Object Oriented Data Analysis of Population of Networks

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DIPARTIMENTO DI MATEMATICA

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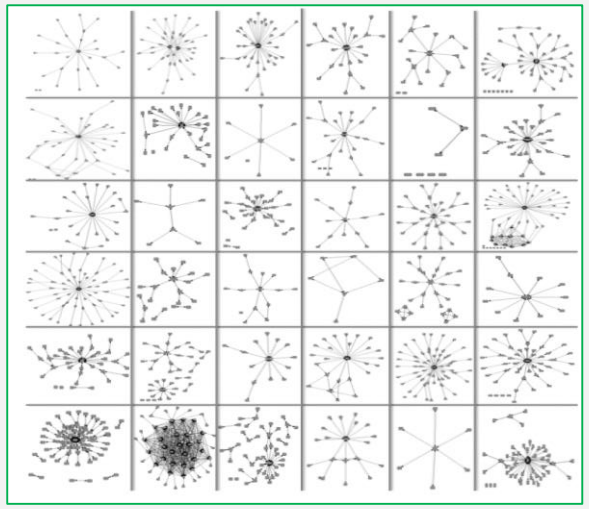
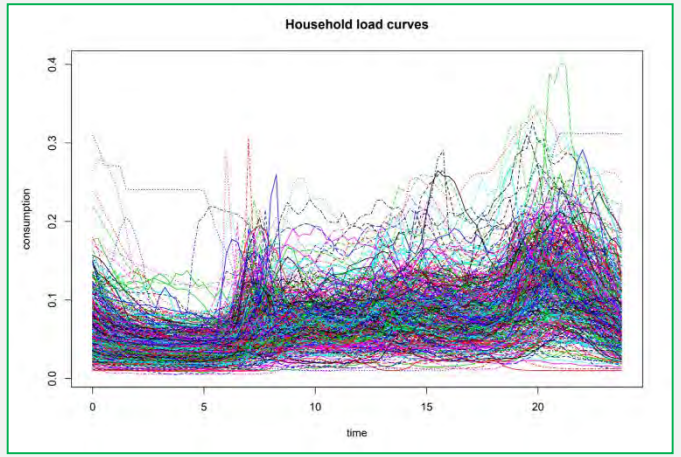
Complex Data

Complex Data





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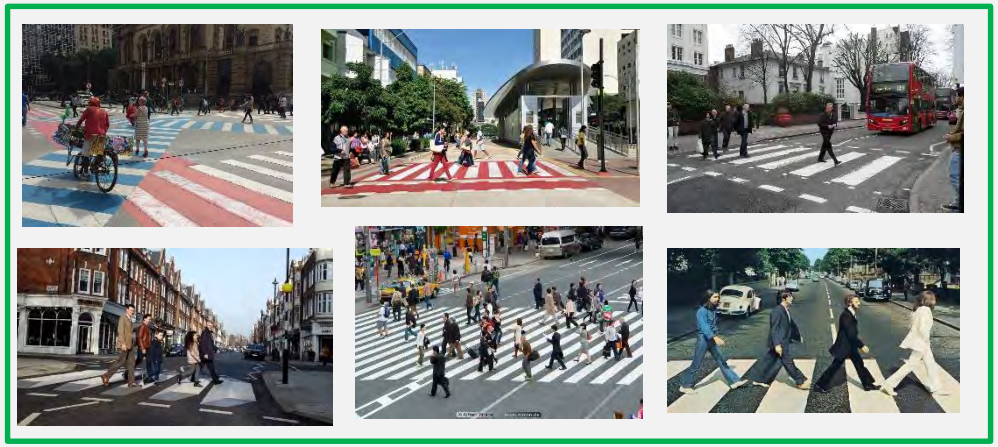

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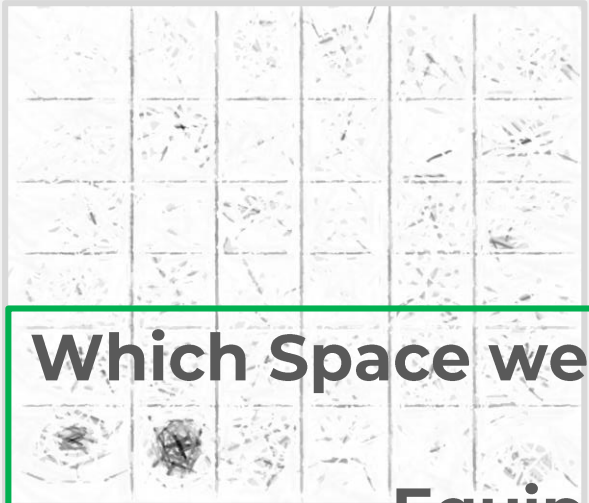

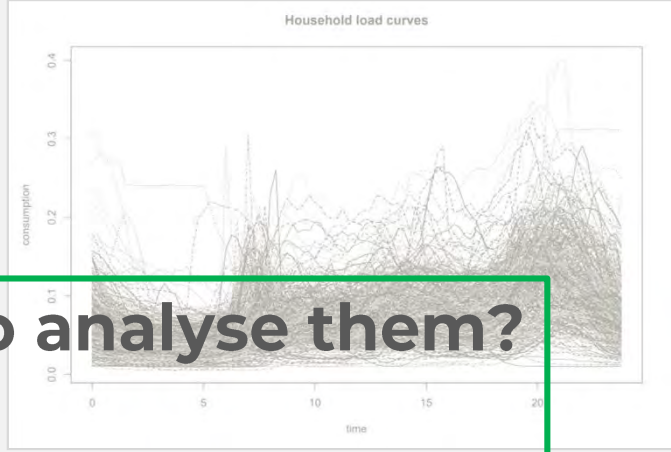

Which Space we should choose to analyse them?

Equipped with which tools?

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Which ingredients to make statistics?

Metric Space	→	Cluster Analysis
Geodesics Space	→	Regression, Principal Components Analysis
Measure Space	→	Probability Distribution, Testing

Which ingredients to make statistics?

Euclidean Vectors (finite and infinite dimension)

- Metric Space → Cluster Analysis
- Geodesics Space → Regression, Principal Components Analysis
- Measure Space → Probability, Distribution, Testing

Which ingredients to make statistics?

Mildly non Euclidean
(functions, covariance matrices, ...)

- Metric Space → Cluster Analysis
- Geodesics Space → Regression, Principal Components Analysis
- Measure Space → Probability, Distribution, Testing

Which ingredients to make statistics?

Strongly non Euclidean
(networks, trees, ...)

↘ Metric Space → Cluster Analysis

? Geodesics Space → Regression, Principal Components Analysis

? Measure Space → Probability, Distribution, Testing

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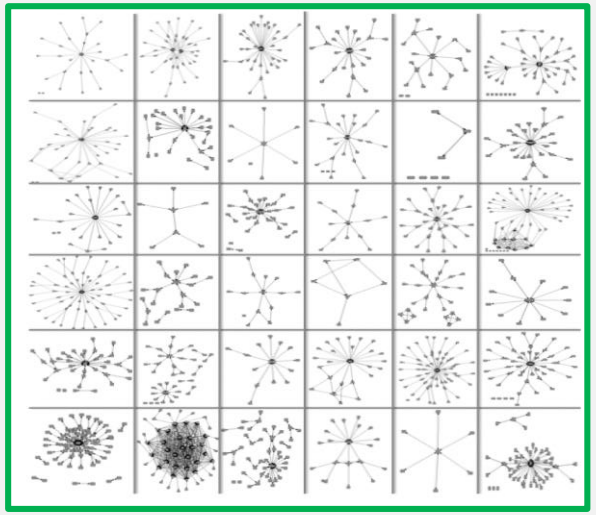

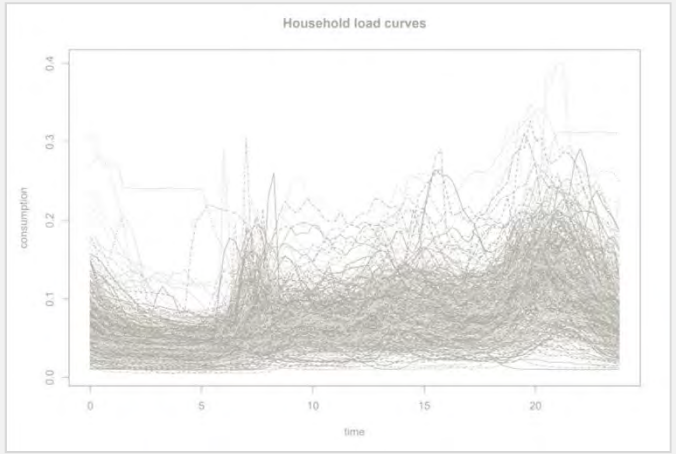

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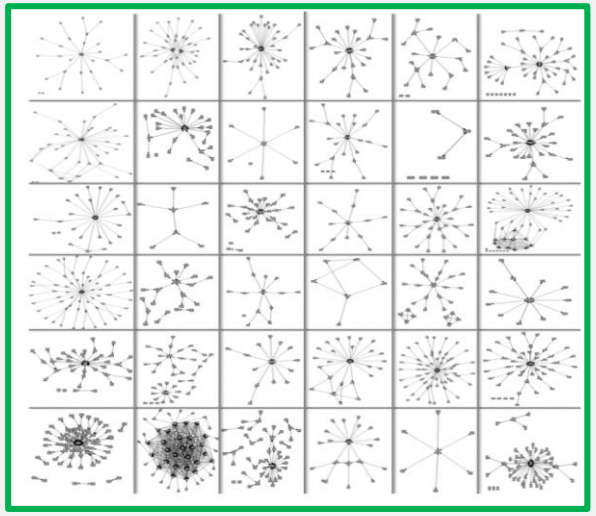
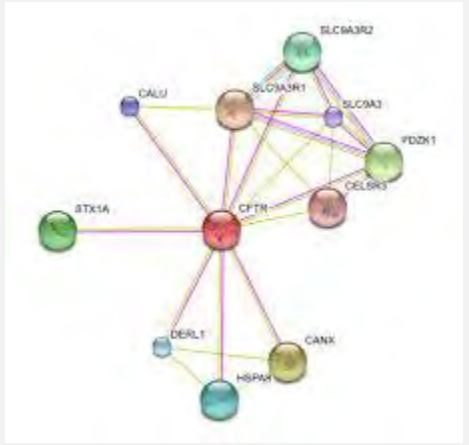
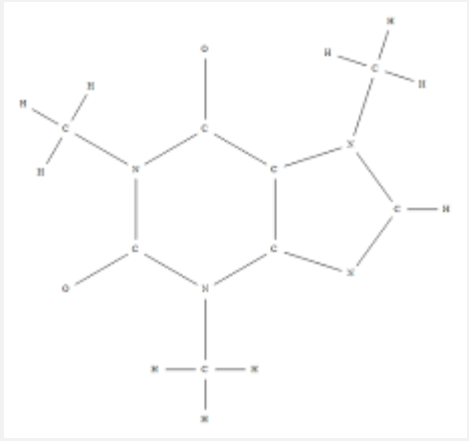
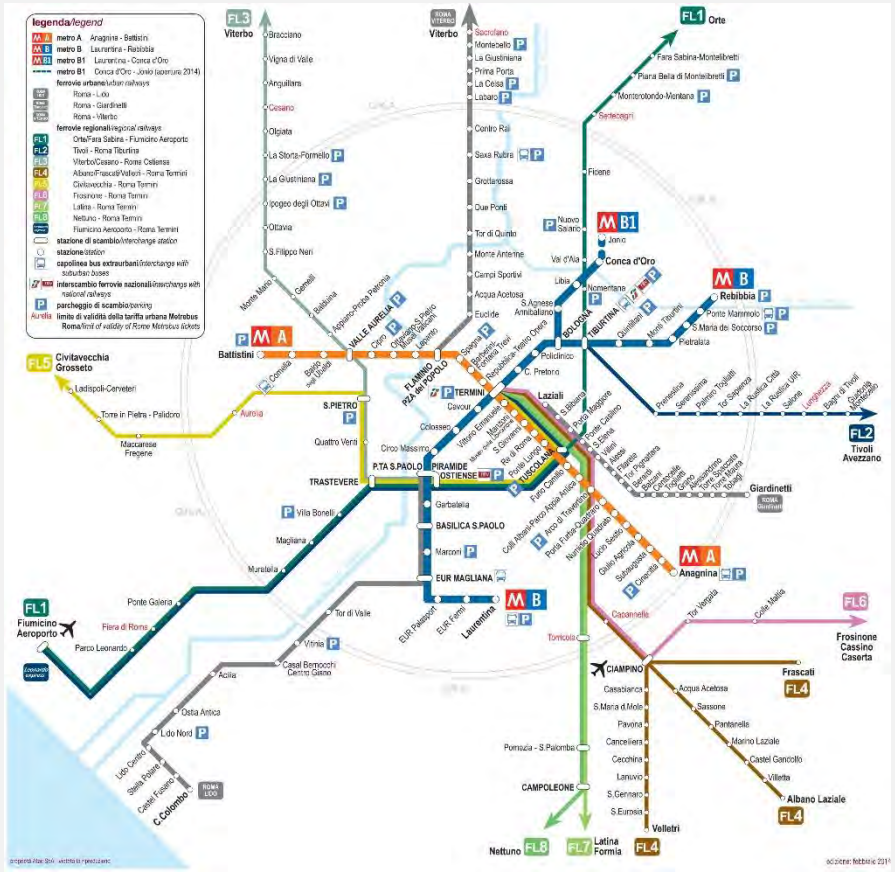






Network Analysis



Rome Public Transport System Network

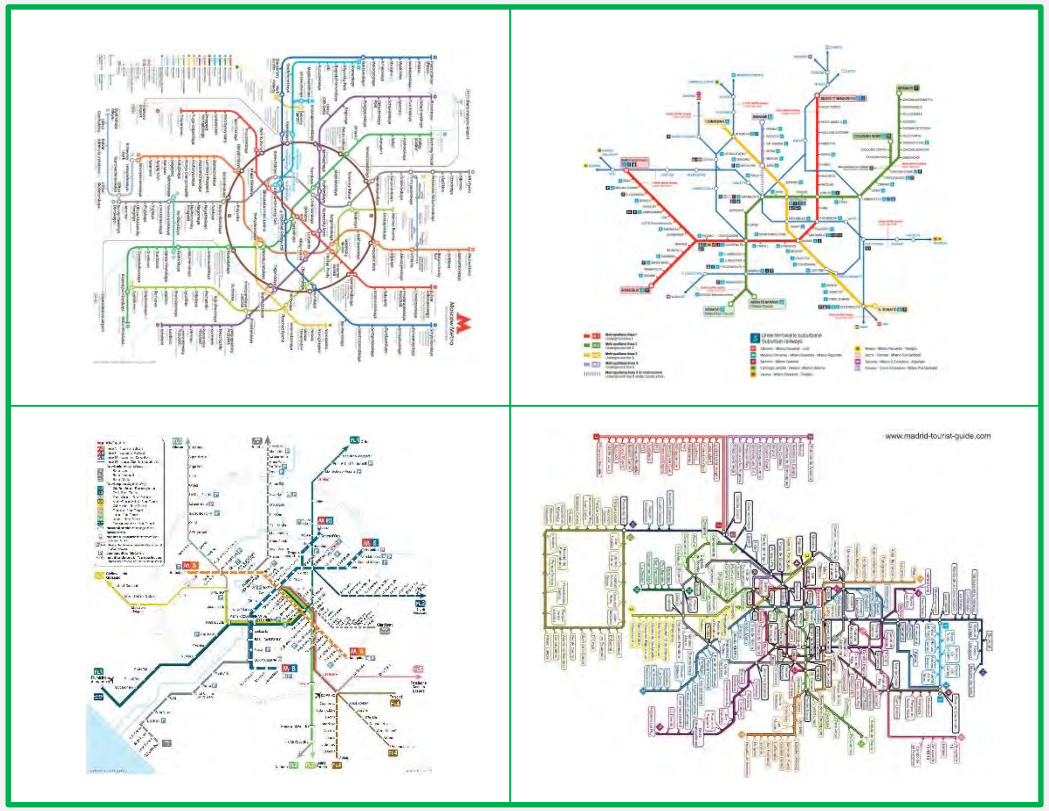
Datum: $x = (P, R, \alpha)$

P- set of nodes

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

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

Network Analysis: from one to many

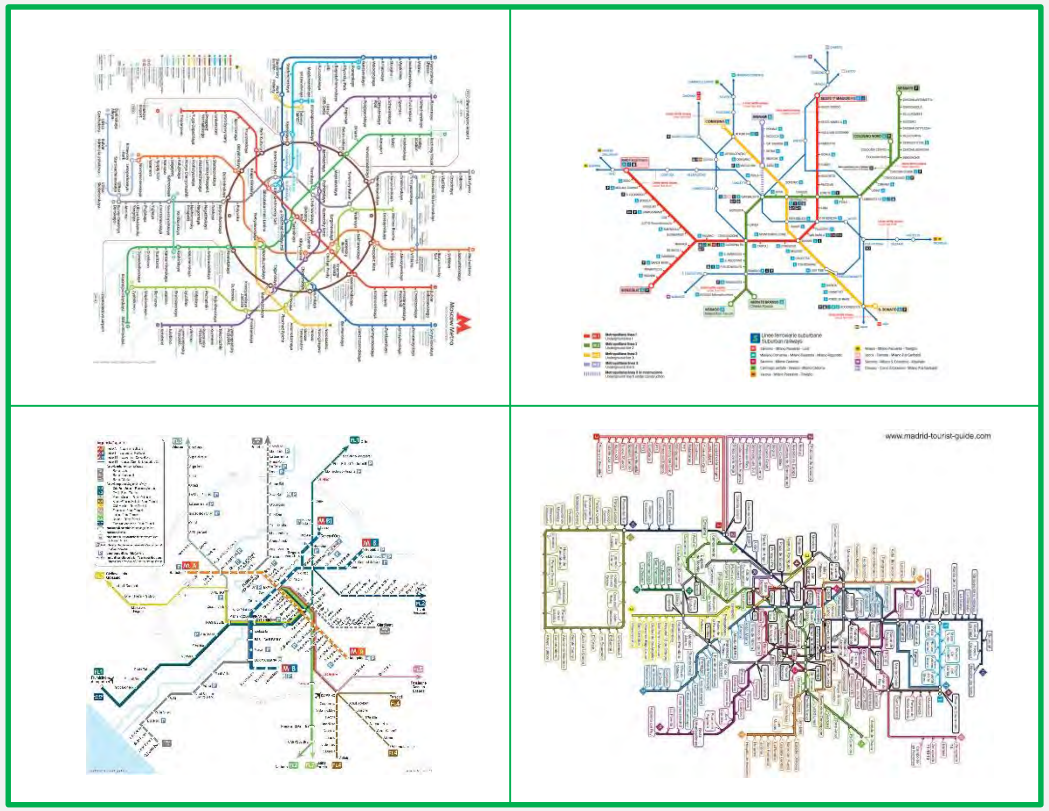


Public Transportation Network in different cities

Data Points are Networks

$$X_1 = (P, R_1), \ldots, X_n = (P, R_n)$$

Network Analysis: from one to many



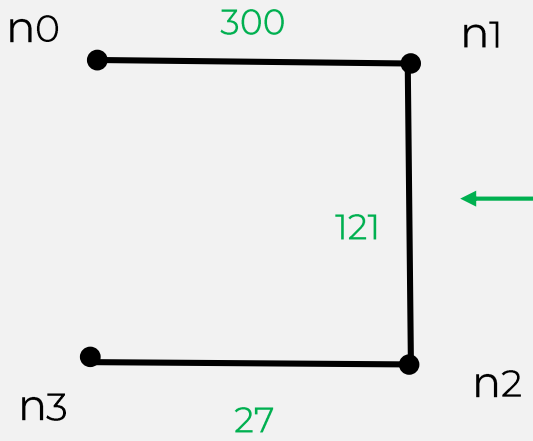
Public Transportation Network in different cities

Many new questions arise:

- How can we describe these networks?
- How can we relate nodes in networks?
- Along which relations/features are different?
- **How can we make statistics?**

Graph Space

Graph Space



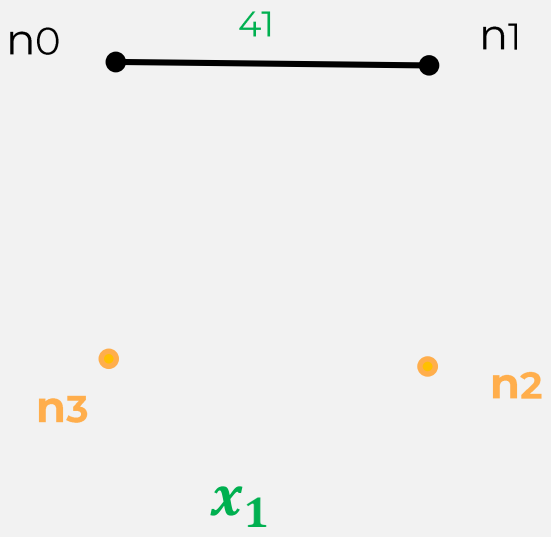
n0	300	0	0
300	n1	121	0
0	121	n2	27
0	0	27	n3

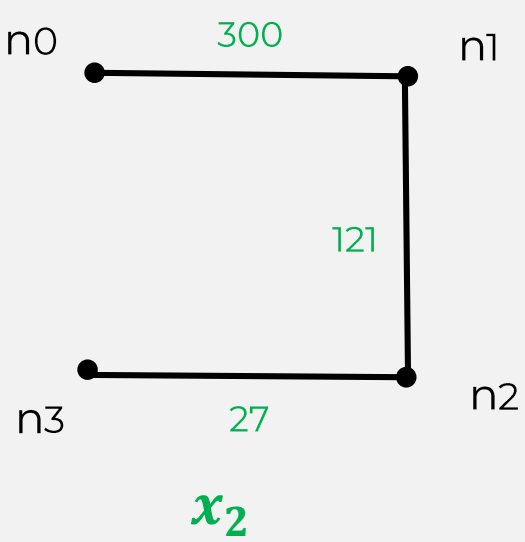
n0	300	0	0	...	n1	121	0	...	27	n3

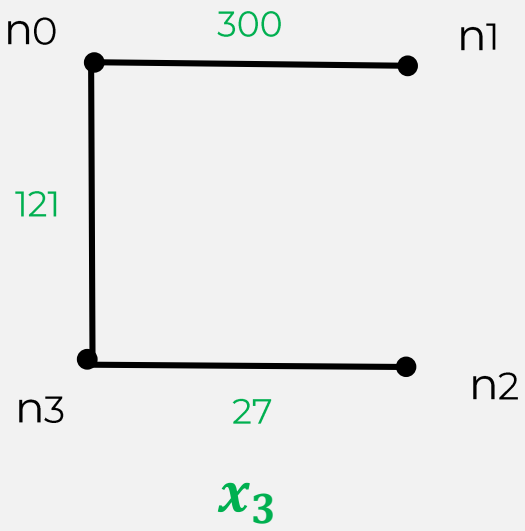
Data Point in

$$\mathbf{X} = \mathbb{R}^{16}$$

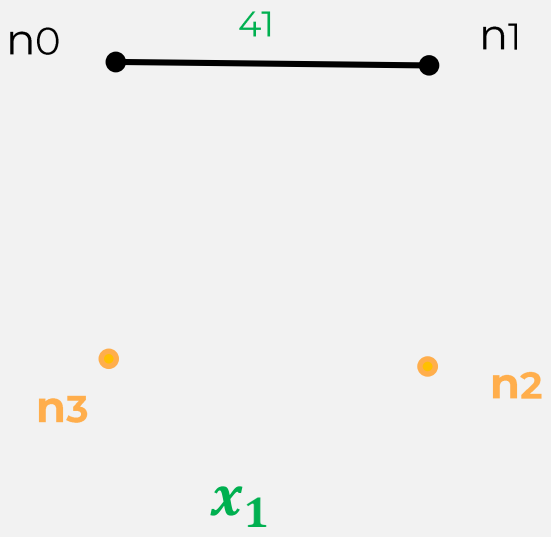
Graph Space



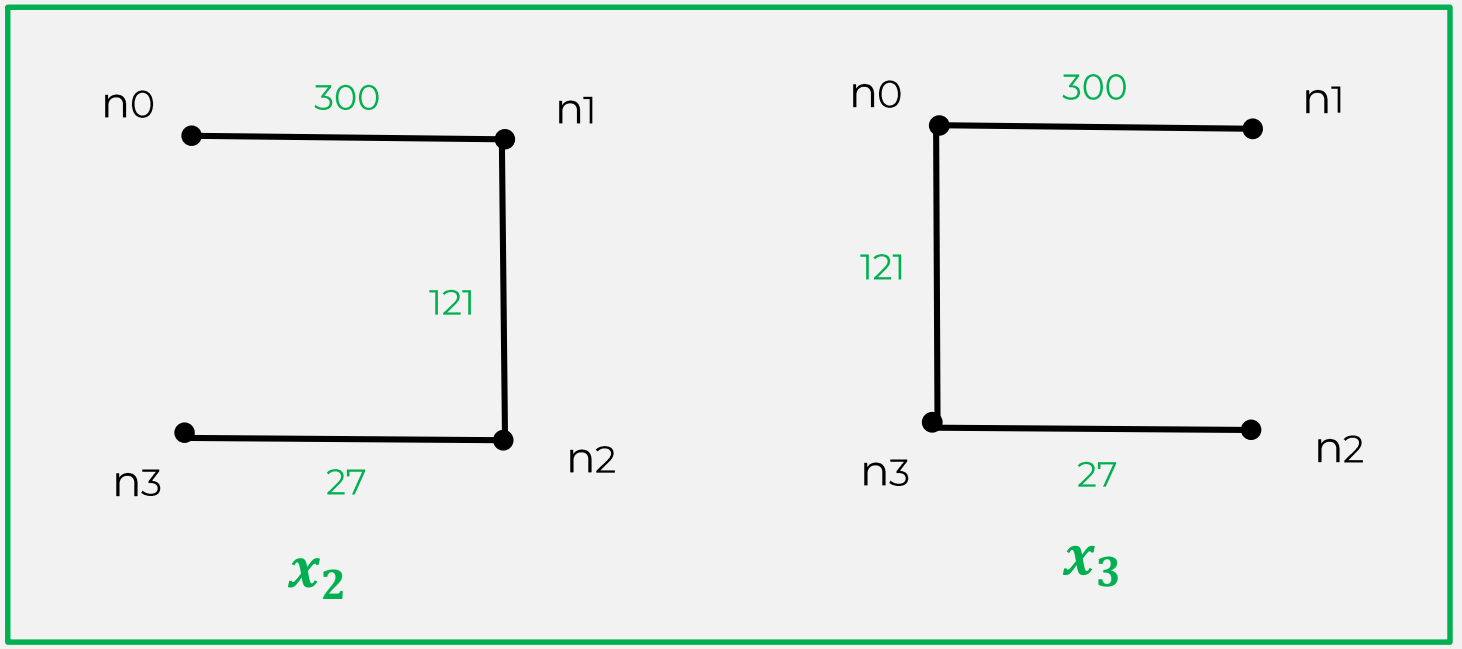




Graph Space



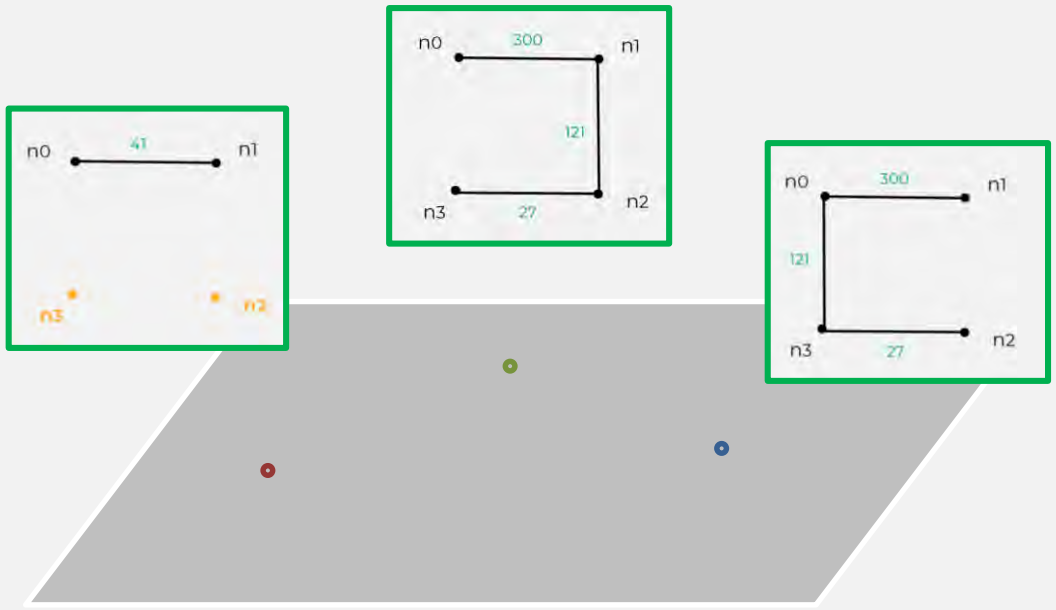
x_1



x_2 x_3

$$x_2 = x_3$$

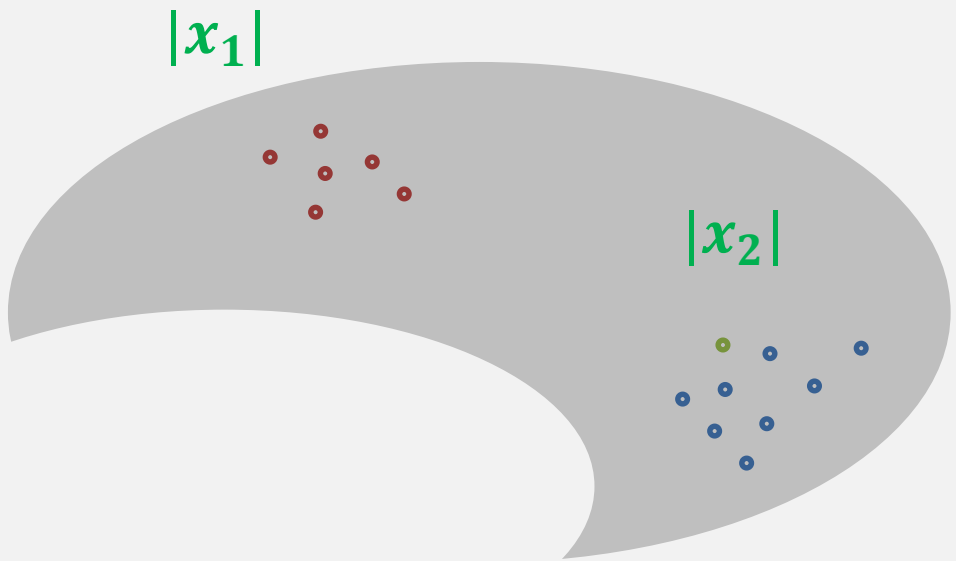
Allowing permutation of nodes



Space: X

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

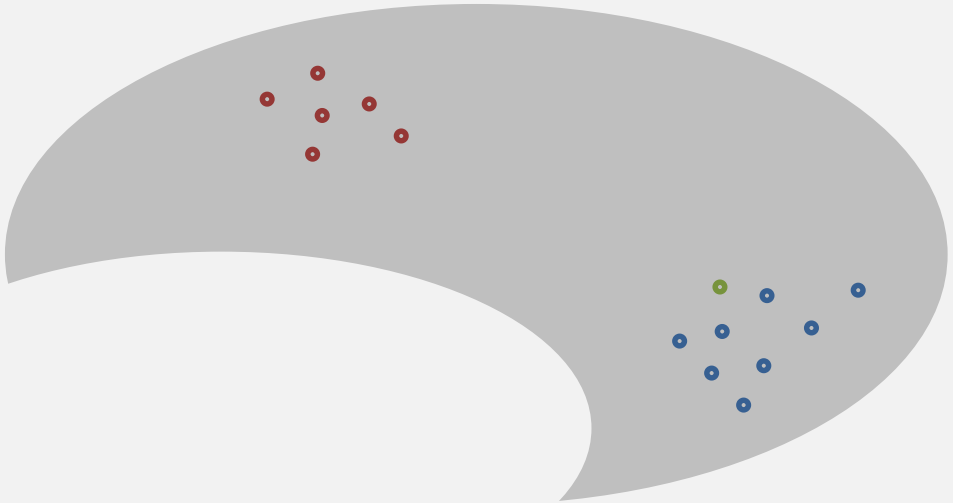
Permuting nodes



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

Quotient Space

Graph Space



Metric Space (X, d_x)
With d_X invariant with respect to permutation

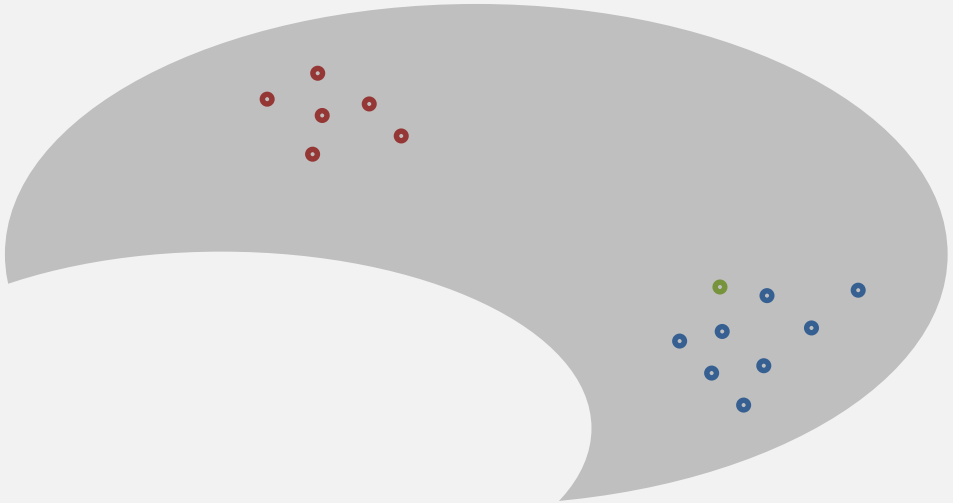
Metric Space $(X/\mathcal{T}, d)$

$$d(|x_1|, |x_2|) = \inf_{t \in \mathcal{T}} d_x(tx_1, x_2)$$

Graph Space

Manifold

$\mathcal{T}$ **action is not Free**



Not a Manifold

Exclude all the literature about
Statistics on Manifold

Graph Space: Novelty

Curvature of the space: unbounded

- → No uniqueness of the geodesics even locally.
- → No uniqueness of the Fréchet Mean

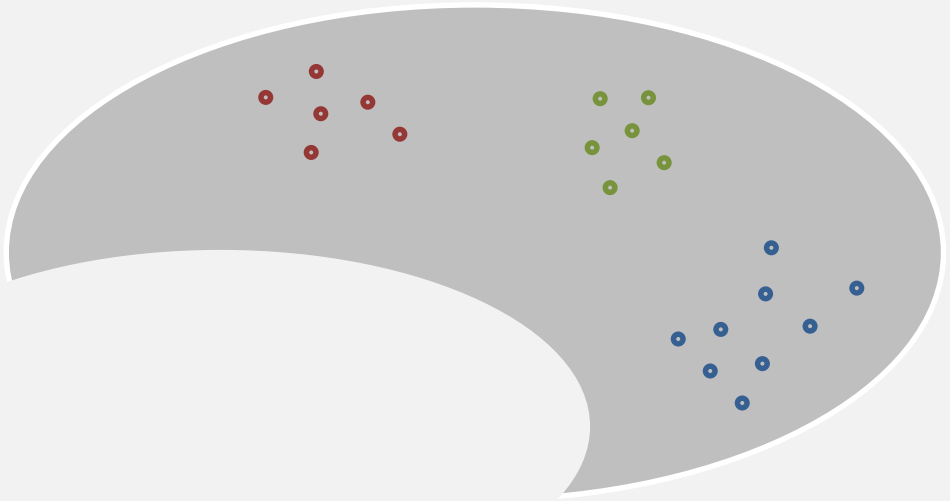
Isometric and Finite Dimension Action:

- → Allows to transfer easily computation from $\mathbb{X}$ to $\mathbb{X}/\mathbb{T}$

Define Geodesic Principal Components and introduce the Align All and Compute Algorithm

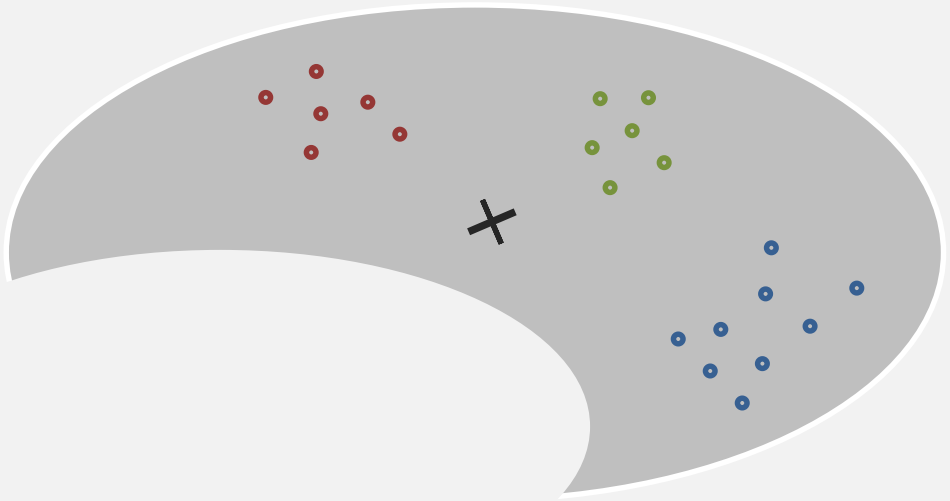
Statistic on Graph Space

Align All and Compute Algorithm



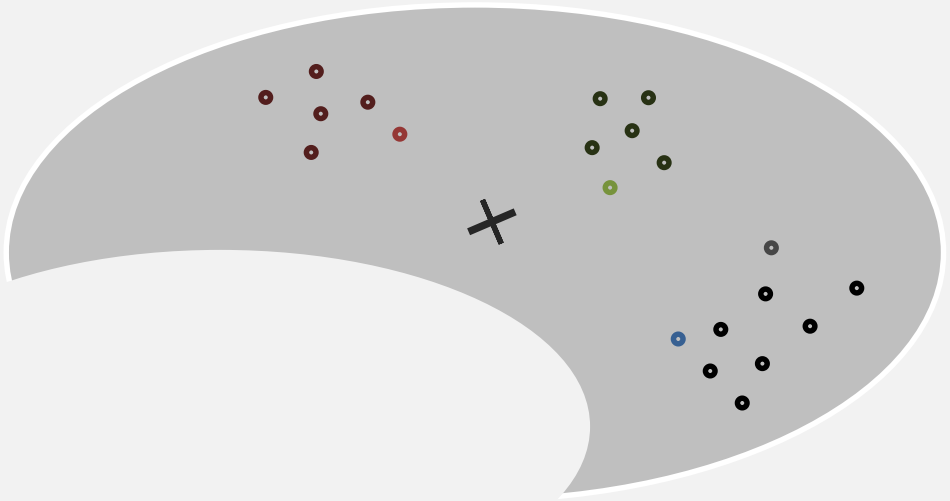
Graph Space: $\mathcal{X}/\mathcal{T}$

Align All and Compute Algorithm



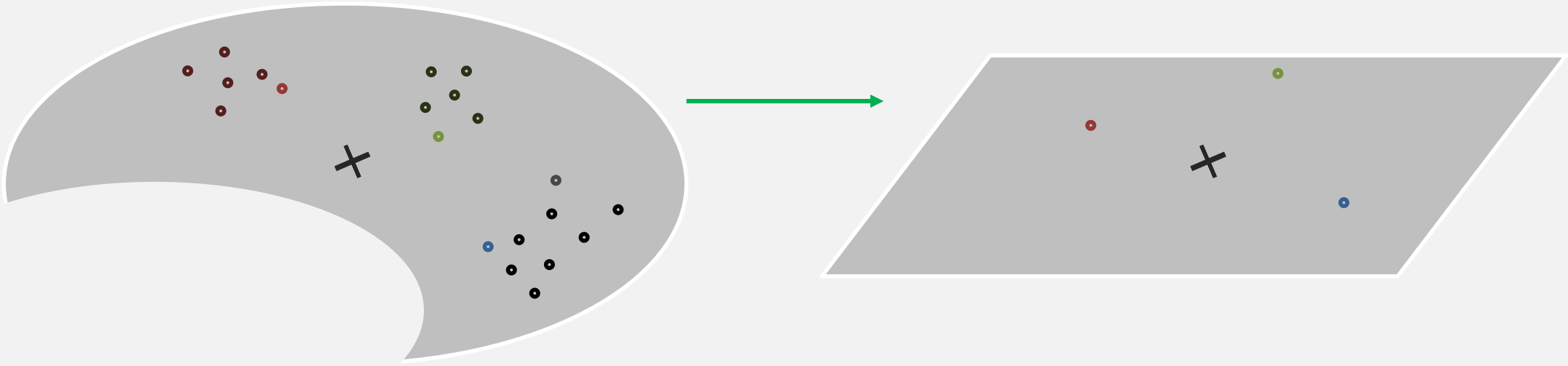
Graph Space: $X/\mathcal{T}$

Align All and Compute Algorithm



Graph Space: X/T

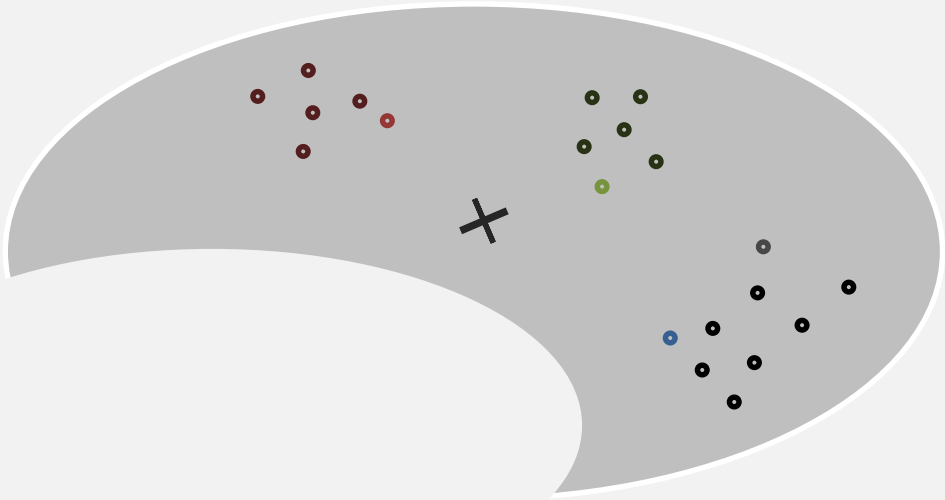
Align All and Compute Algorithm



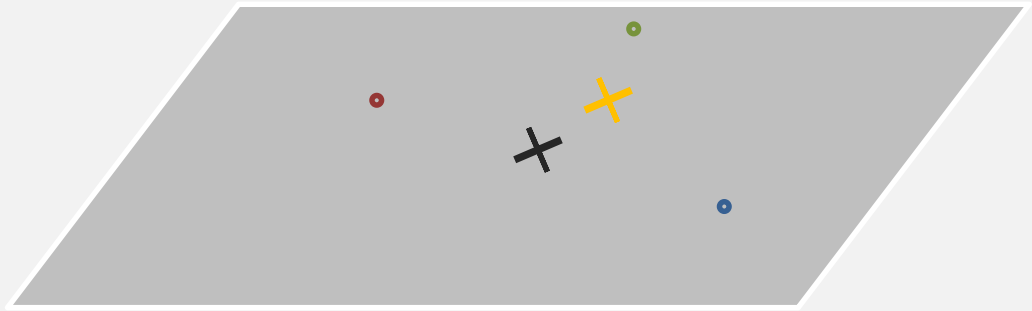
Graph Space: $X/\mathcal{T}$

Space: X

Align All and Compute Algorithm

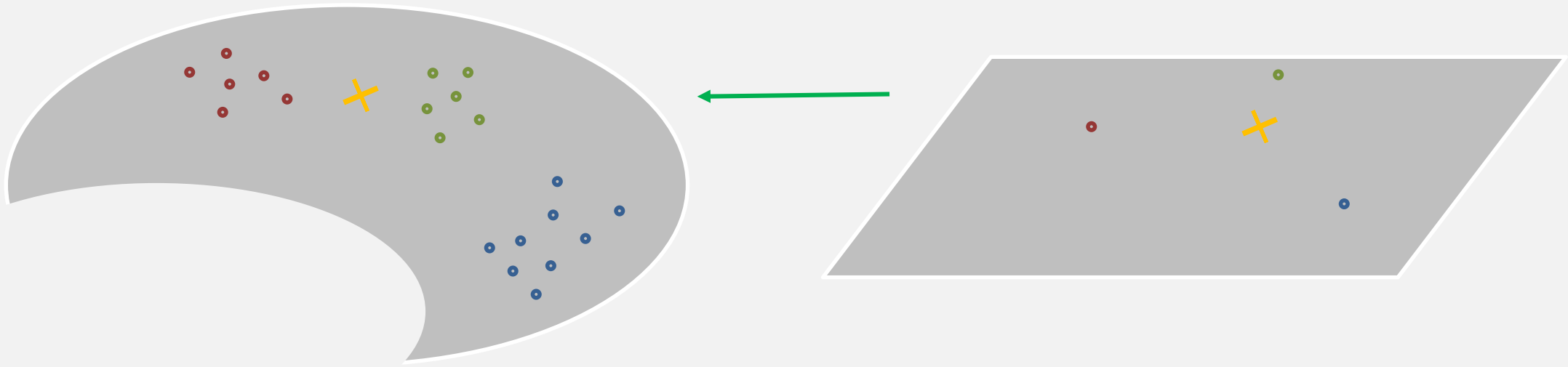


Graph Space: X/T



Space: X

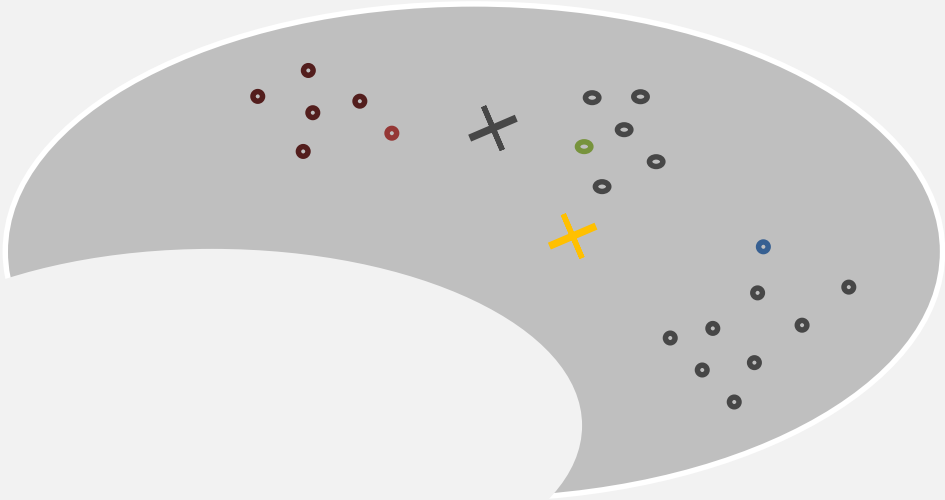
Align All and Compute Algorithm



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

Space: X

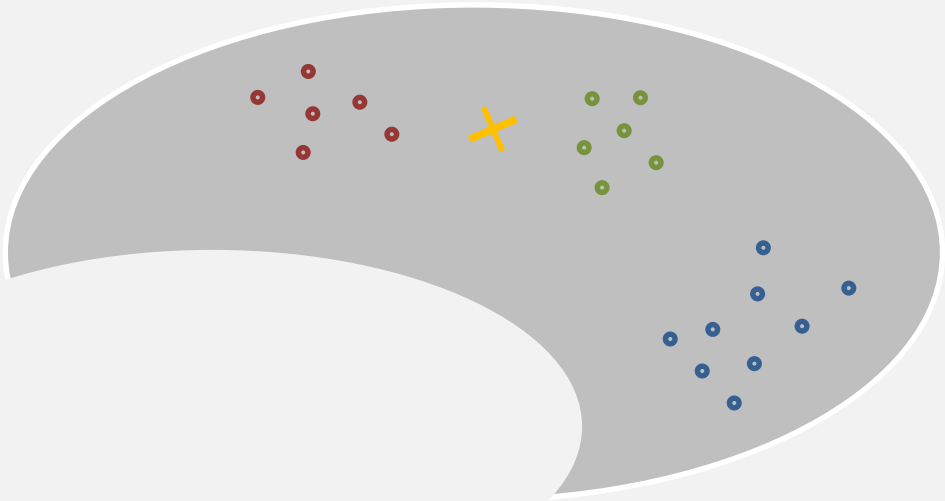
Align All and Compute Algorithm



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

Space: X

Align All and Compute Algorithm



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

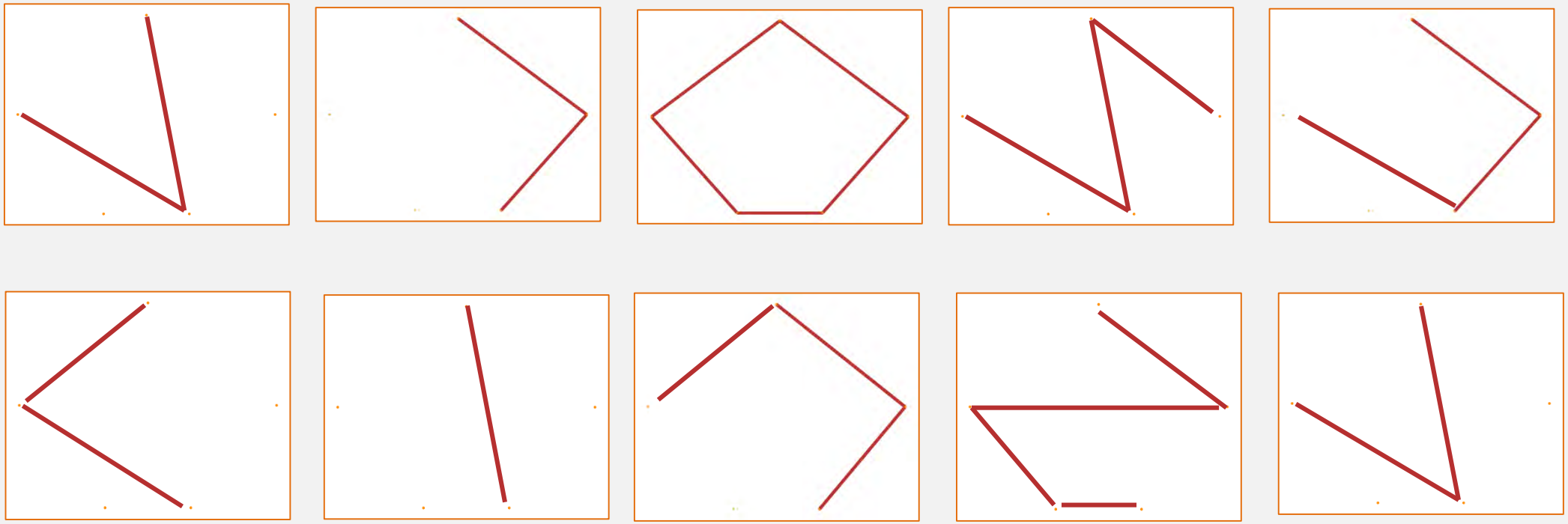
Can be a Fréchet Mean, a Geodesic, etc.

Example 1: Simulation

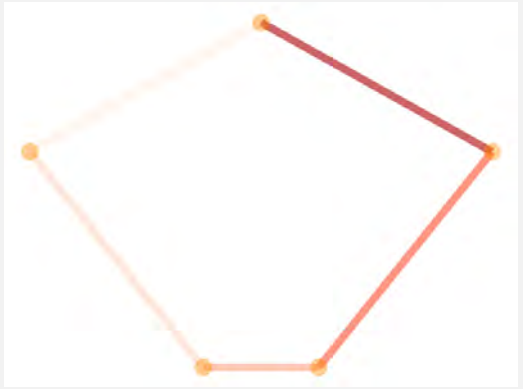
Topological Variation

Topological Variation

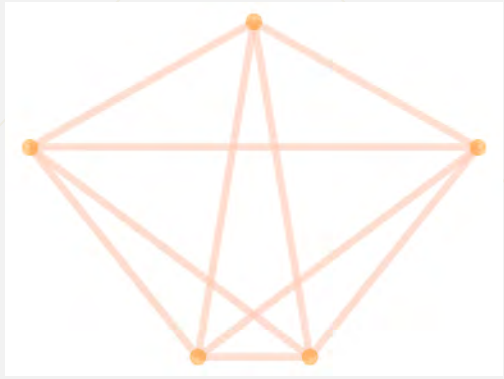
Generated 5000 observation randomly sampled from the 5 orbits. Here a subsample:



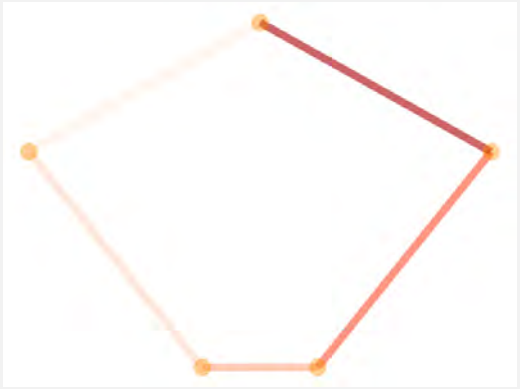
A Frèchet mean



Theoretical Fréchet Mean

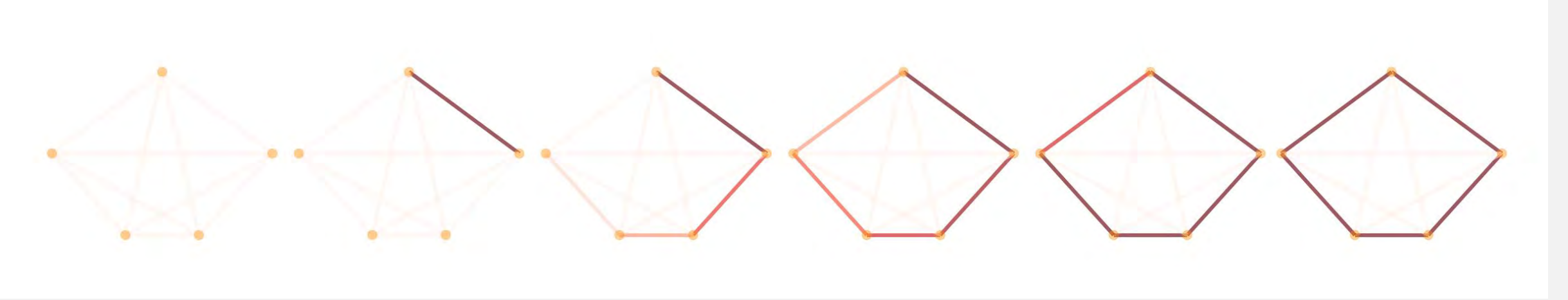


Estimation of Fréchet Mean without Alignment



Estimation of Fréchet Mean with Alignment

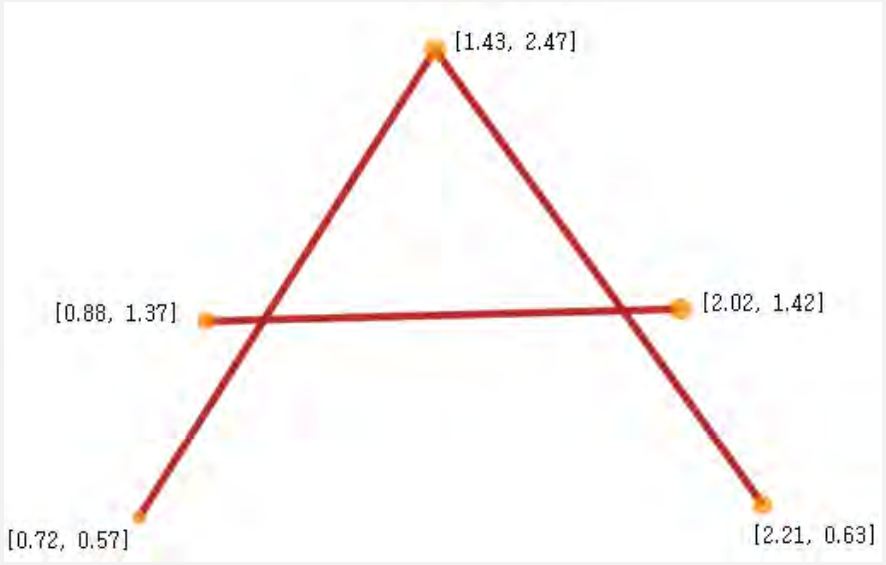
First Geodesic Principal Component



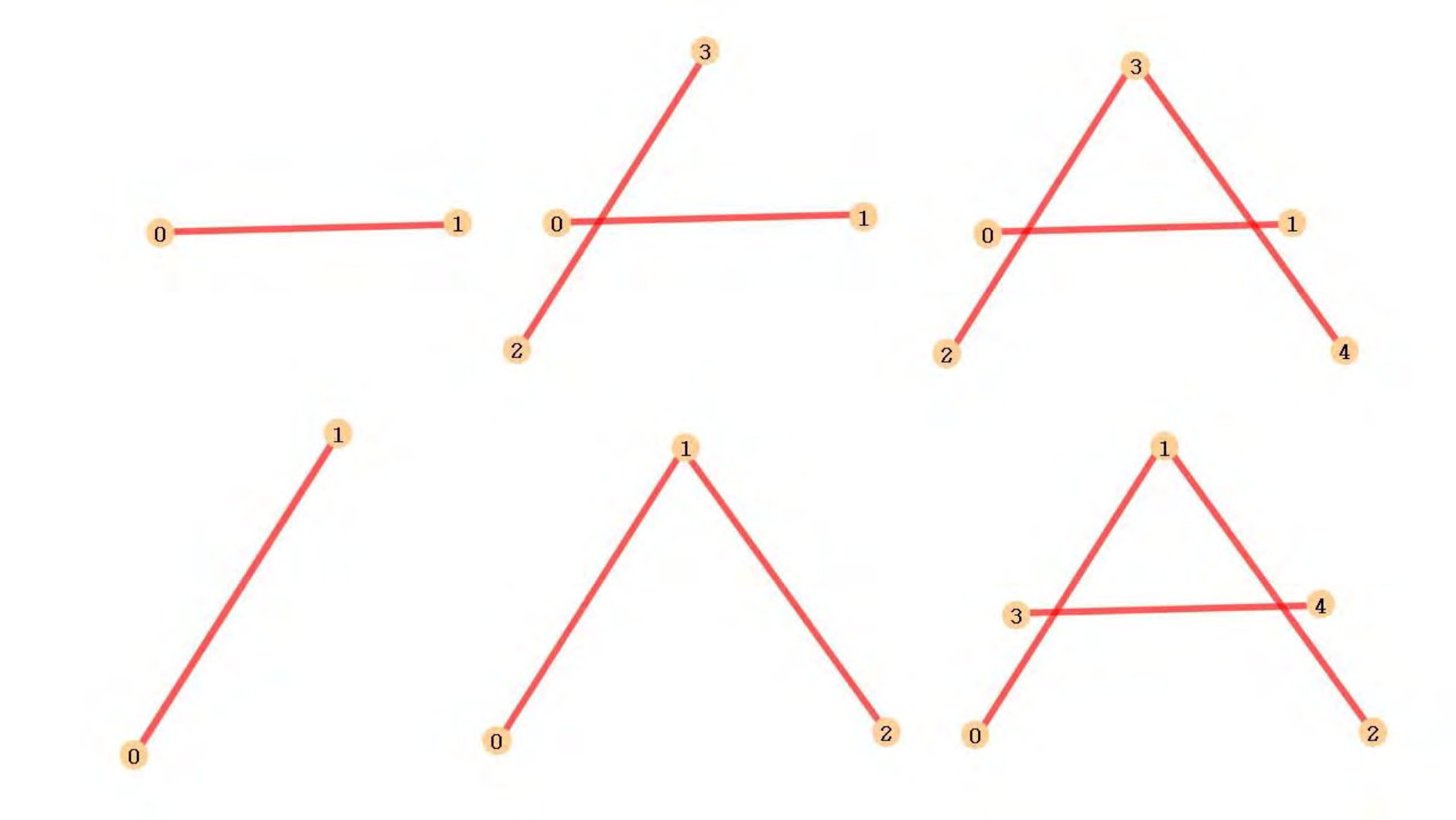
Projection along the 1st GPCA explaining
60% of the total variance

Example 2: Letters

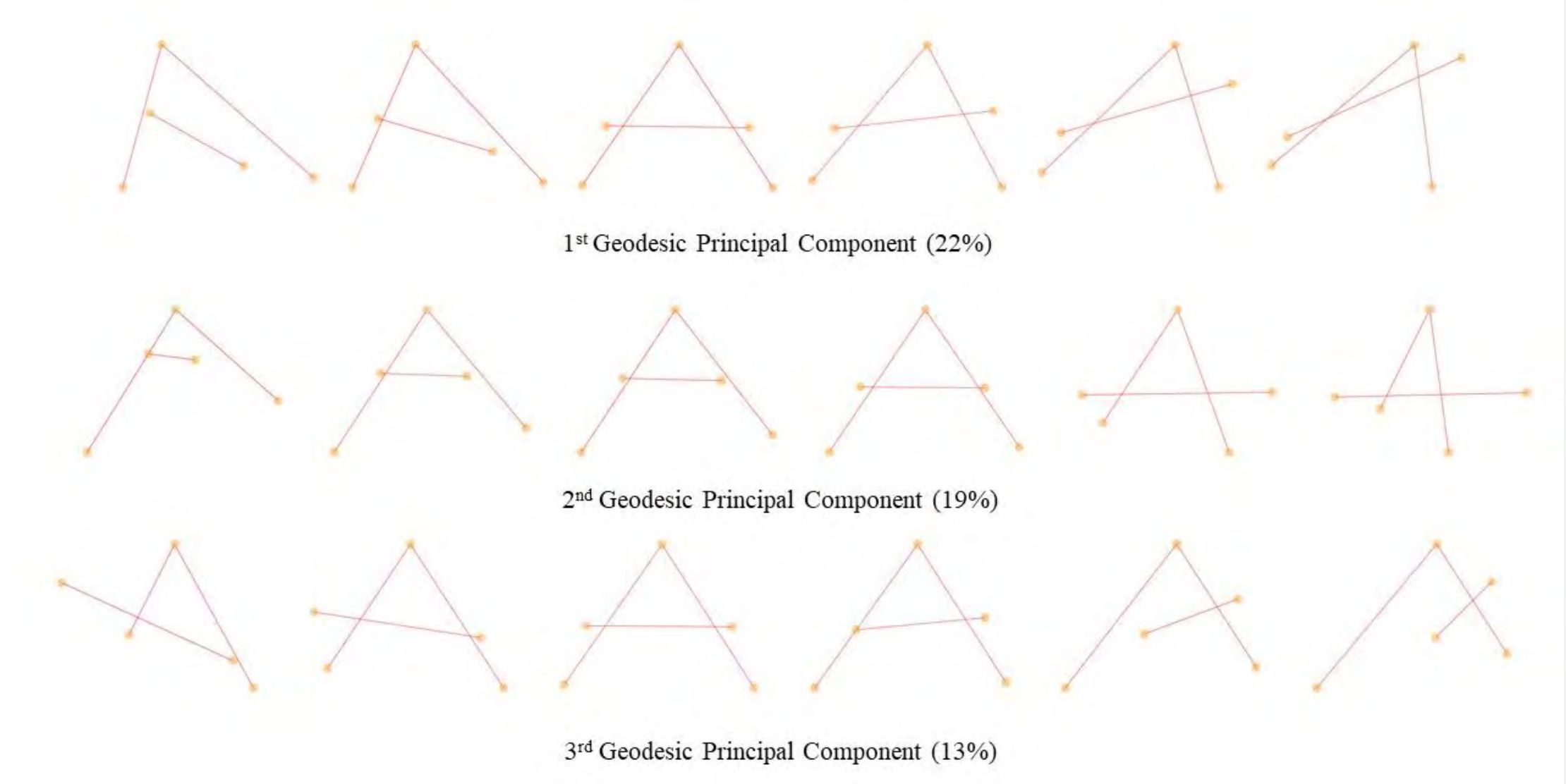
Letters



Letters



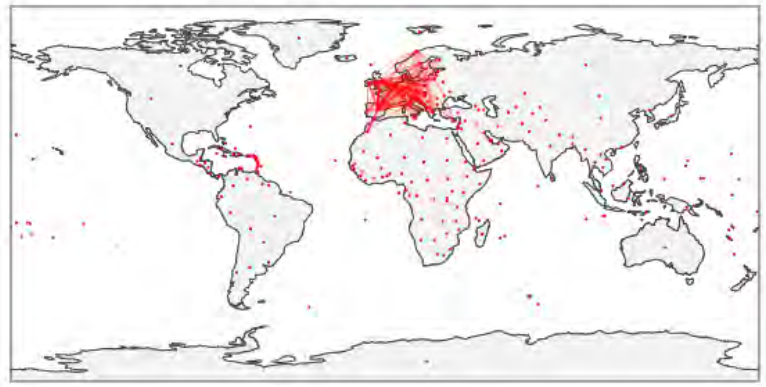
Letters GPCAnalysis



Example 2: Clustering

Airlines Dataset

Alitalia



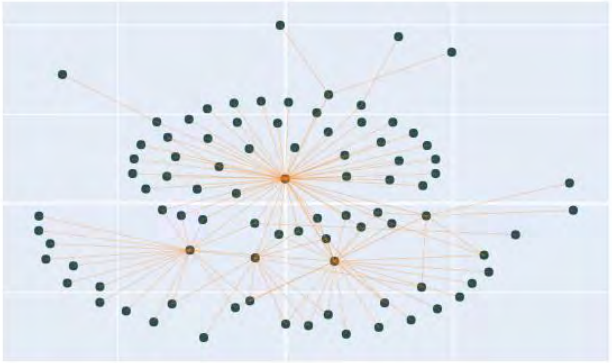
RyanAir

Luftansa

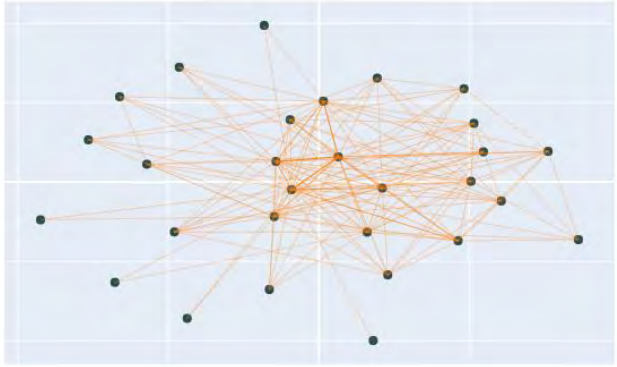
KLM

12 airlines companies OpenFlights Project

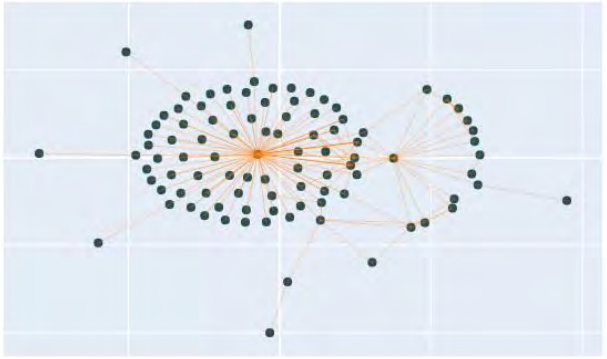
Airlines Dataset



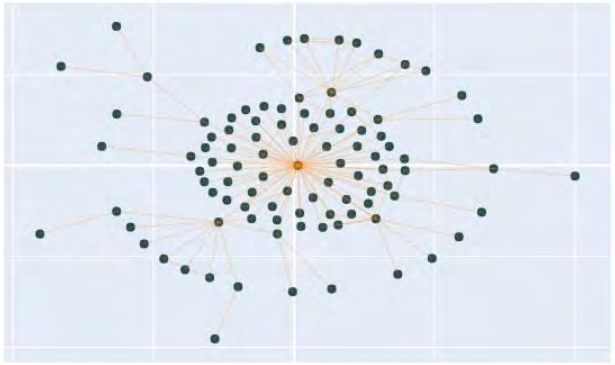
Alitalia



RyanAir

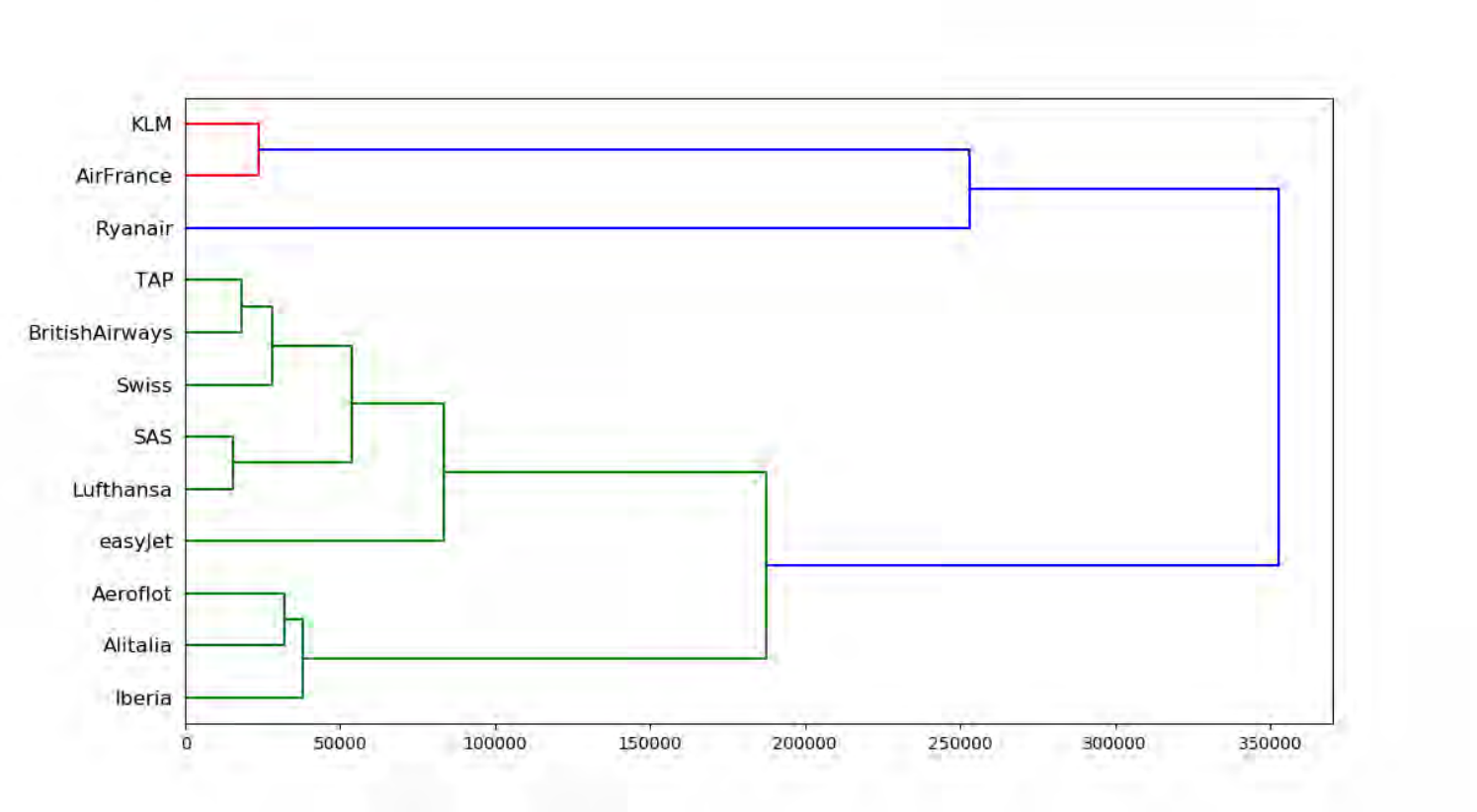


Luftansa



KLM

Cluster



Graduate Assignment Graph Matching, Euclidean Distance, Ward Linkage

Conclusions

Conclusions

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

⟹ Geometrical Properities of the Space (e.g. Curvature)

⟹ Geodesic Principal Component

⟹ Align All and Compute Algorithm

Next Step:

⟹ Introduce a Measure on the Space

⟹ Define a Regression Model Network-on-Network

Object Oriented Data Analysis of Population of Networks

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DIPARTIMENTO DI MATEMATICA

Some References

Aydın, Burcu, et al. "A principal component analysis for trees." *The Annals of Applied Statistics* 3.4 (2009): 1597-1615.

Brenner and Katsikis, Nighttime Lights and Population Density in North Dakota, 2016

Dumont, J. “Object Oriented Data Analysis in the study of two population of texts” sup. Calissano, Vantini *Thesis KTH-Polimi* (2017)

Durante, Daniele, and David B. Dunson. "Bayesian inference and testing of group differences in brain networks." *Bayesian Analysis* 13.1 (2018): 29-58.

Durante, Daniele, David B. Dunson, and Joshua T. Vogelstein. "Nonparametric Bayes modeling of populations of networks." *Journal of the American Statistical Association* 112.520 (2017): 1516-1530.

Duvenaud, David K., et al. "Convolutional networks on graphs for learning molecular fingerprints." *Advances in neural information processing systems*. 2015.

Feragen, Aasa, et al. "Tree-space statistics and approximations for large-scale analysis of anatomical trees." *International Conference on Information Processing in Medical Imaging*. Springer, Berlin, Heidelberg, 2013.

Fletcher, Thomas. "Geodesic regression on Riemannian manifolds." *Proceedings of the Third International Workshop on Mathematical Foundations of Computational Anatomy-Geometrical and Statistical Methods for Modelling Biological Shape Variability*. 2011.

Ginestet, Cedric E., et al. "Hypothesis testing for network data in functional neuroimaging." *The Annals of Applied Statistics* 11.2 (2017): 725-750.

Gehl and Svarre. How to study public life. Island press, 2013.

Some References

Guo, Xiaoyang, Anuj Srivastava, and Sudeep Sarkar. "A Quotient Space Formulation for Statistical Analysis of Graphical Data." arXiv preprint arXiv:1909.12907 (2019).

Huckemann, Stephan, Thomas Hotz, and Axel Munk. "Intrinsic shape analysis: Geodesic PCA for Riemannian manifolds modulo isometric Lie group actions." *Statistica Sinica* (2010): 1-58.

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

Jain, Brijnesh, and Klaus Obermayer. "On the sample mean of graphs." *2008 IEEE International Joint Conference on Neural Networks (IEEE World Congress on Computational Intelligence)*. IEEE, 2008.

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

Nathan Keyfitz. Individual mobility in a stationary population. Population Studies, 27(2):335–352, 1973

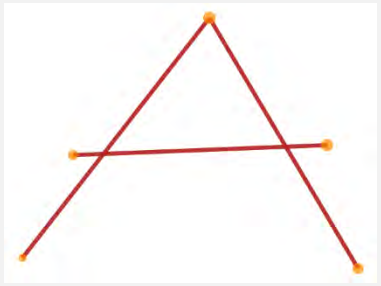
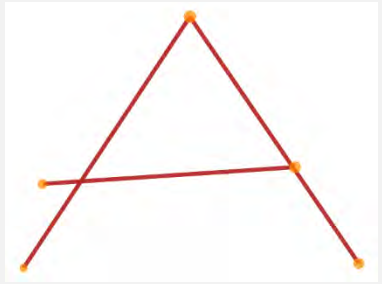
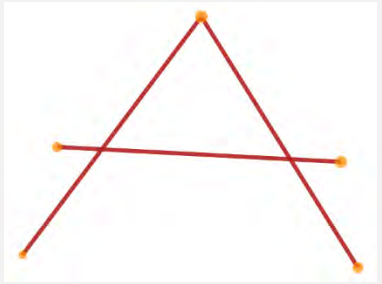
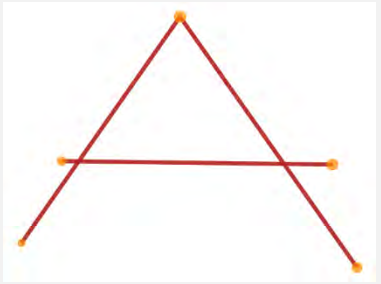
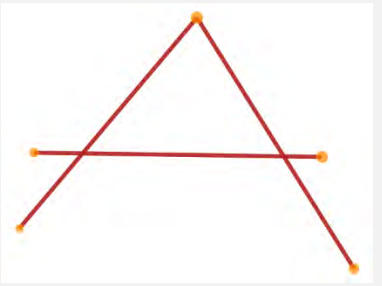
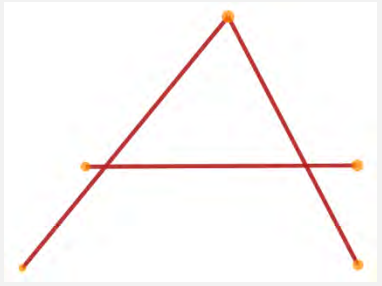
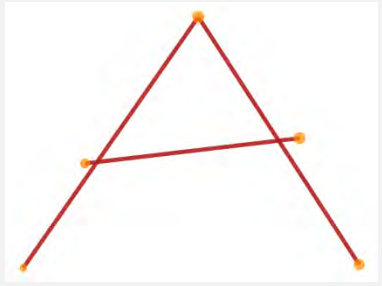
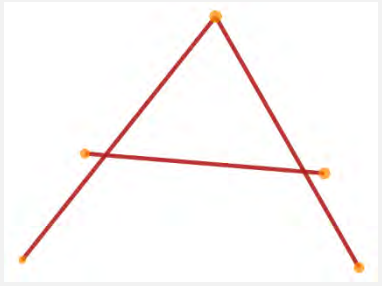
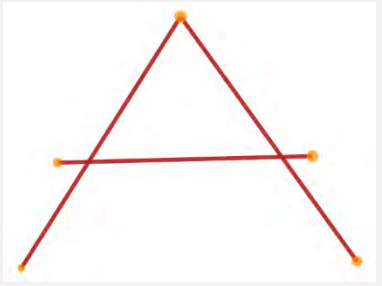
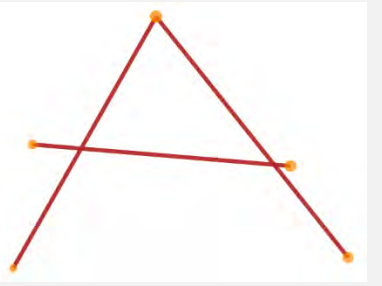
Nye, Tom MW, et al. "Principal component analysis and the locus of the Fréchet mean in the space of phylogenetic trees." *Biometrika* 104.4 (2017): 901-922

Ramsay, James O., and Bernard W. Silverman. *Applied functional data analysis: methods and case studies*. *Springer,* 2007.

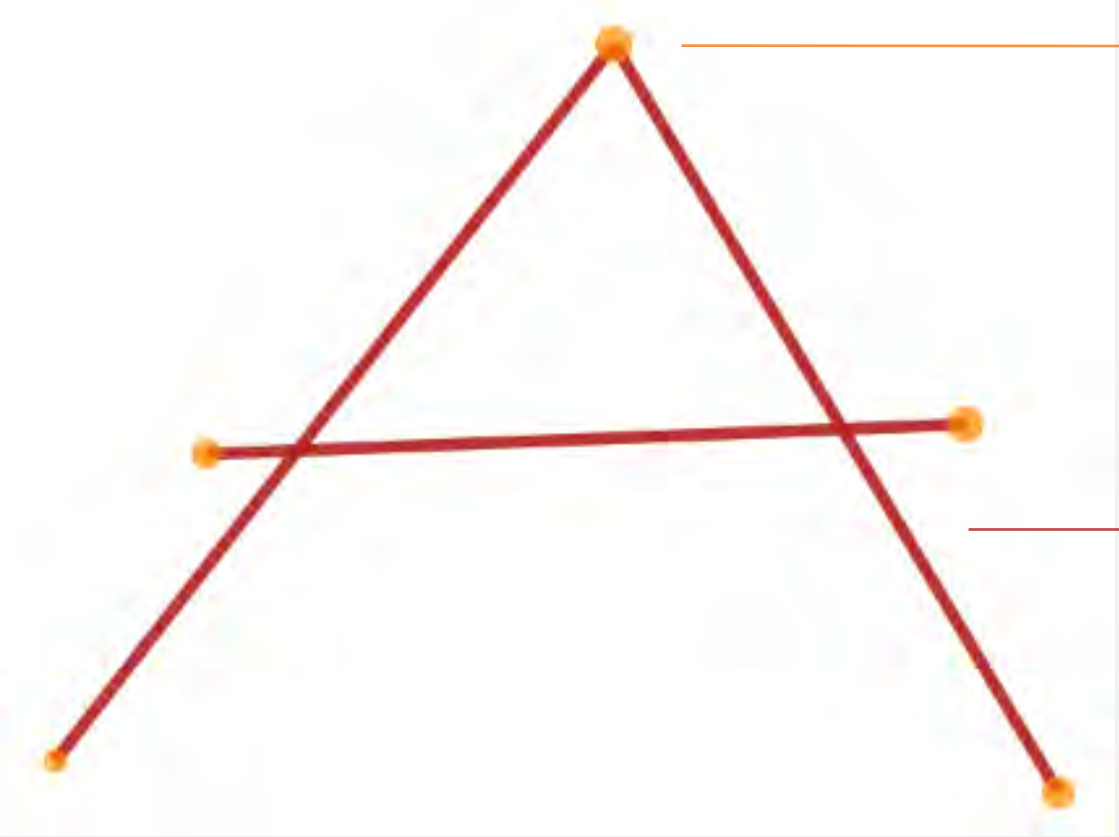
Simpson, Sean L., F. DuBois Bowman, and Paul J. Laurienti. "Analyzing complex functional brain networks: fusing statistics and network science to understand the brain." *Statistics surveys 7* (2013): 1.

Examples

Example: Attributes and Topology

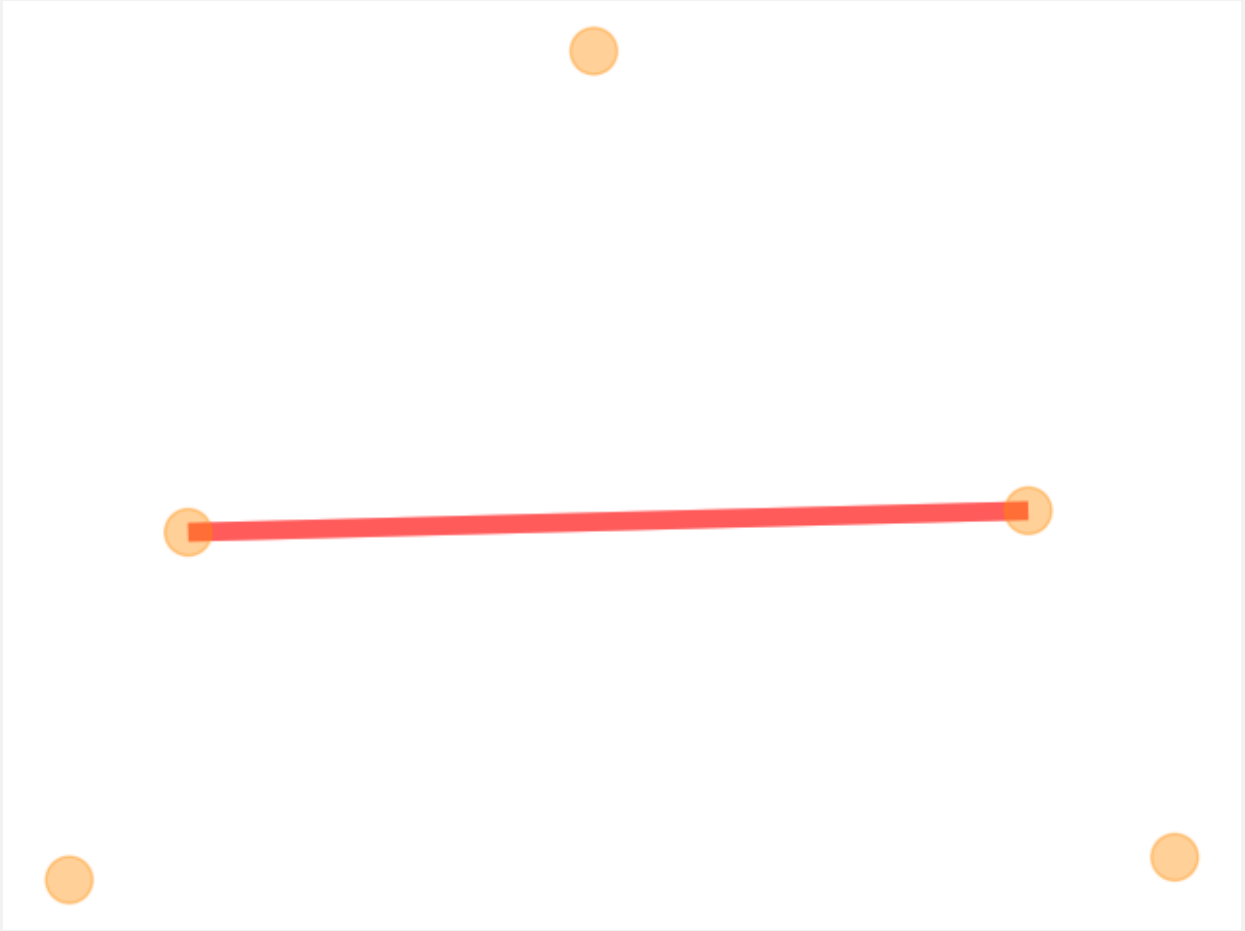
Letters DataSet



(x,y) coordinates

Presence of a drawn line

Letters DataSet



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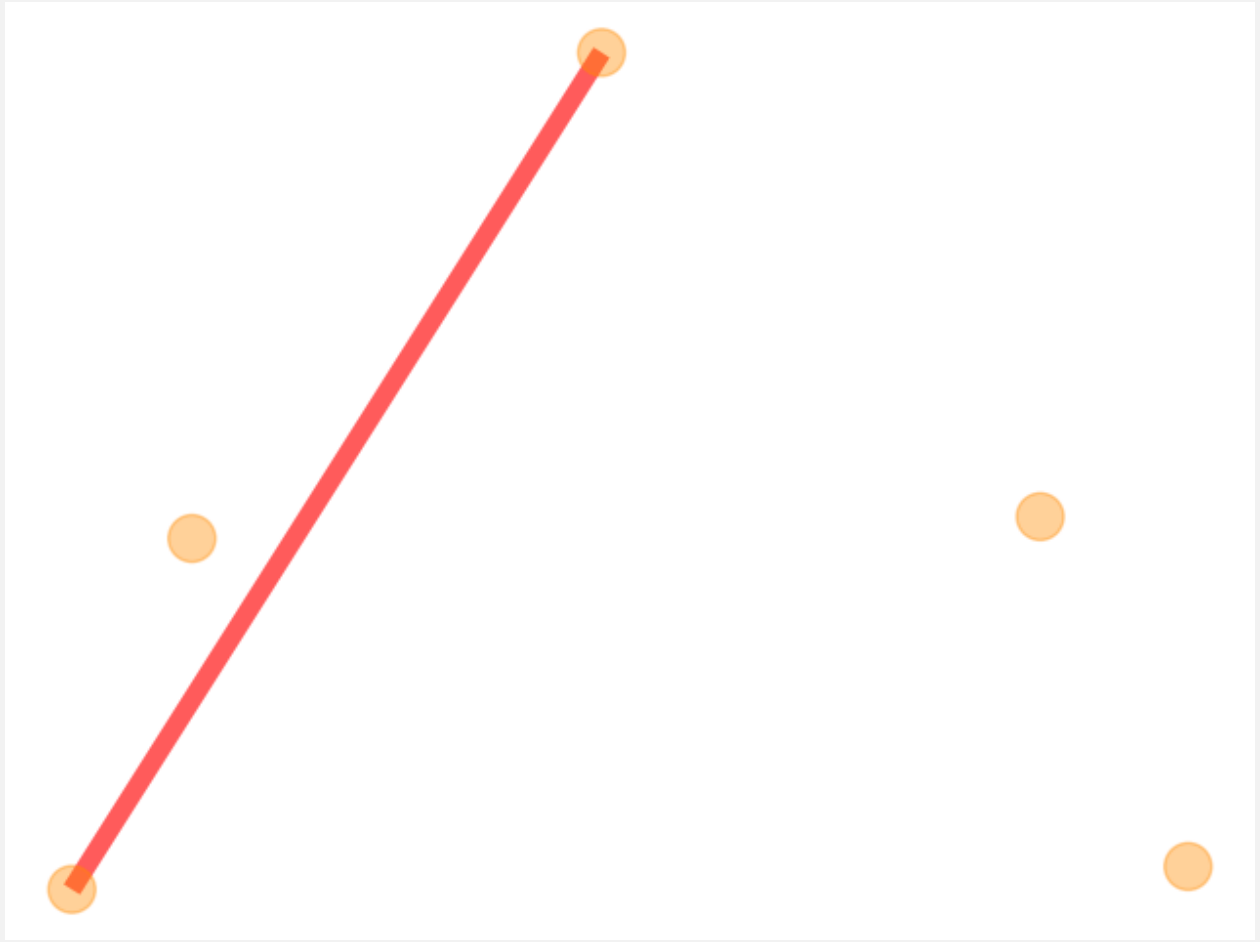
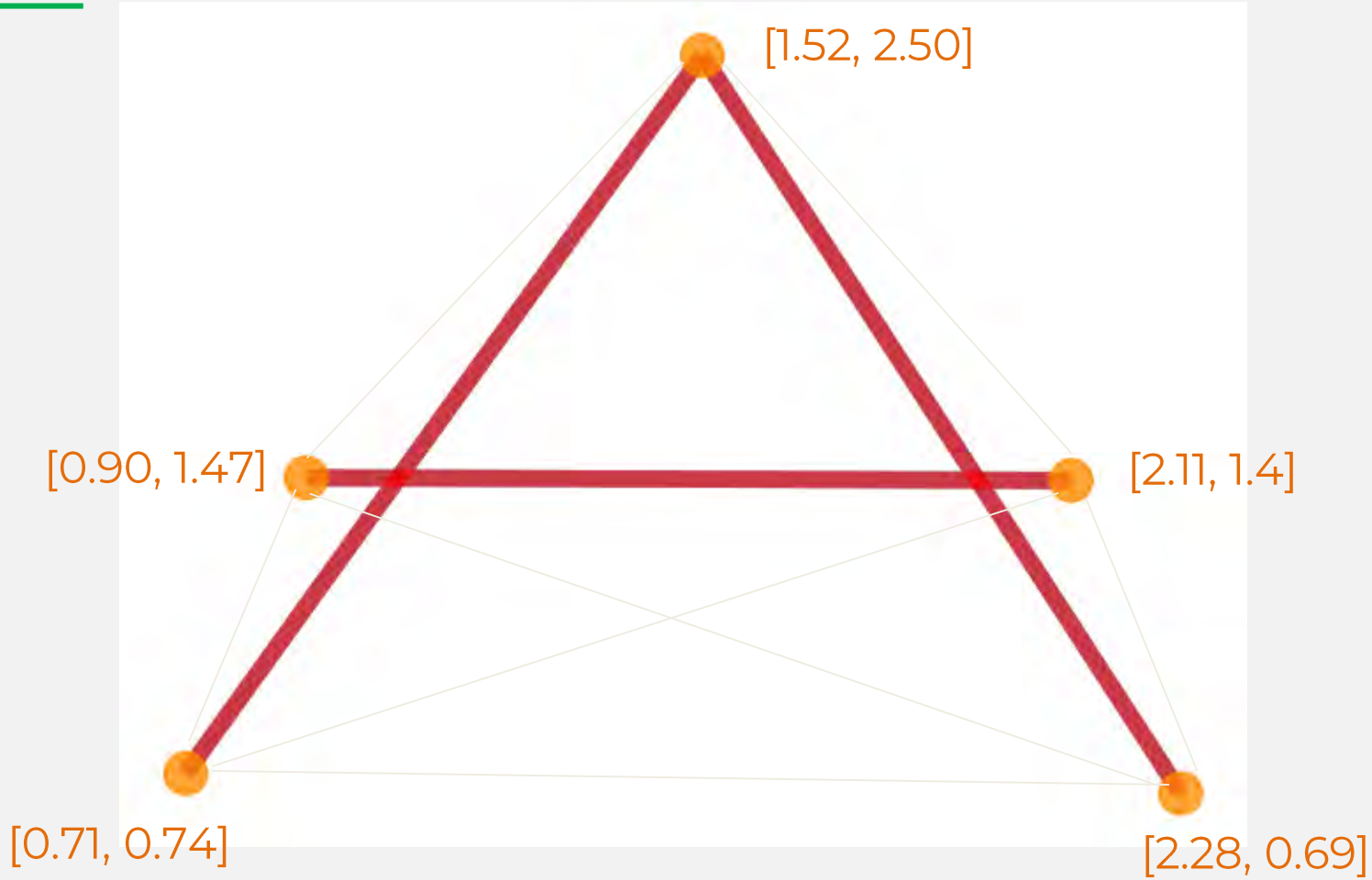
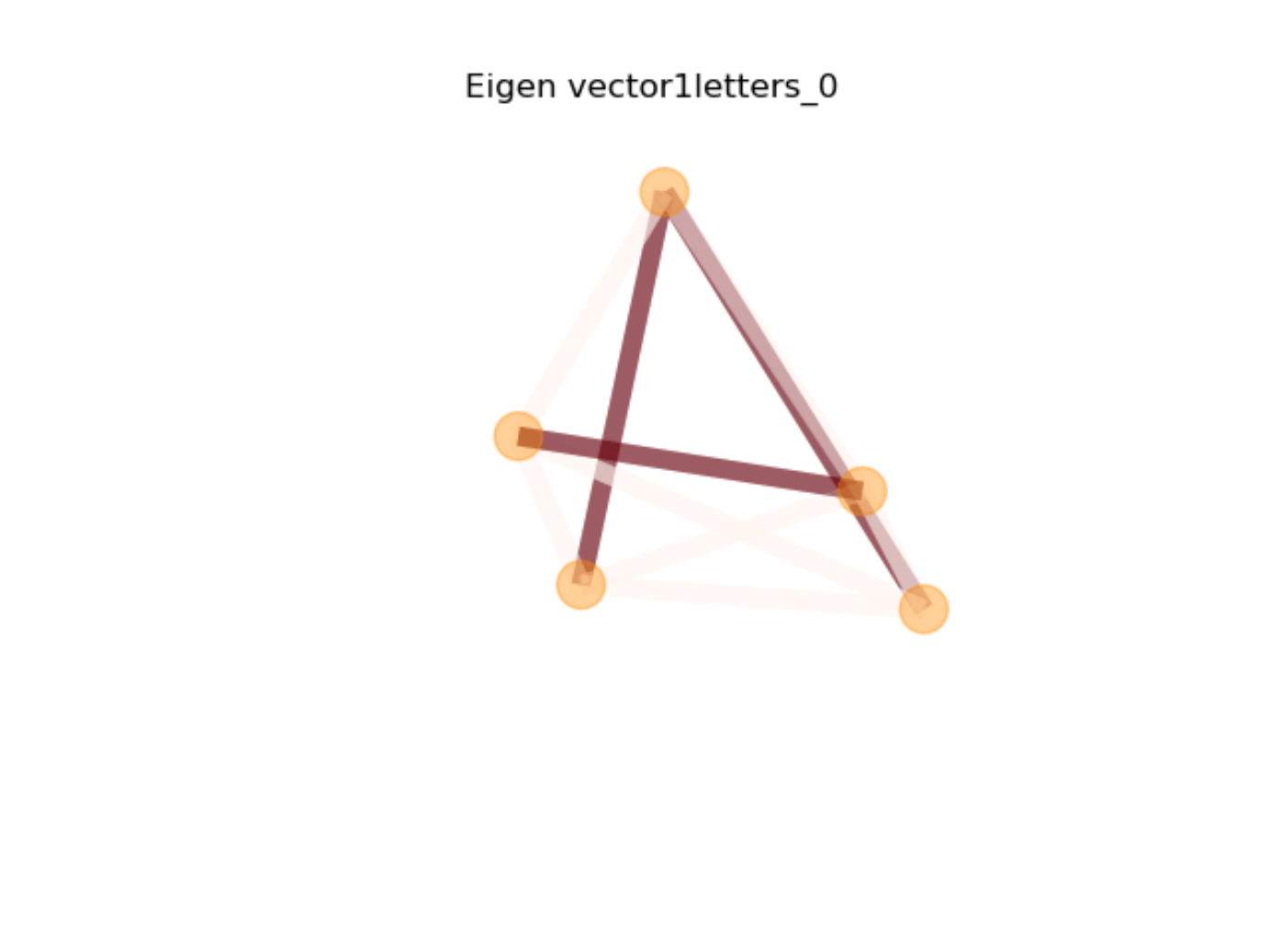


A mean



Geodesic Principal Component Analysis

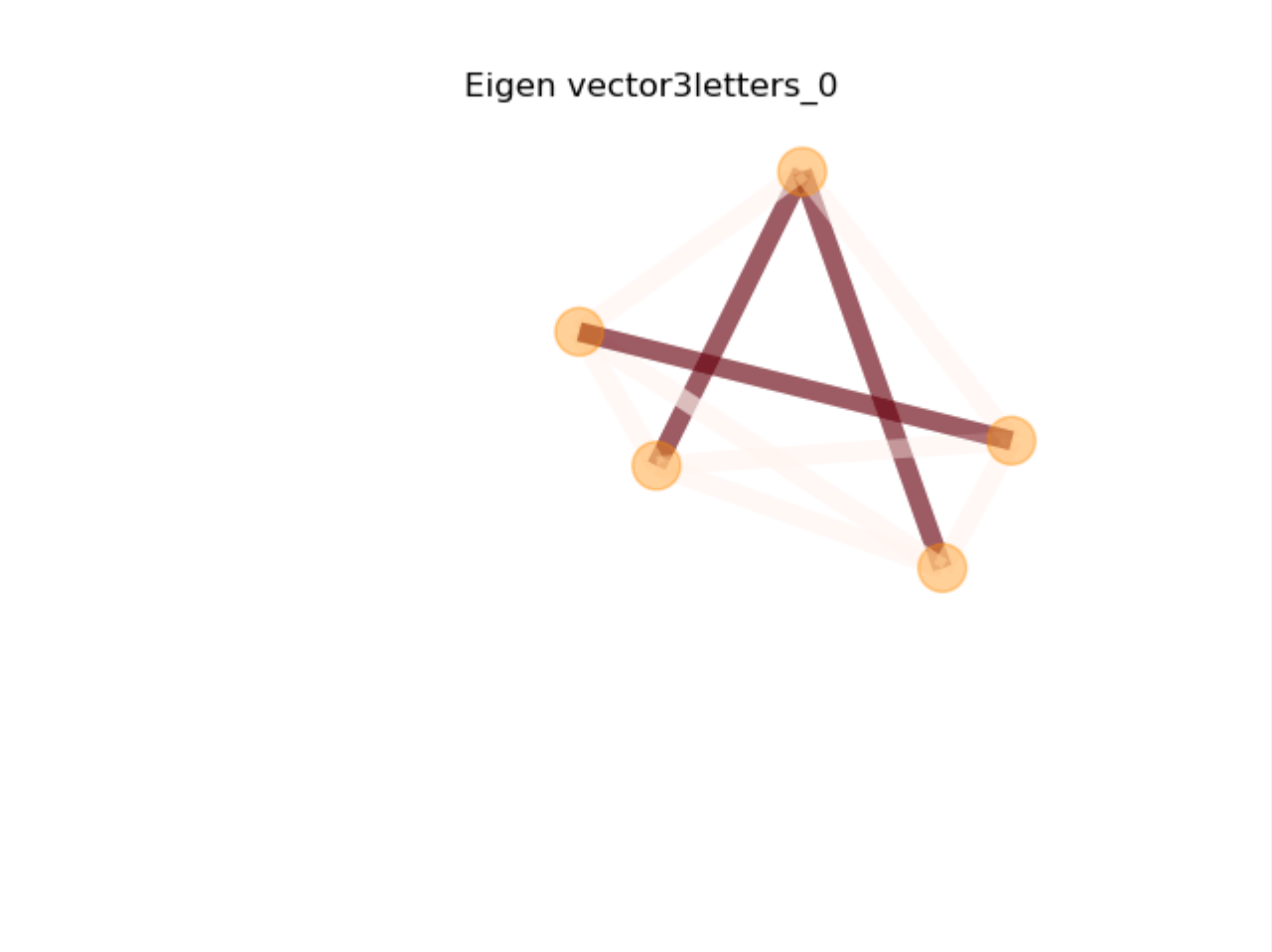


Capturing 18% of the total variance

Geodesic Principal Component Analysis

Capturing 16% of the total variance

Geodesic Principal Component Analysis



Capturing 14% of the total variance

Observation about different cases

	EDGES: All	EDGES: Not All
NODES: All same number	✓	✓ With intensity edge attributes or no attribute
NODES: Different number	✗	✓ With intensity edge and nodes attributes or no attribute