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Analysis of Populations of Networks:

Graph Spaces and the Computation of Summary Statistics.

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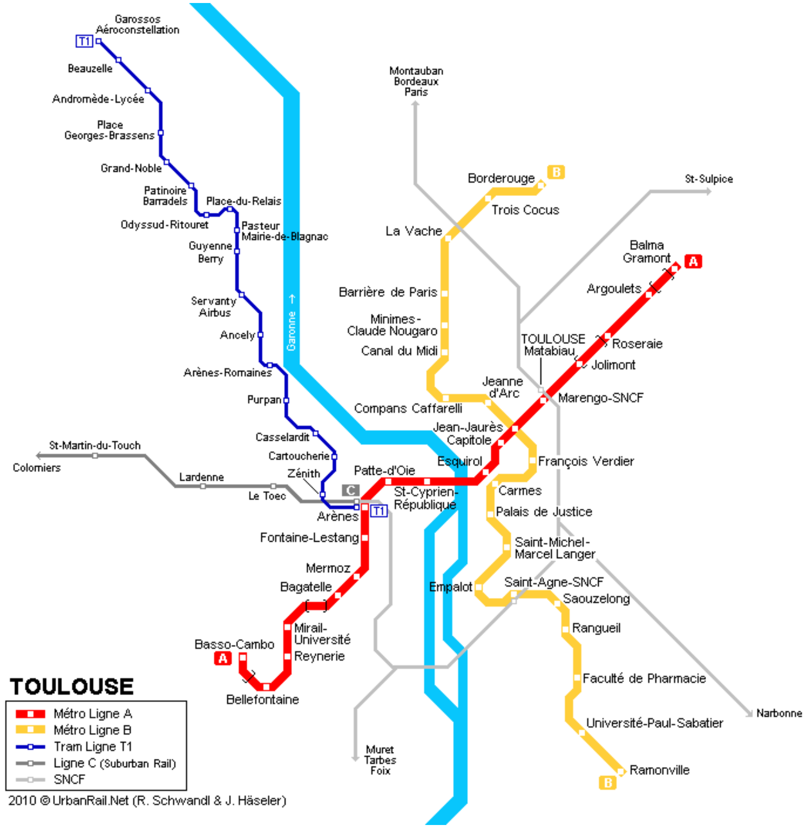
Object Oriented Data Analysis: Population of Networks

Structure Spaces: Graph Space as a particular case

Summary Statistics: Mean and Geodesic PCA

Population of Networks

Network Analysis



Datum:
Nodes and Edges

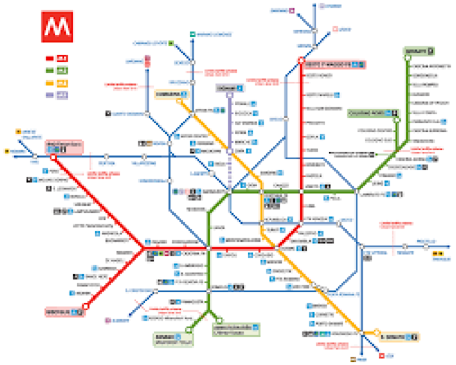
Analysis focusing on:
Features: nodes and edge attributes

Relations: how nodes influence each other

«1° Generation Approach»

Marron, J. Steve, and Andrés M. Alonso. "Overview of object oriented data analysis." *Biometrical Journal* 56.5 (2014): 732-753.

Network Analysis: from one to many

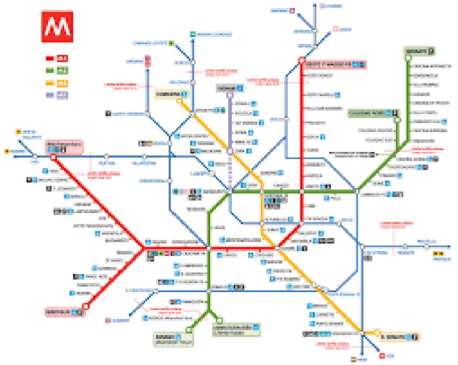


Objects are Networks $X_1, X_2, \ldots$

«2° Generation Approach»

Marron, J. Steve, and Andrés M. Alonso. "Overview of object oriented data analysis." *Biometrical Journal* 56.5 (2014): 732-753.

Network Analysis: from one to many



Many new questions arise:

- How can we describe these networks?
- How can we relate nodes in networks?
- Along which relations/features are different?
- Can we do any statistical analysis and how?

OODA for Networks

OODA for Networks: State of the Art

OODA for trees Wang and Marron (2007), Aydın, et al. (2009), Feragen et al. (2013), Nye, et al. (2017),

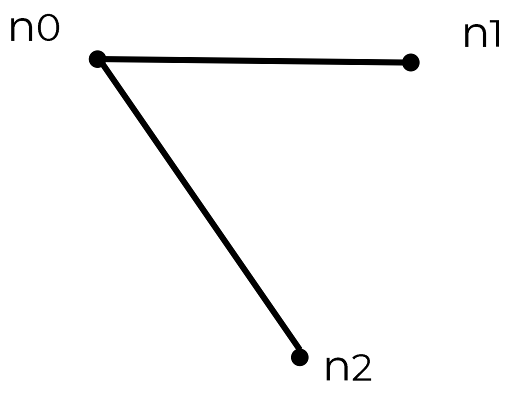
Hypothesis Testing Simpson, et al. (2013), Ginestet, et al. (2017), Lovato, et al. (2017)

Bayesian Generative Models Durante et al. (2017), Durante and Dunson (2018)

Graph Embedding Duvenaud et al. (2015)

Structure Spaces Jain et al. (2009)

Structure Spaces



A-attributed R-structure: $x = (P, R, \alpha)$

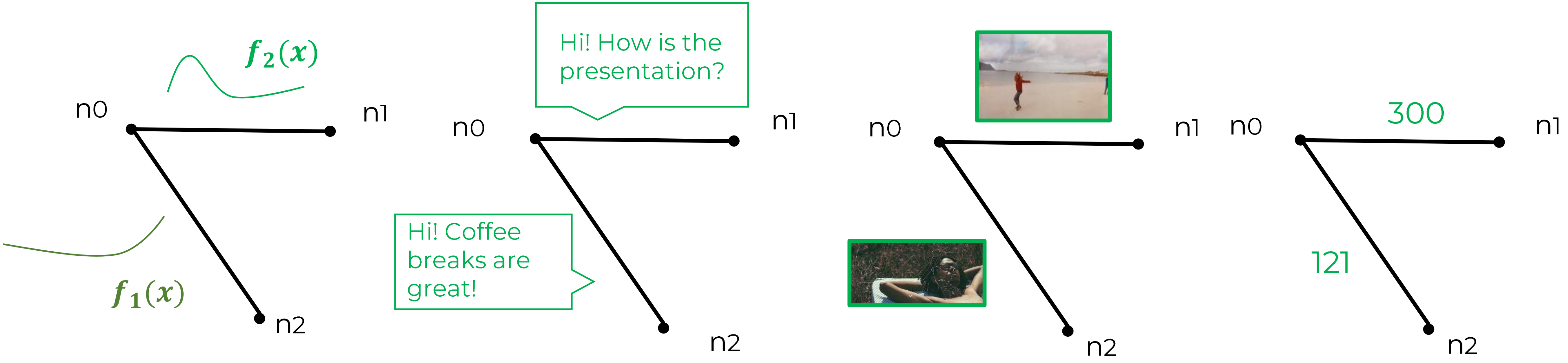
P- set of nodes

$R \in P^r$ - set of relations (edges if r=2).

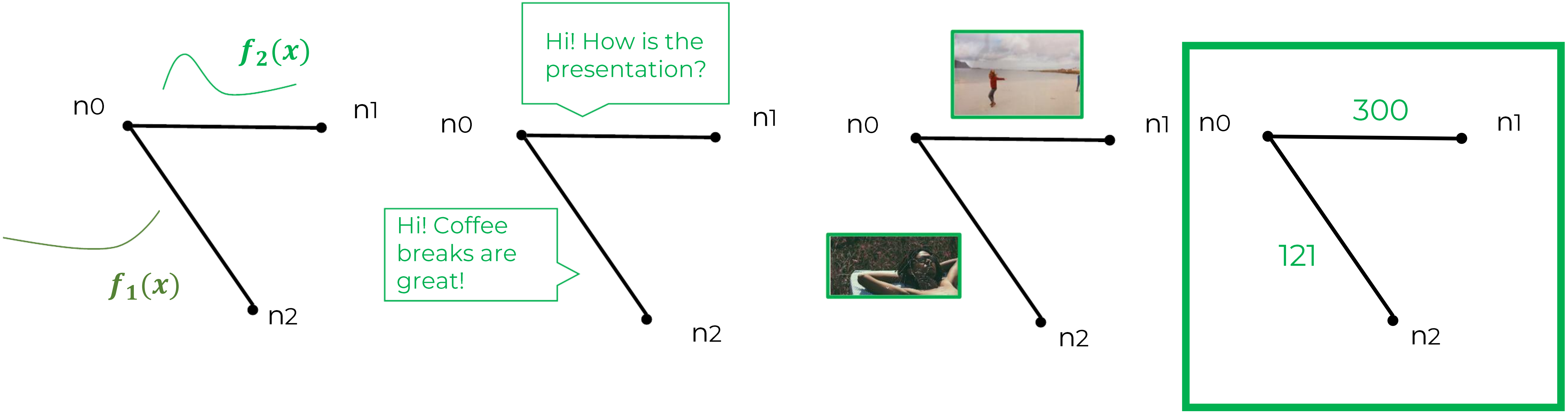
$\alpha: R \rightarrow M$ - function assigning attributes to edges

Jain, Brijnesh J., and Klaus Obermayer. "Structure spaces." *Journal of Machine Learning Research* 10.Nov (2009): 2667-2714.

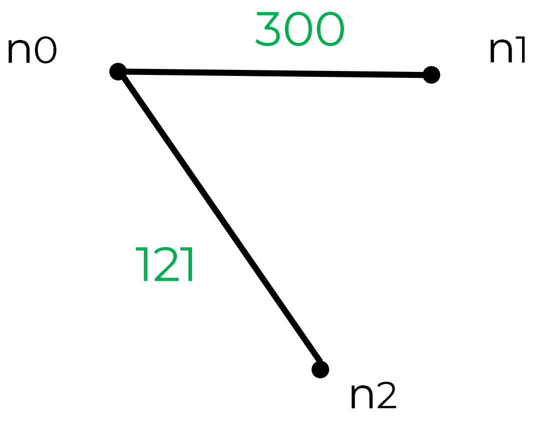
Structure Spaces



Structure Spaces



Graph Spaces



A-attributed R-structure: $\mathrm{x} = (P, R, \alpha)$

$\mathrm{P}=\{0,1,2\}$- set of nodes

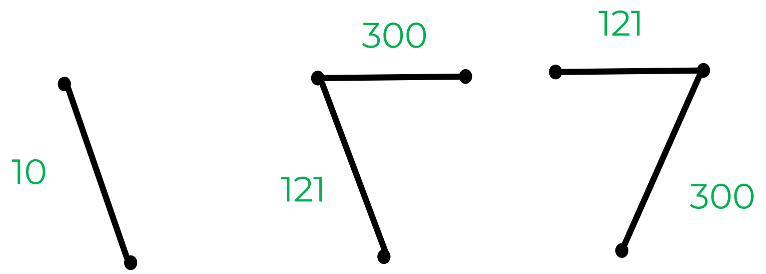
$R \in P^2, R = \{(0,1), (0,2)\}$ - set of relations

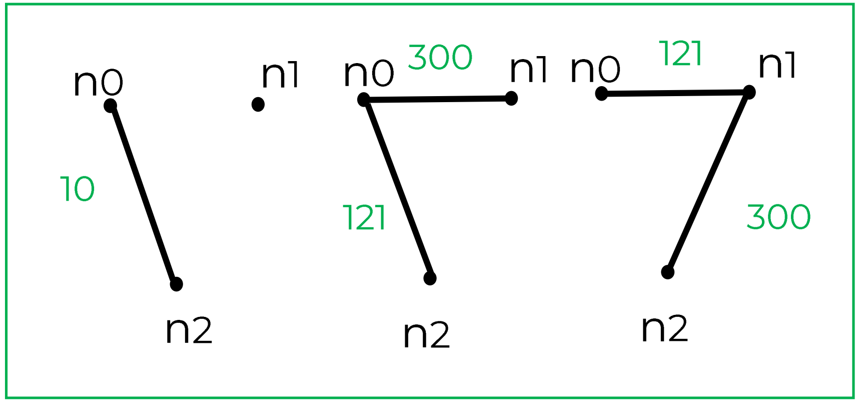
$\alpha\colon \mathrm{R} \rightarrow \mathbb{R}$ - weights

$\alpha\big((0,1)\big) = 300$

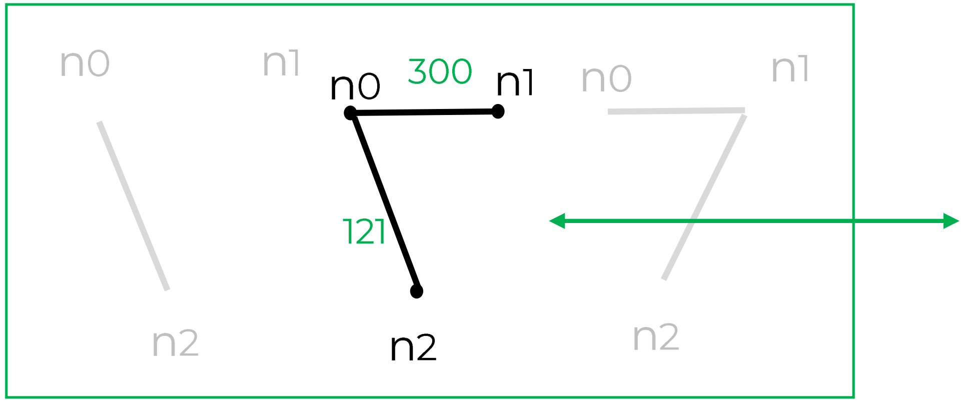
$\alpha\big((0,2)\big) = 121$

Graph Spaces





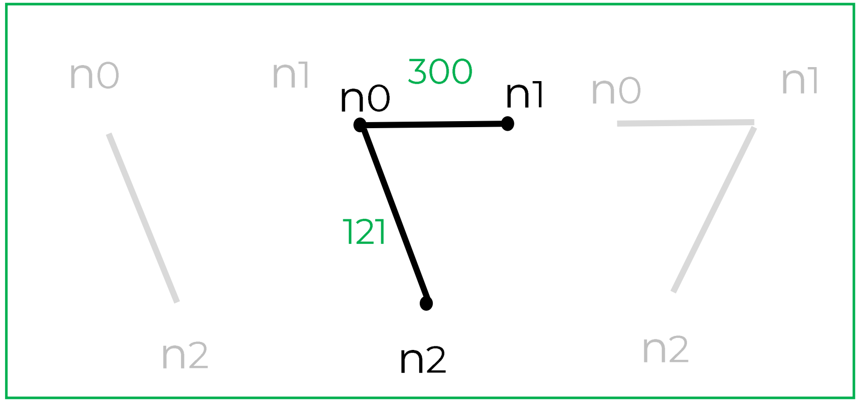
Graph Spaces



n0	300	121
300	n1	0
121	0	n2

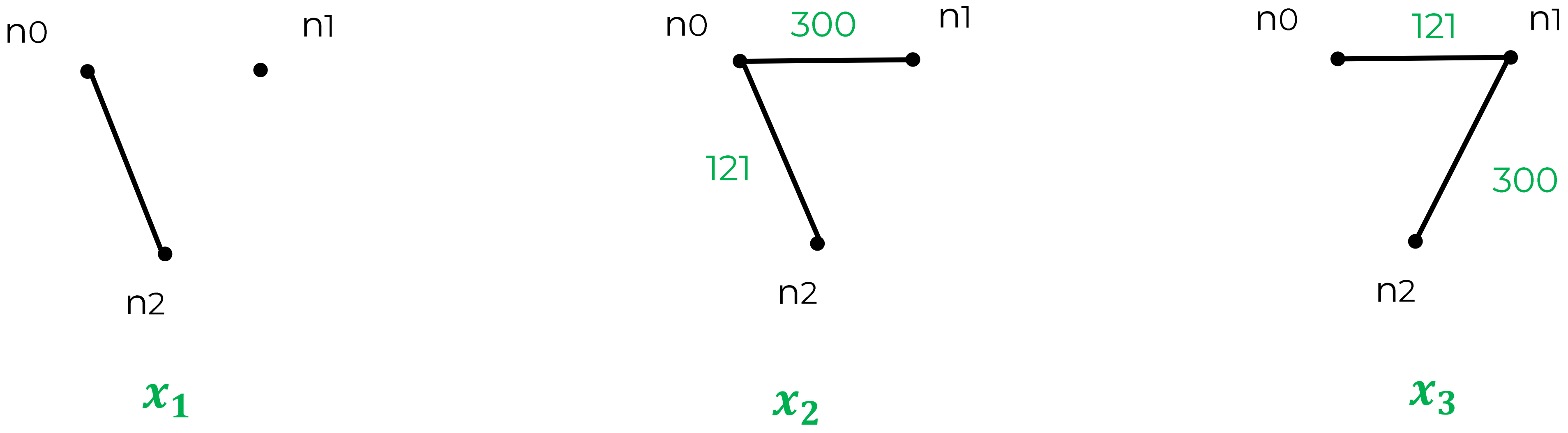
n0	300	121	300	n1	0	121	0	n2

Graph Spaces

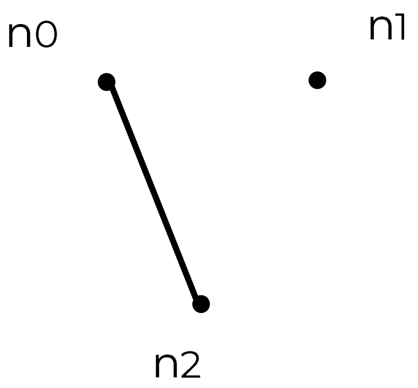


Space: $\mathbf{X} = \mathbb{R}^9$

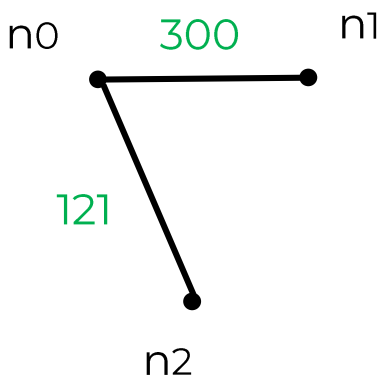
Graph Spaces



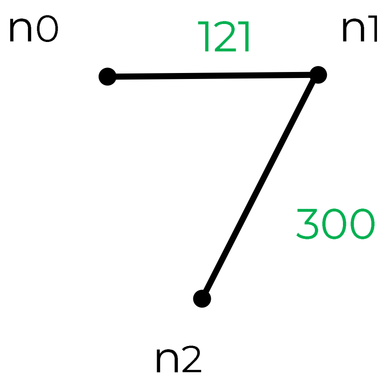
Graph Spaces



x_1



x_2

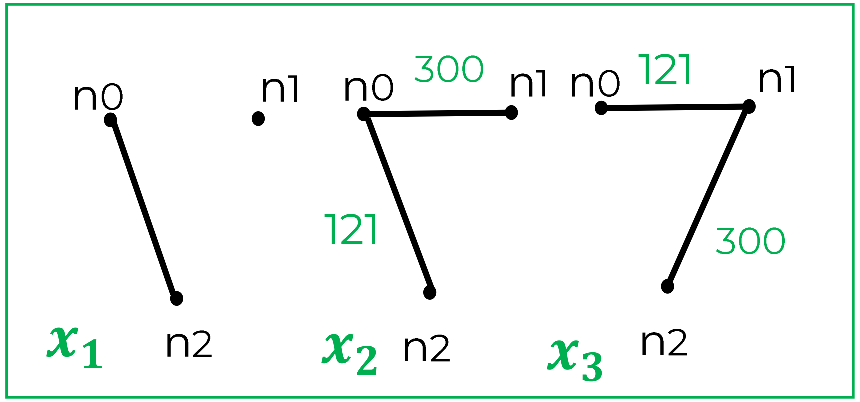


x_3

$x_2 = x_3$

Allowing permutation of nodes

Graph Spaces



$$\lfloor x_1 \rfloor = \{T x_1 : T \in \mathcal{T}\}$$

$$\lfloor x_2 \rfloor = \{T x_2 : T \in \mathcal{T}\}$$

Space: X

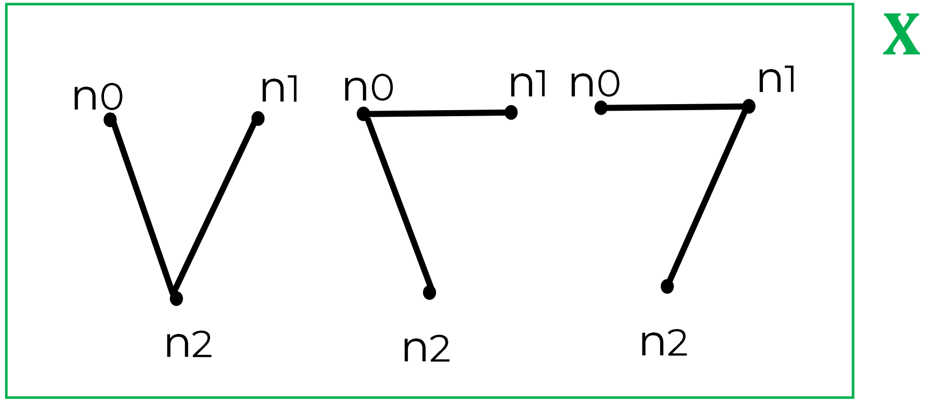
$\mathcal{T}$: **Permutation Action**

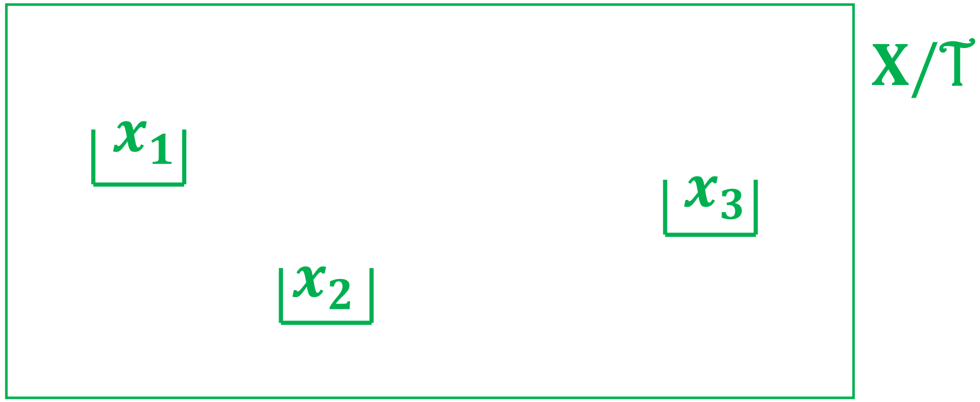
Permuting nodes

Graph Space: $X/\mathcal{T}$

Graph Space Properties

Metric Space

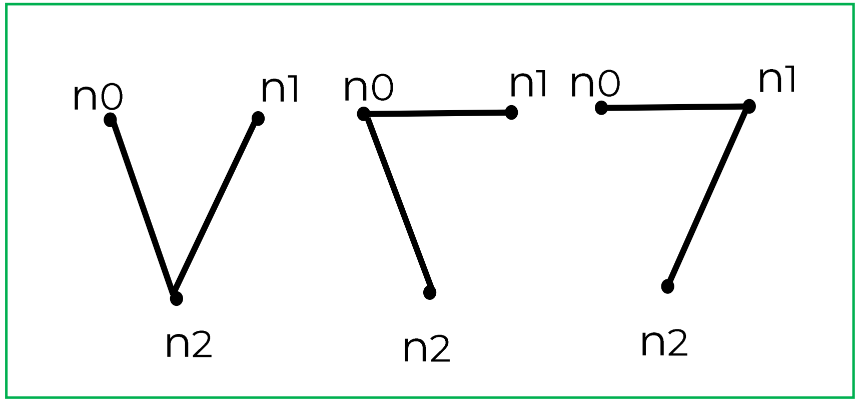




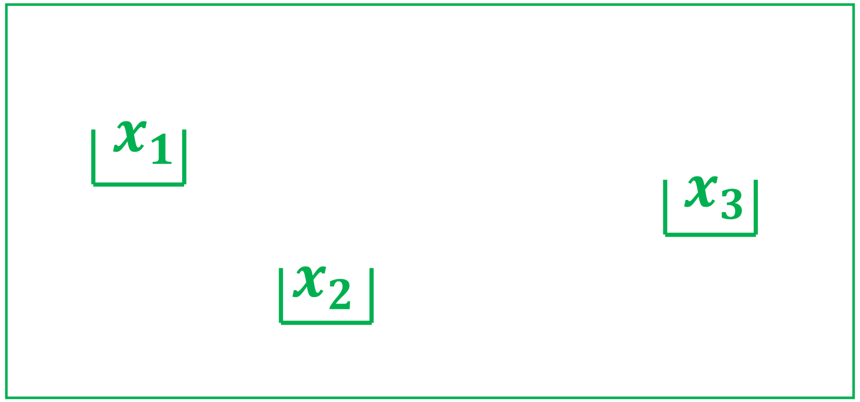
Metric Space
invariant with respect to permutation

Metric Space
Given two equivalent classes, find the permuted elements that have minimum distance

Geodesic Space



$\mathbf{X}$



$\mathbf{X}/\mathcal{T}$

Geodesic Space

Euclidean Space, complete, locally compact.

$\mathcal{T}$: **Finite Group Action**

Geodesic Space

Properties and Consequences

Not a Manifold (Not Free Action):

→ Can’t use all the literature about Manifold statistics

Unbounded:

→ No uniqueness of the geodesic even locally.

Isometric and Finite Dimension Action:

→ Allows to transfer easily computation from X to X/T

Properties and Consequences

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→ Can't all the literature about Manifold statistics

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Properties and Consequences

Isometric and Finite Dimension Action:

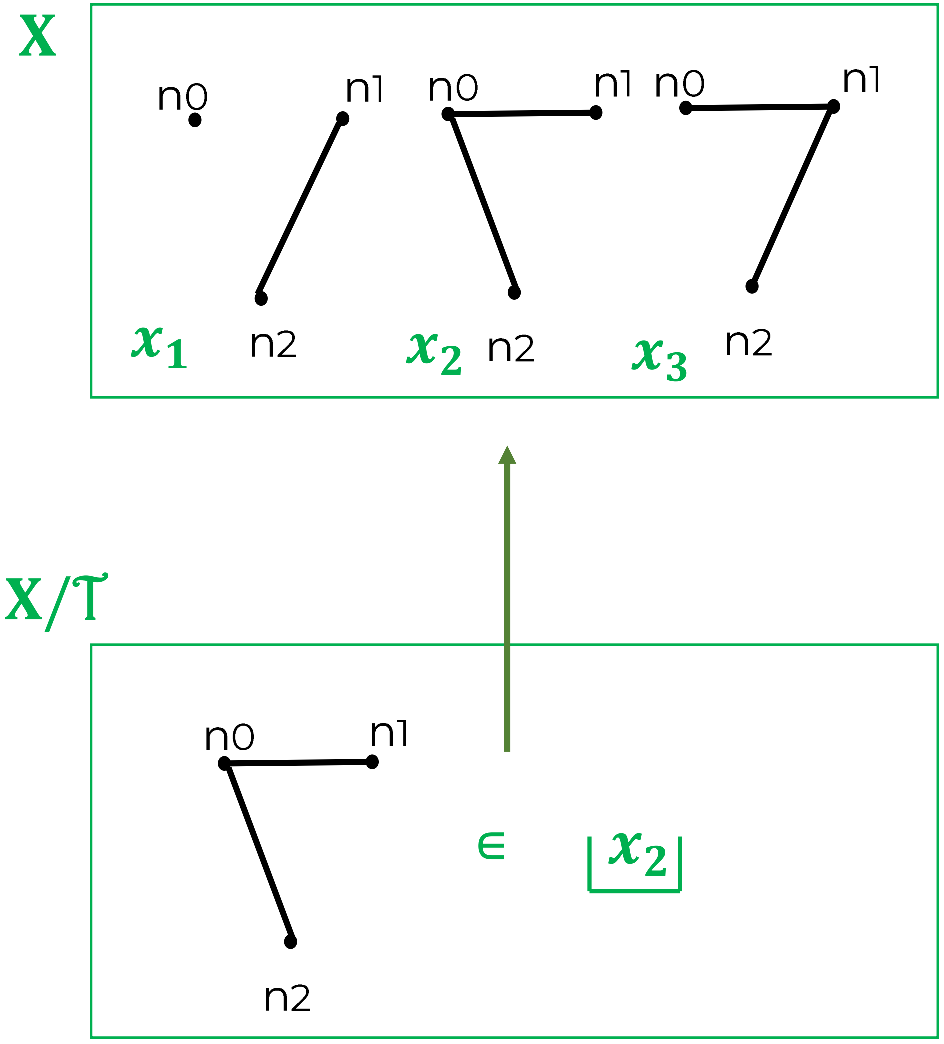
→ Allows to transfer easily computation from X to X/T

↓

Align All and Compute Algorithm to be able to compute statistics on this space.

Align All and Compute

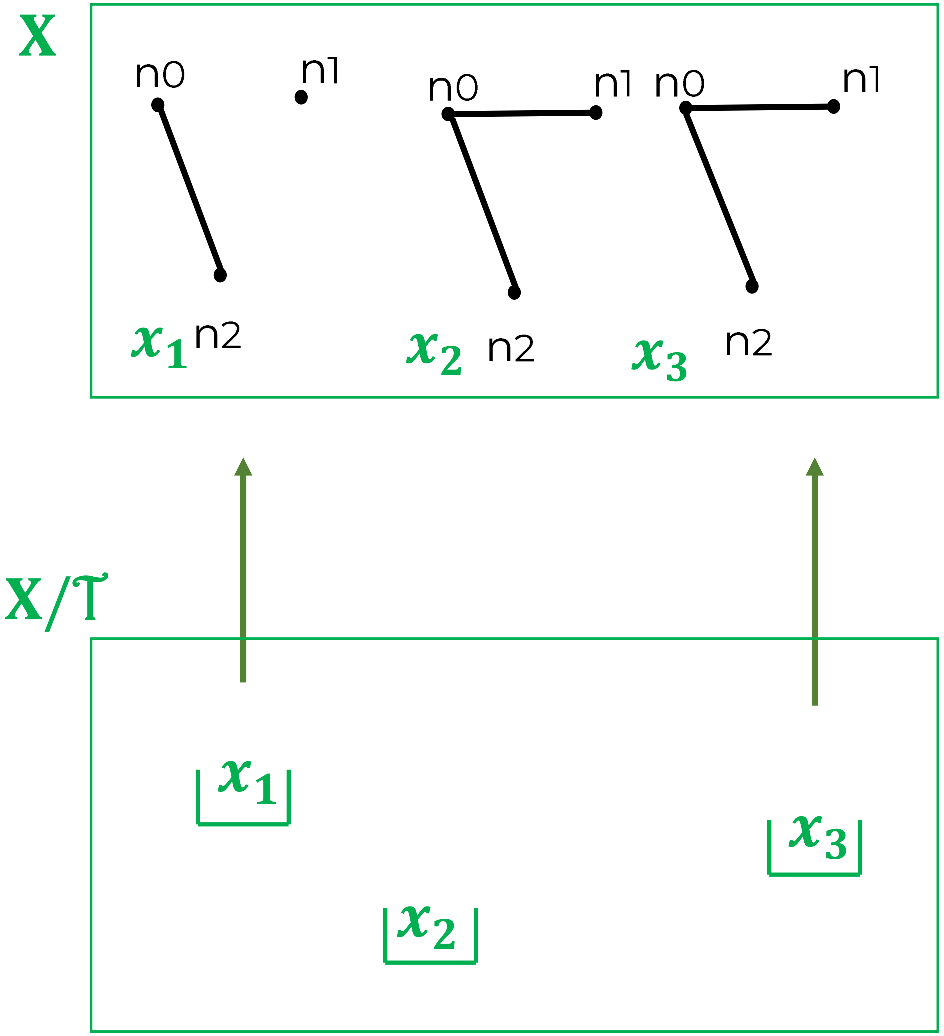
Align All and Compute



Based on the Generalized Procrustes Algorithm:

1) Select a random candidate point $\varkappa \in \lfloor x_2 \rfloor$ in **X/T**

Align All and Compute

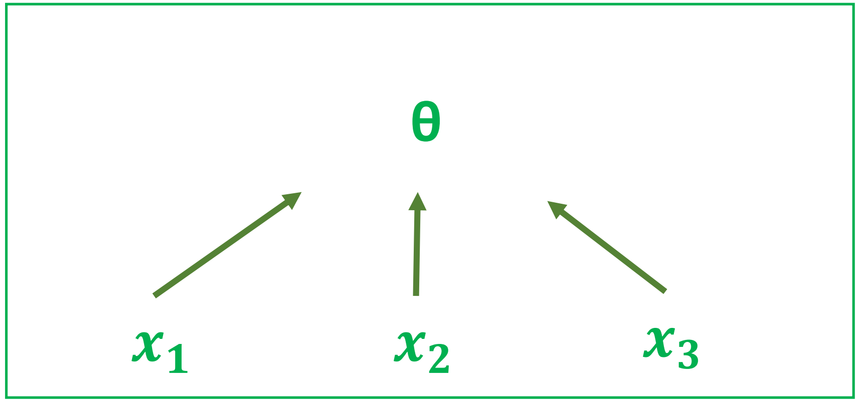


Based on the Generalized Procrustes Algorithm:

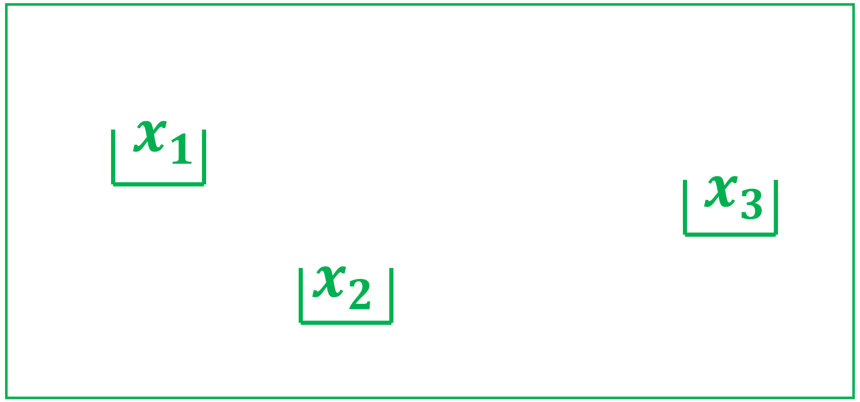
1) Select a random candidate point $\varkappa \in \lfloor x_2 \rfloor$ in $\mathbf{X/T}$
2) Align all the points to $\varkappa$ obtaining $x_1, x_2, \ldots, x_n$ in $\mathbf{X}$

Align All and Compute

X



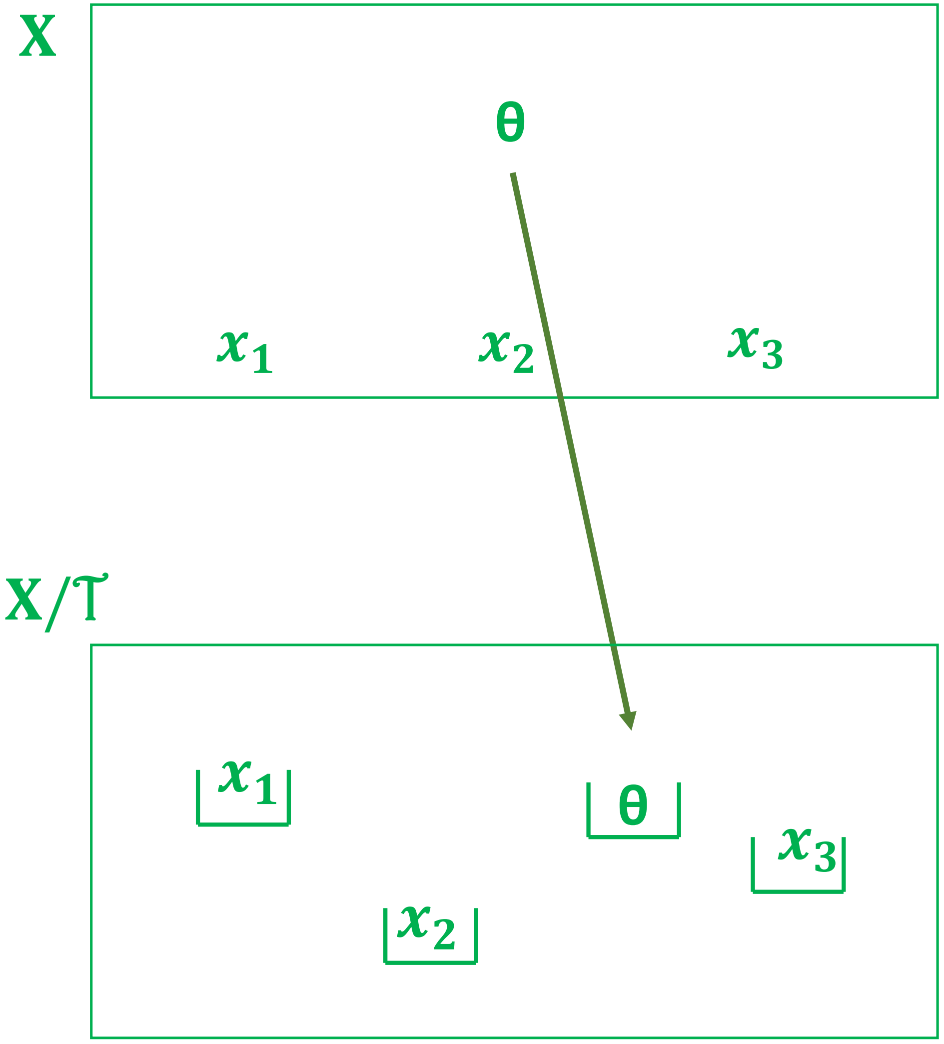
X/T



Based on the Generalized Procrustes Algorithm:

1) Select a random candidate point $\varkappa \in \lfloor x_2 \rfloor$ in **X/T**
2) Align all the points to $\varkappa$ obtaining $x_1, x_2, \ldots, x_n$ in **X**
3) Compute the Statistics θ in X

Align All and Compute



Based on the Generalized Procrustes Algorithm:

1) Select a random candidate point $\tilde{x} \in \lfloor x_2 \rfloor$ in $\mathbf{X/T}$
2) Align all the points to $\tilde{x}$ obtaining $x_1, x_2, \ldots, x_n$ in $\mathbf{X}$
3) Compute the Statistics θ in X
4) Set the $\varkappa = \theta$
5) Do 1 – 4 until the algorithm converge

AAC in Action

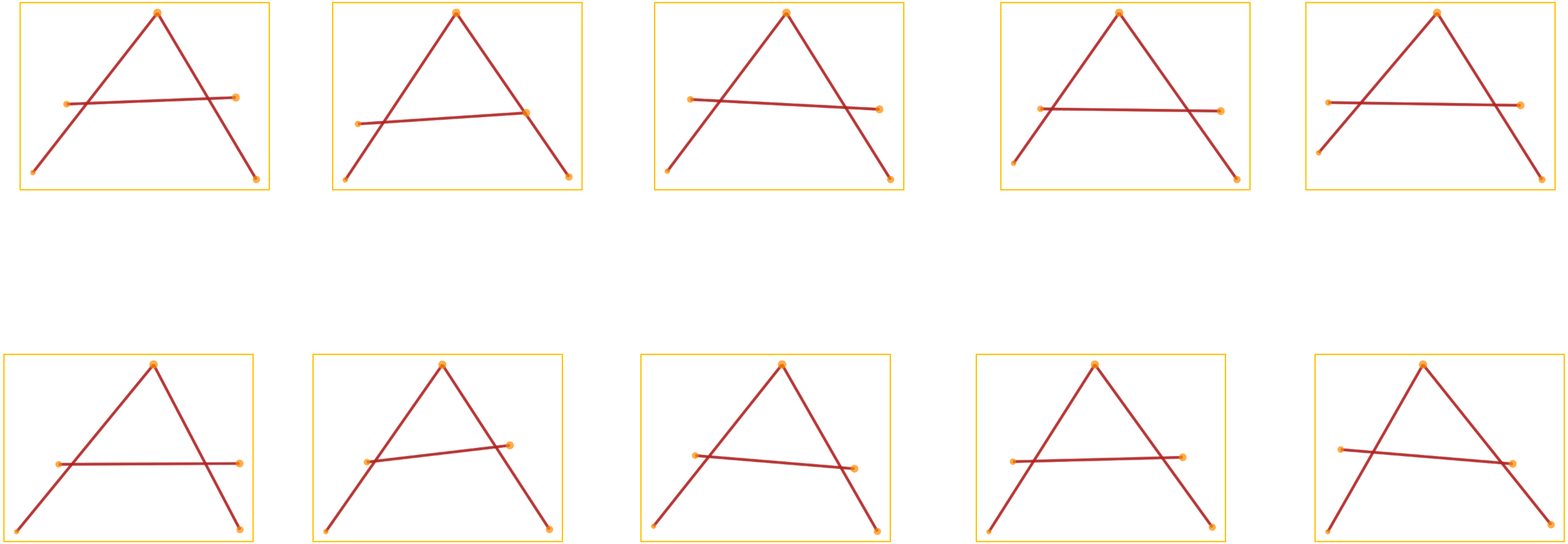
Align All and Compute Algorithm to be able to compute statistics on this space:

→ Fréchet Mean

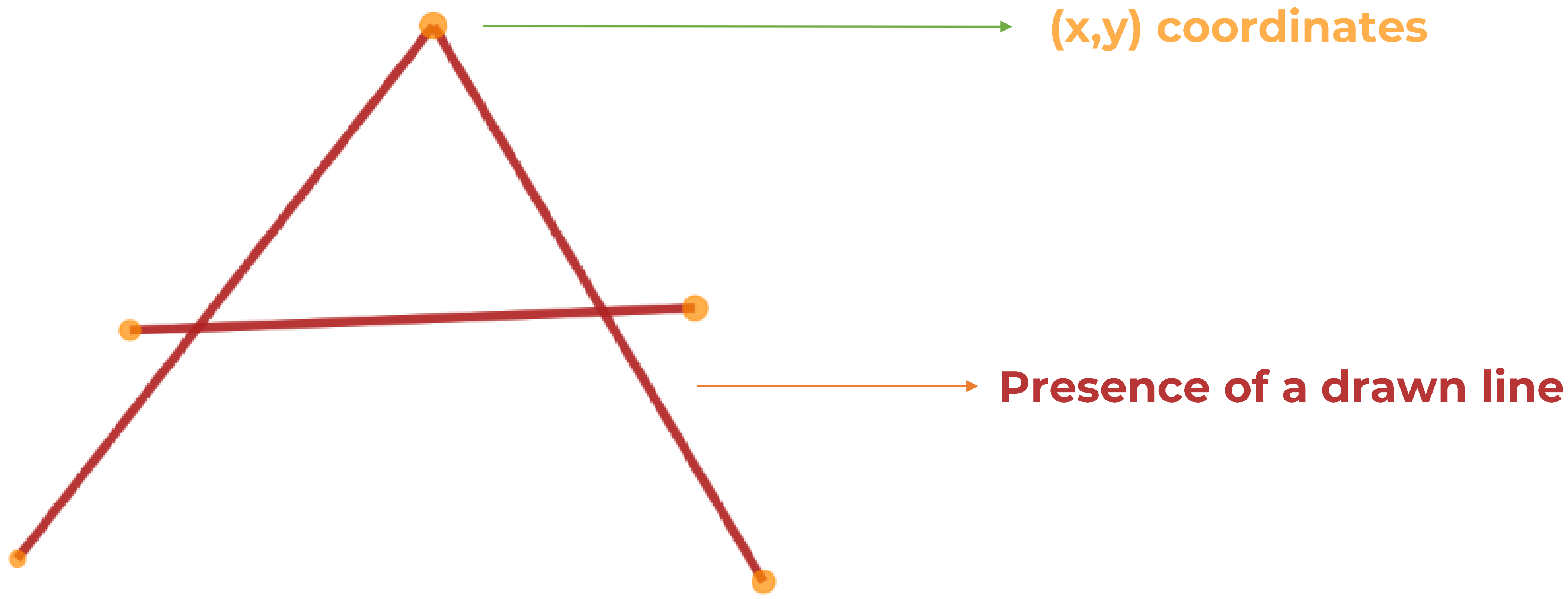
→ Geodesic Principal Components Analysis: following the framework introduced in Huckemann, Hotz, & Munk (2010)

Example

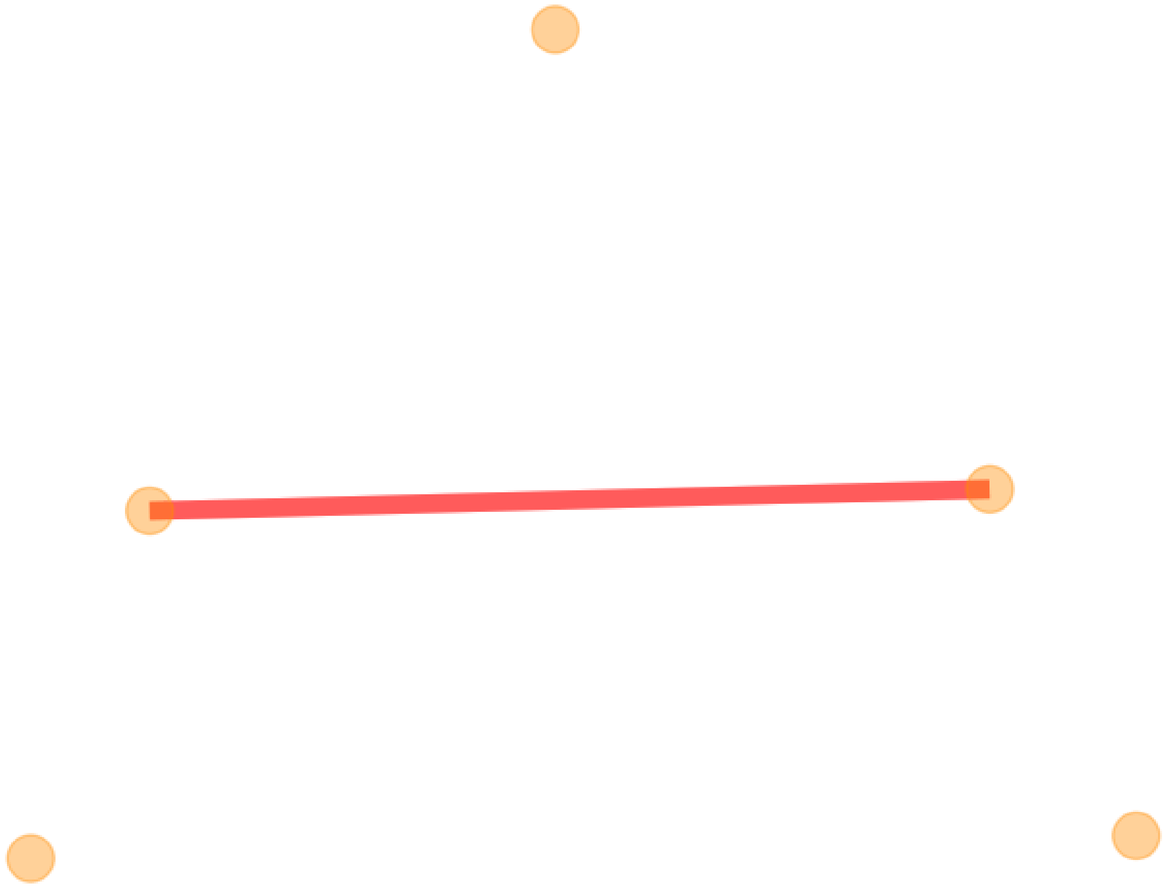
Example: Attributes and Topology



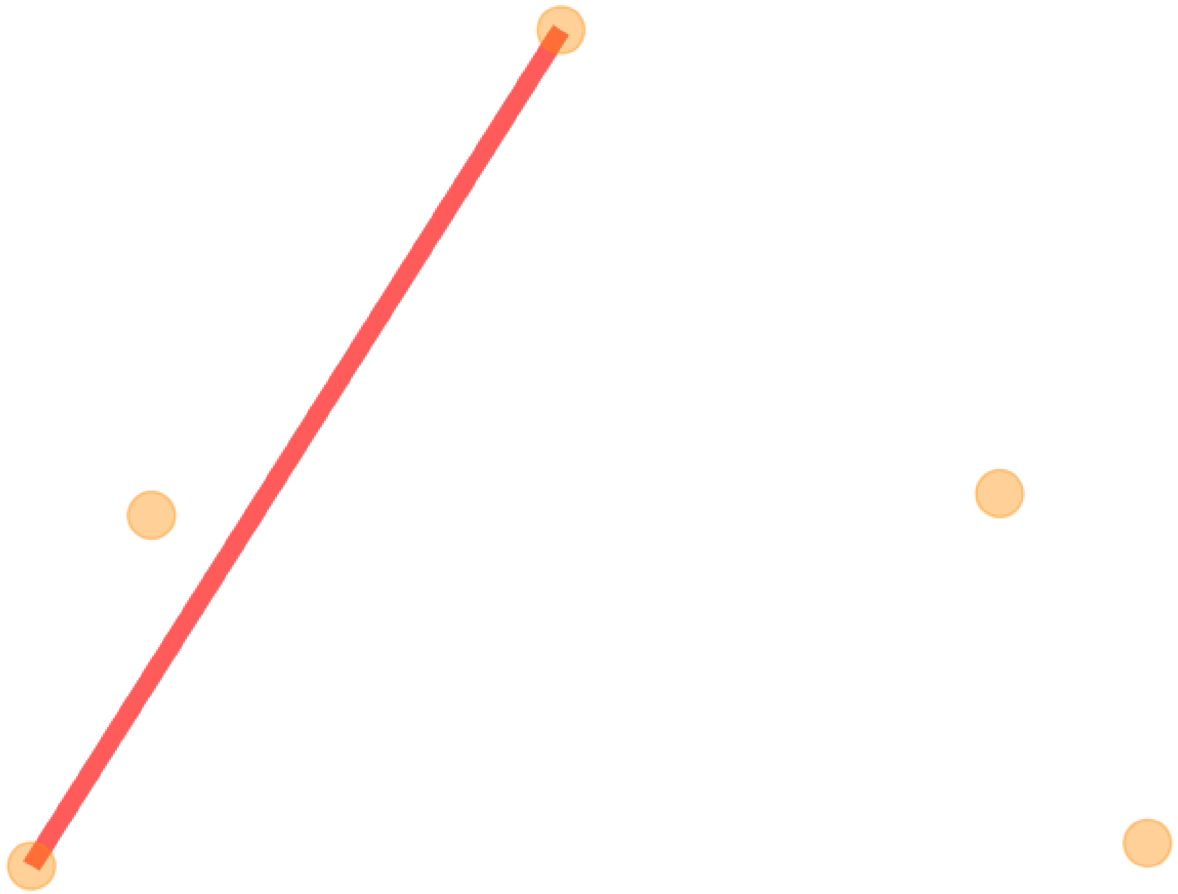
Example: Letters



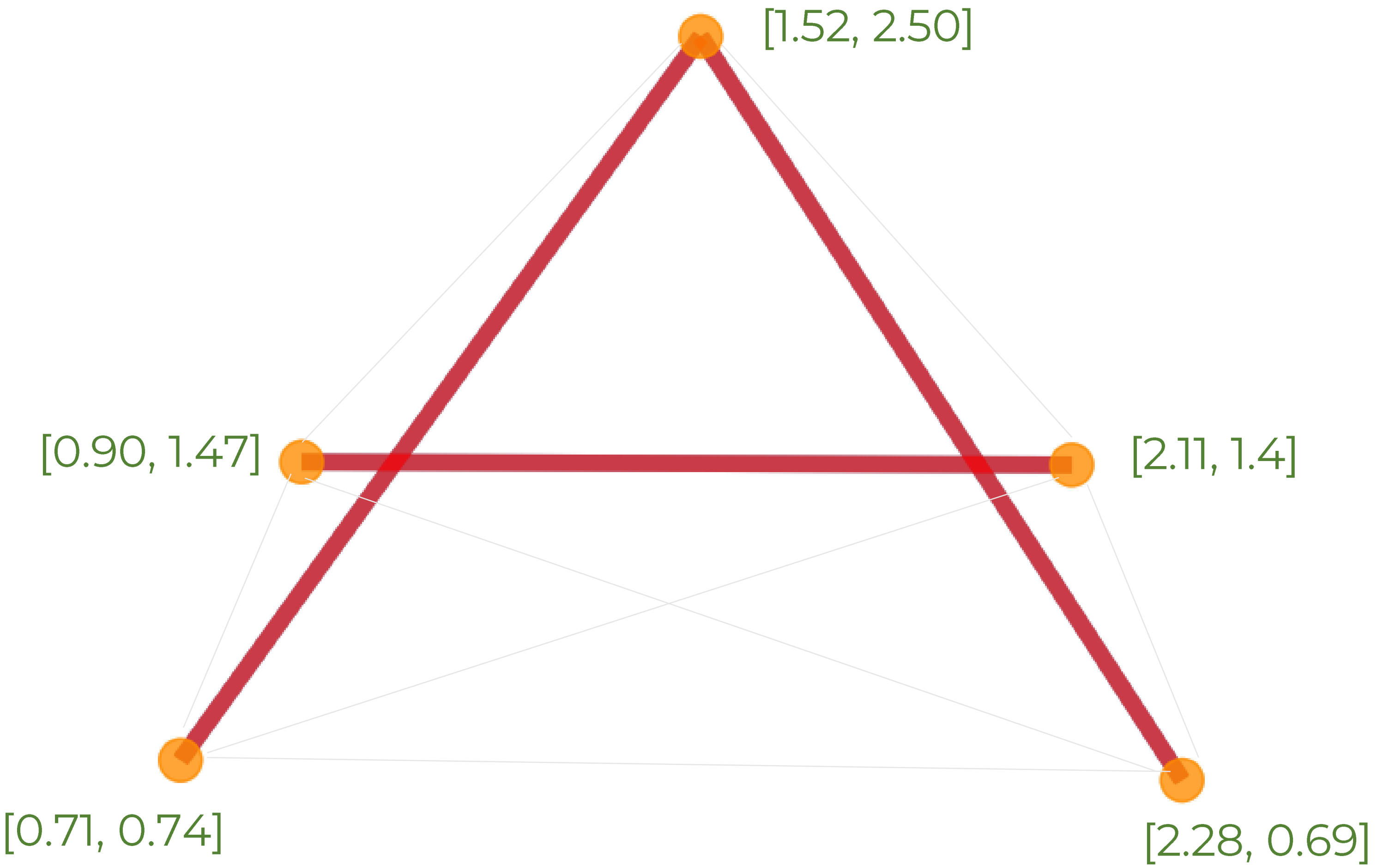
Example: Letters



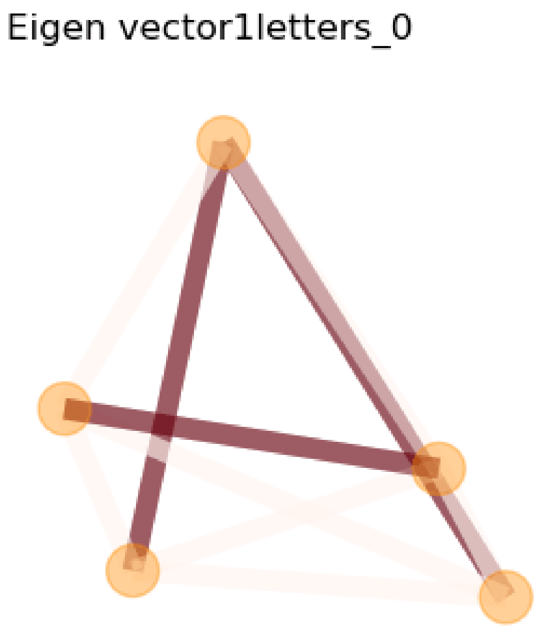
Example: Letters



A mean

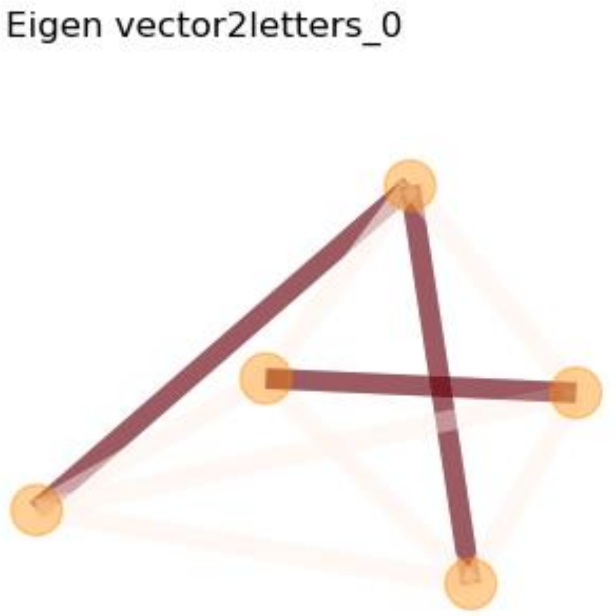


Geodesic Principal Component Analysis



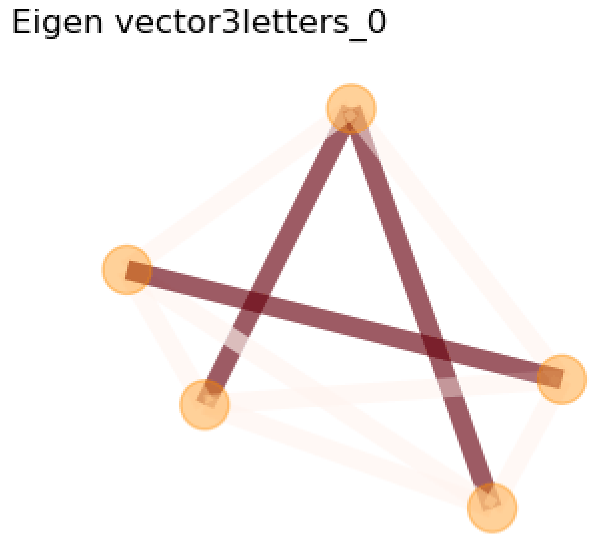
Capturing 18% of the total variance

Geodesic Principal Component Analysis



Capturing 16% of the total variance

Geodesic Principal Component Analysis



Capturing 14% of the total variance

Conclusion and Further Developments

Starting from Strcuture Spaces defined by Jain and Obermayer (2009), we introduced:

⟹ the GPCA for the Graph Space

⟹ AAC Algorithm for computing statistics such as the Fréchet Mean

⟹ Python Package

Next Step:

- Pure Topological Geodesic Principal Component
- Network on Network Regression Model

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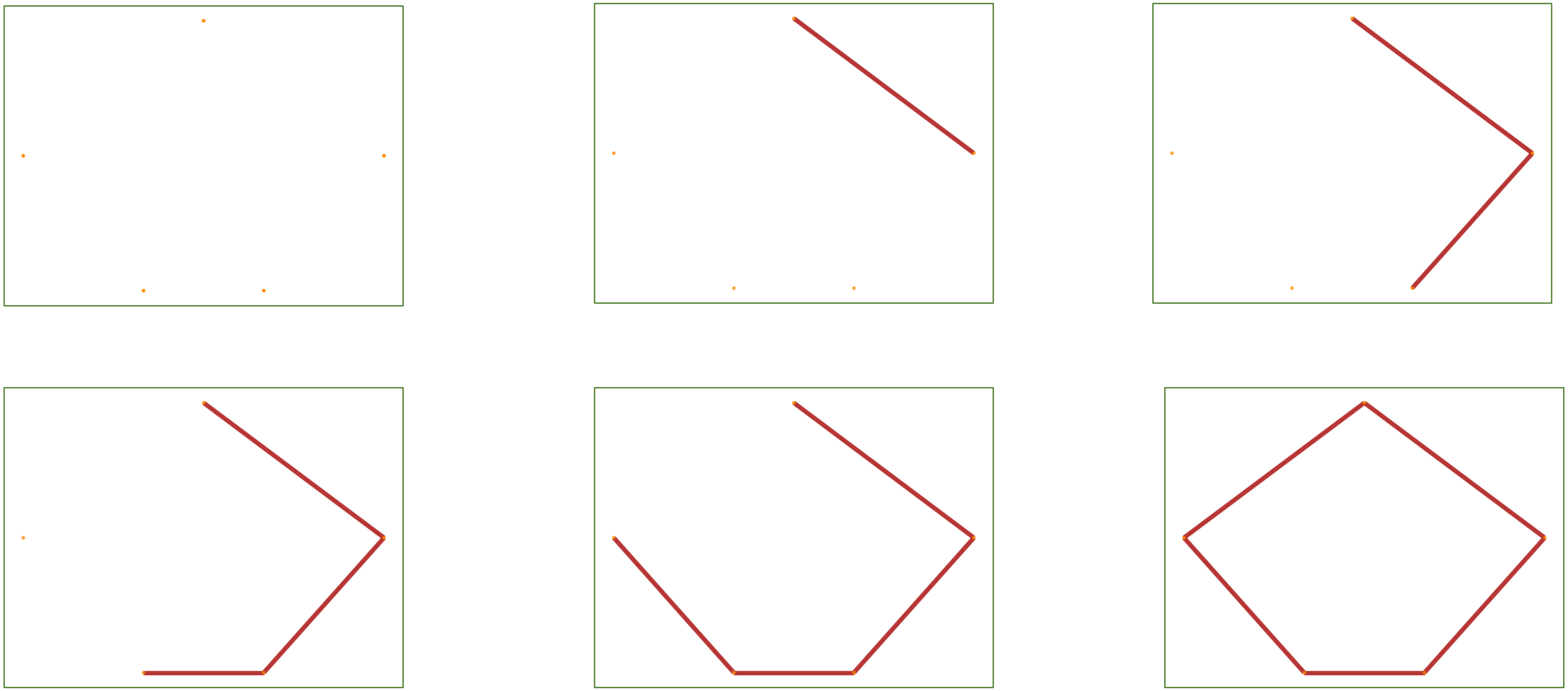
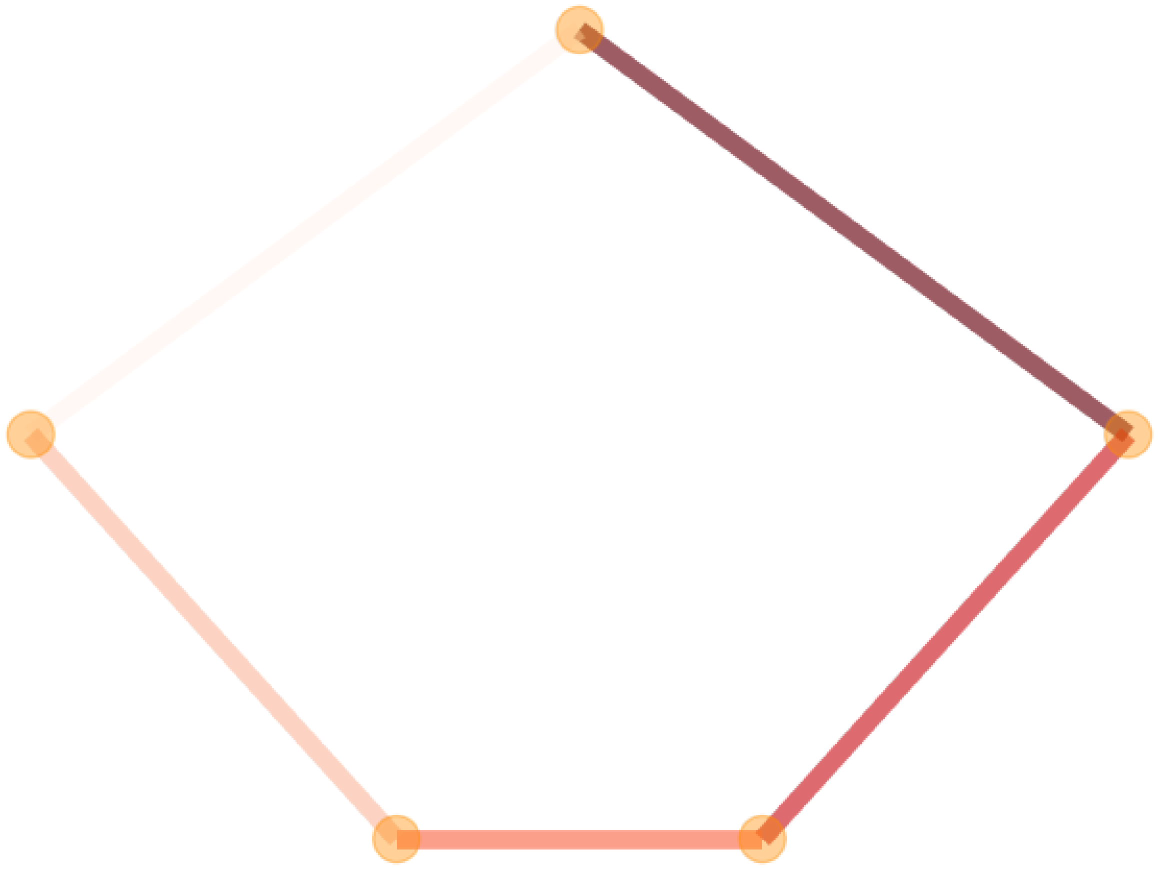
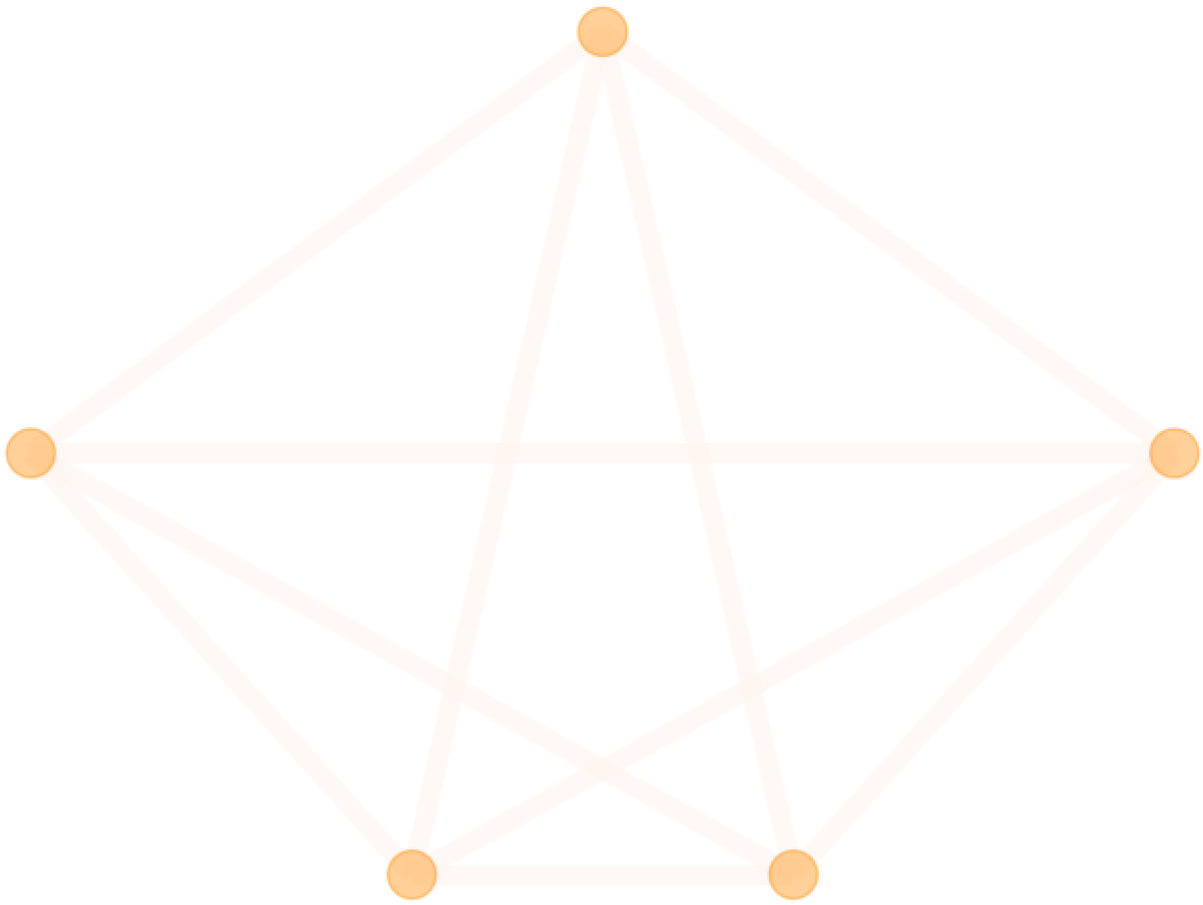
Example 1: Topological Variation



A Mean



Geodesic Principal Component Analysis



Capturing 60% of the total variance