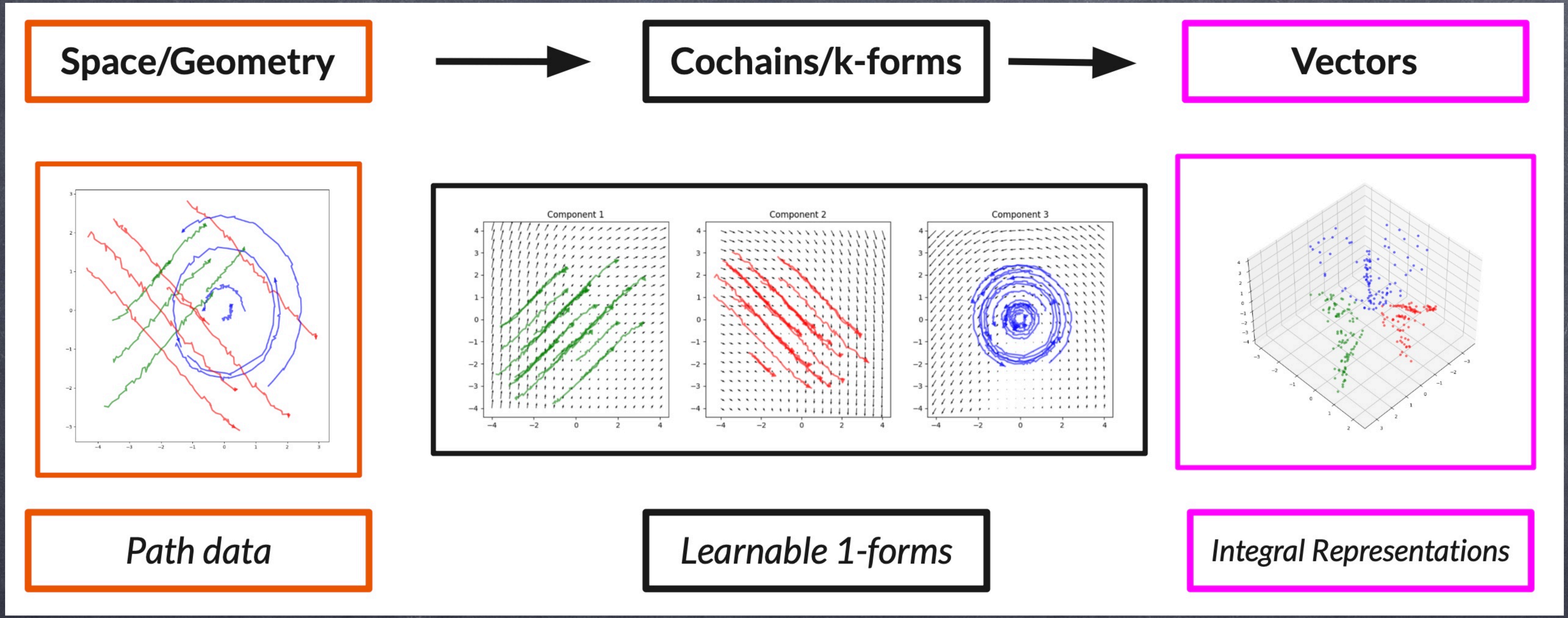
  $\Rightarrow$ matrices $M^t_{\vec{\varphi}, \vec{\beta}}(\vec{\omega}) \in \mathbb{R}^{m_t, \ell}$
- **Readout**: $\Psi : \mathbb{R}^{m_t, \ell} \longrightarrow \mathbb{R}^\ell$
- Classify and evaluate against a loss function

Remarks

① Realizable by any deep learning framework appropriate for training MLP's.

② No message passing involved.

Experiment ①



Objective function: maximize path integrals within classes, minimize else

Experiment ②

AUROC ± std. deviation of 5 runs

	Params.	BACE	BBBP	HIV
GAT [Vel+18]	135K	69.52 ± 17.52	76.51 ± 3.36	56.38 ± 4.41
GCN [KW17]	133K	66.79 ± 1.56	73.77 ± 3.30	68.70 ± 1.67
GIN [Xu+19]	282K	42.91 ± 18.56	61.66 ± 19.47	55.28 ± 17.49
NkF (ours)	9K	**83.50 ± 0.55**	**86.41 ± 3.64**	**76.70 ± 2.17**

Benchmark datasets from the MoleculeNet database, reporting only best results for GNNs.

Cochains in computational biology

Maggs-Youssef-Nguyen-Pulver

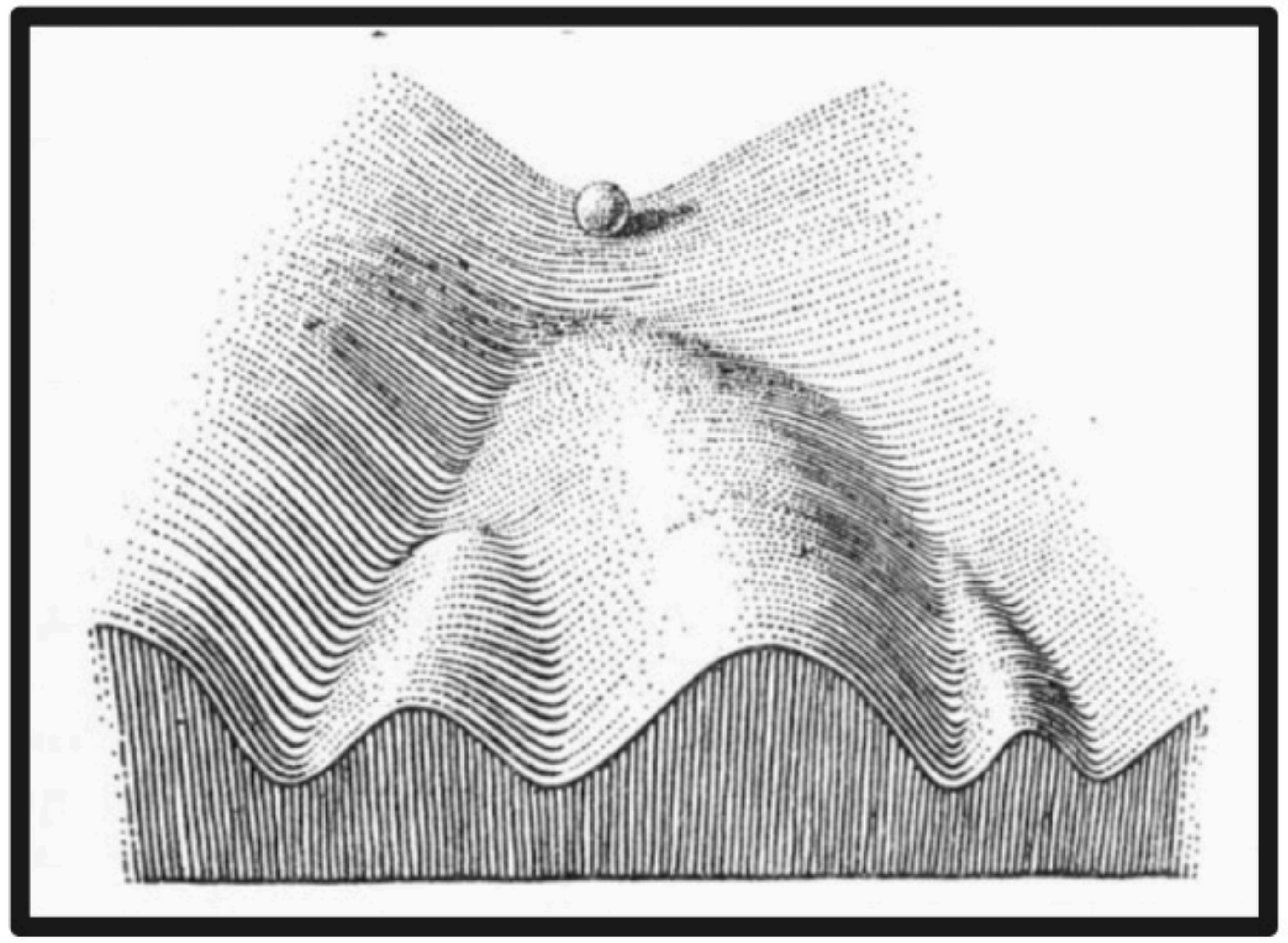
In progress

The geometry of biology

Space/Geometry

Biology

Gradient Descent



Cell Development

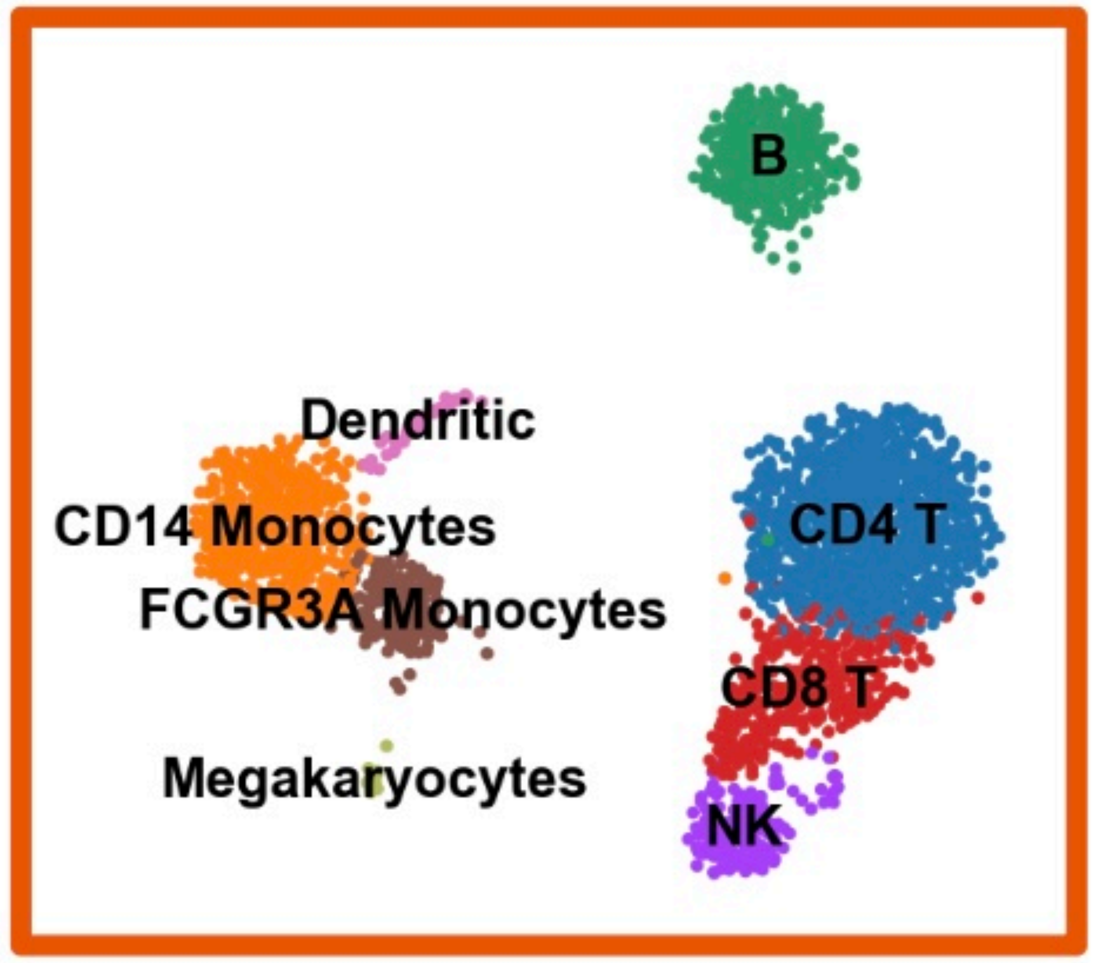
The Epigenetic Landscape

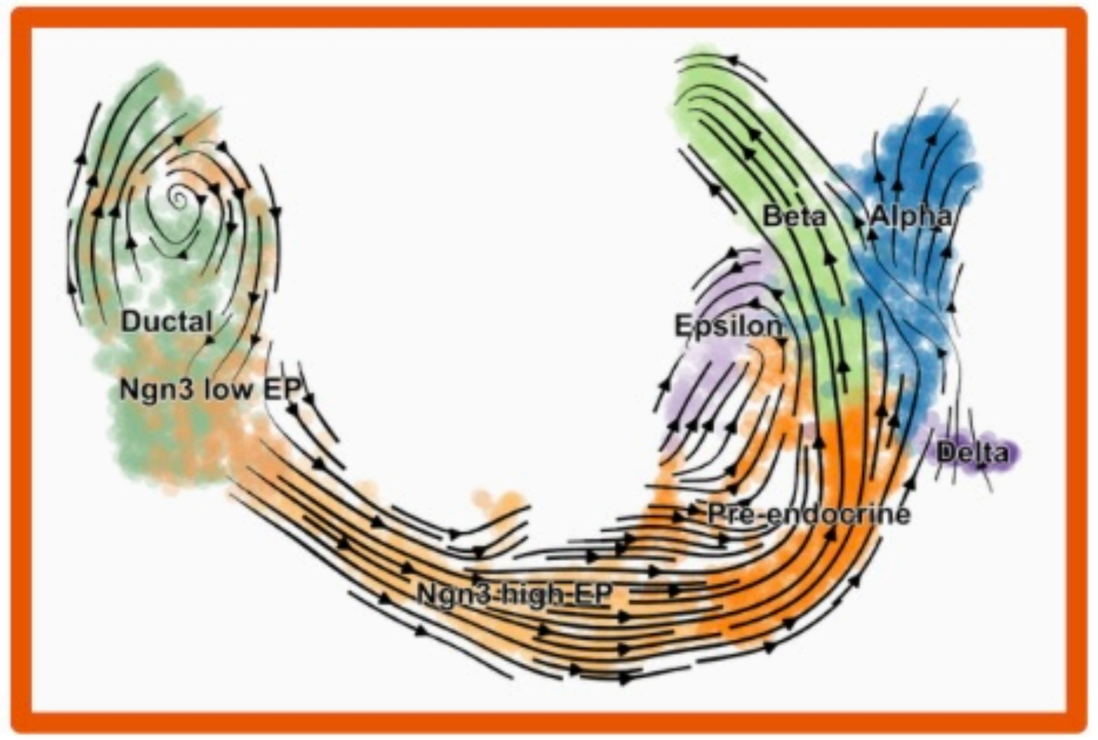
C.H. Waddington. *The Strategy of the Genes.* Routledge. (1957)

The phase space of single-cell data

Space/Geometry

Gene x Cell Matrix

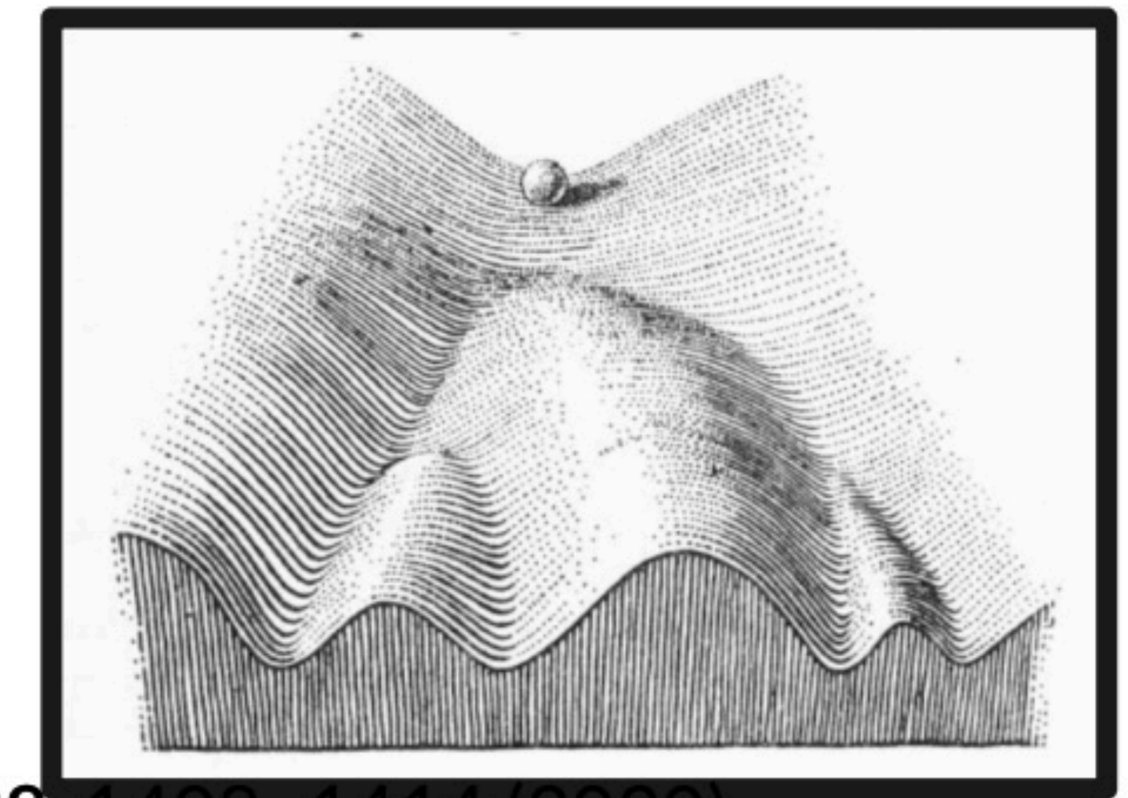




Cell Type

Differentiation

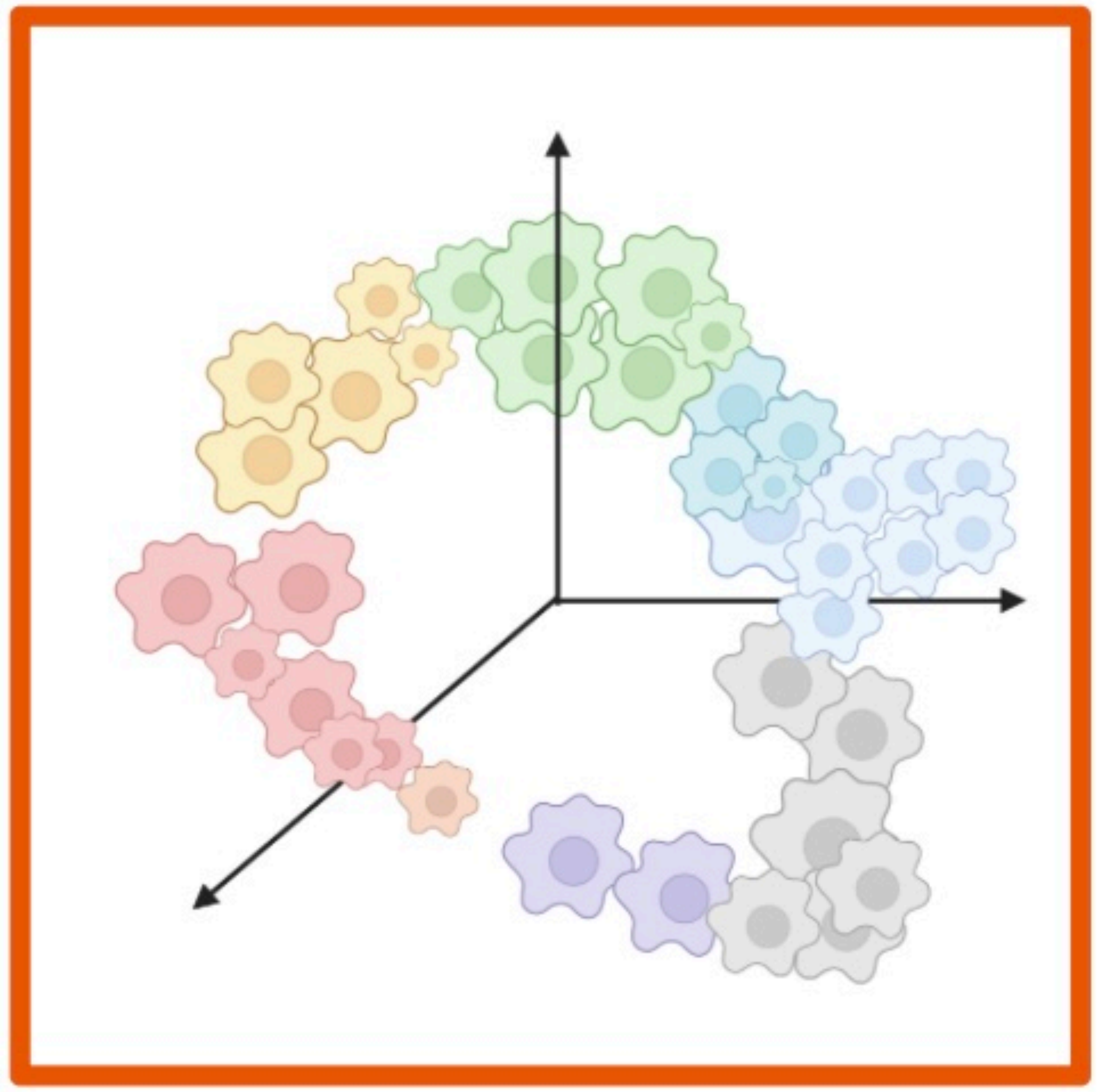
Biology



Bergen, V *et al*. Generalizing RNA velocity to transient cell states through dynamical modeling. *Nat Biotechnol* **38**, 1408–1414 (2020).

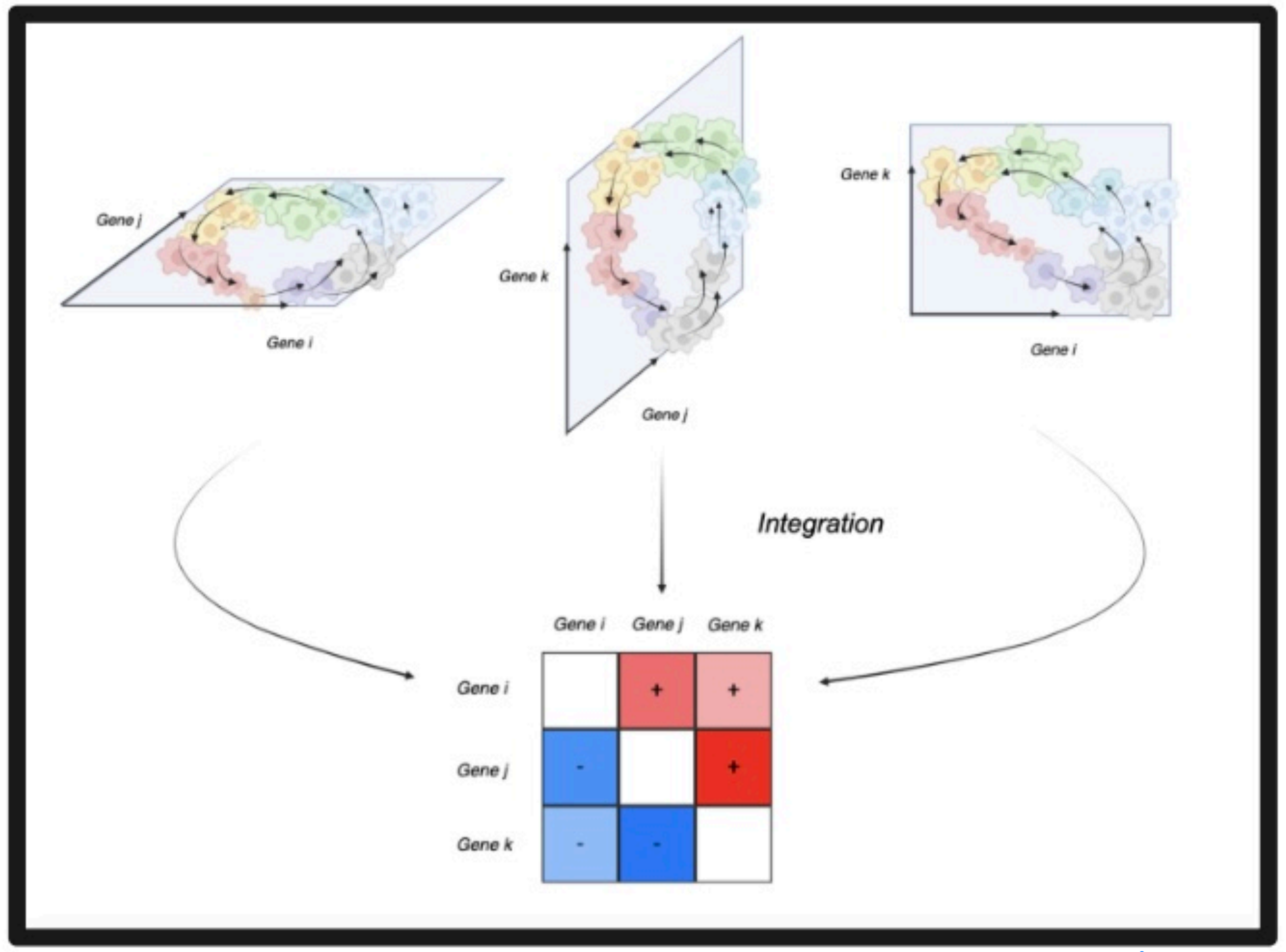
From circular structure to gene cascades

Space/Geometry → **Cochains/k-forms** → **Biology**



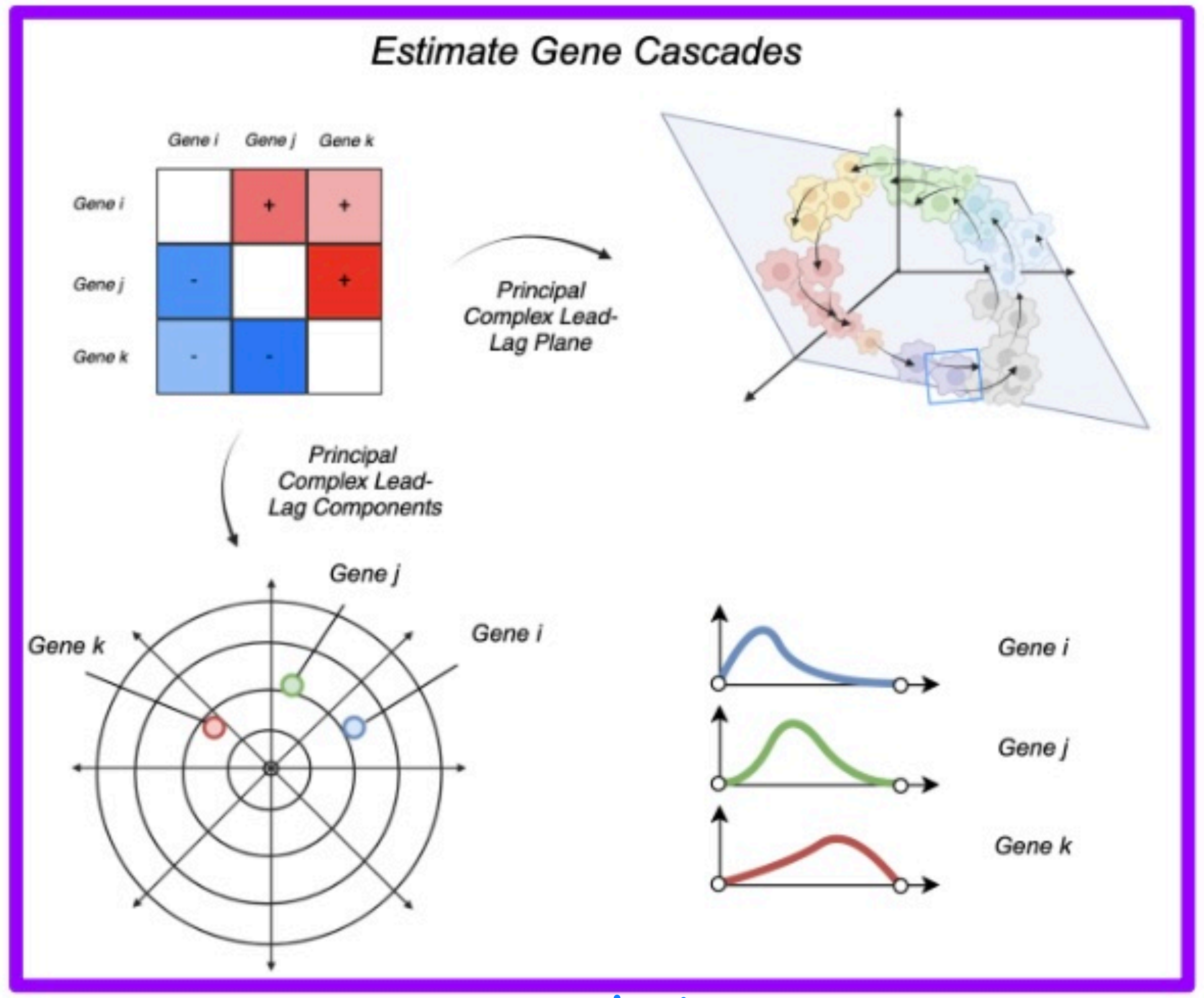
Persistent cohomology

Structural: cohomology class



Discrete Hodge theory + simplicial cyclicity analysis

Dynamical



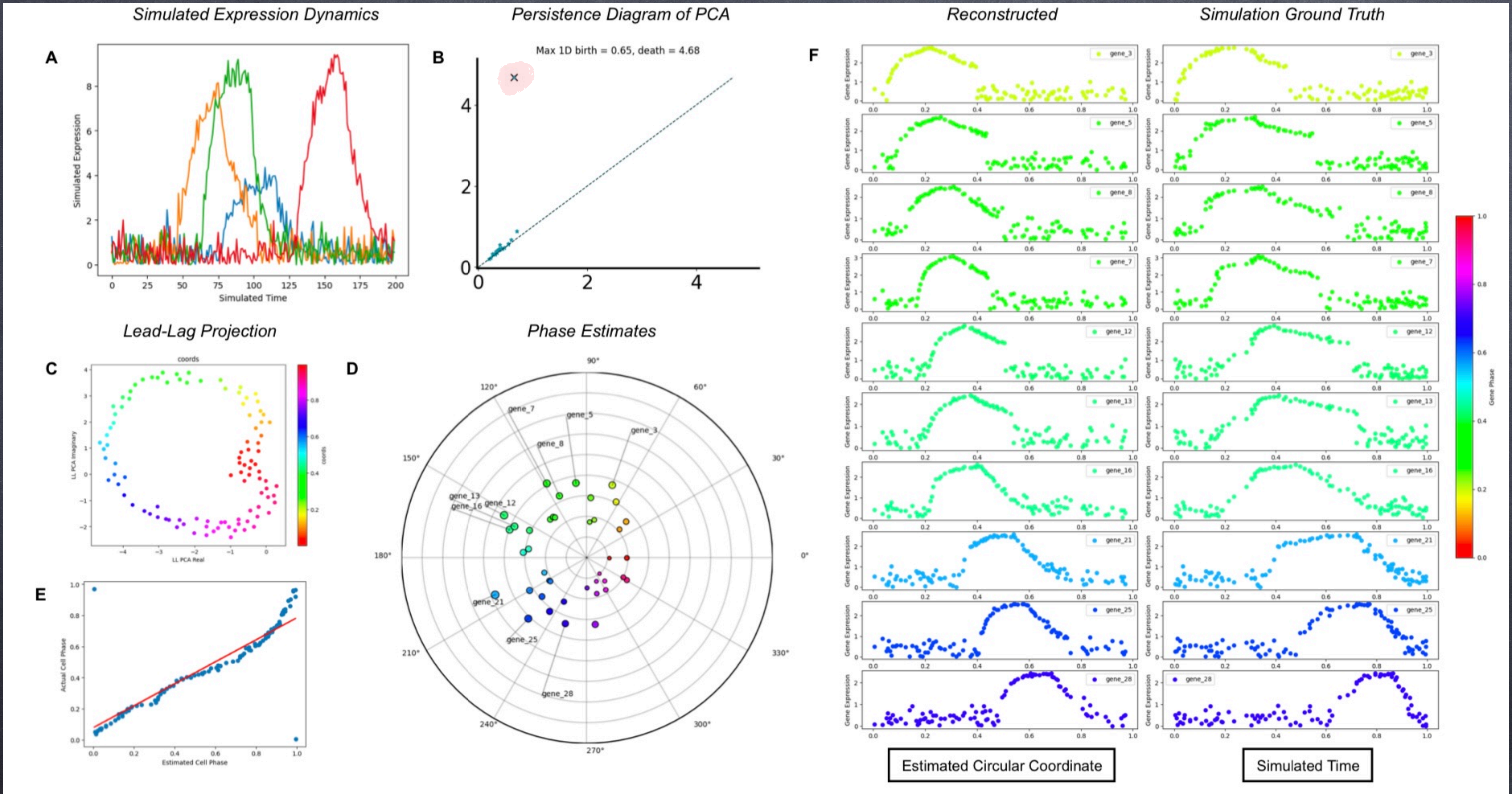
Interpretation

Estimate gene cascades

The pipeline

The pipeline

Testing the pipeline (synthetic data)



Thank you!