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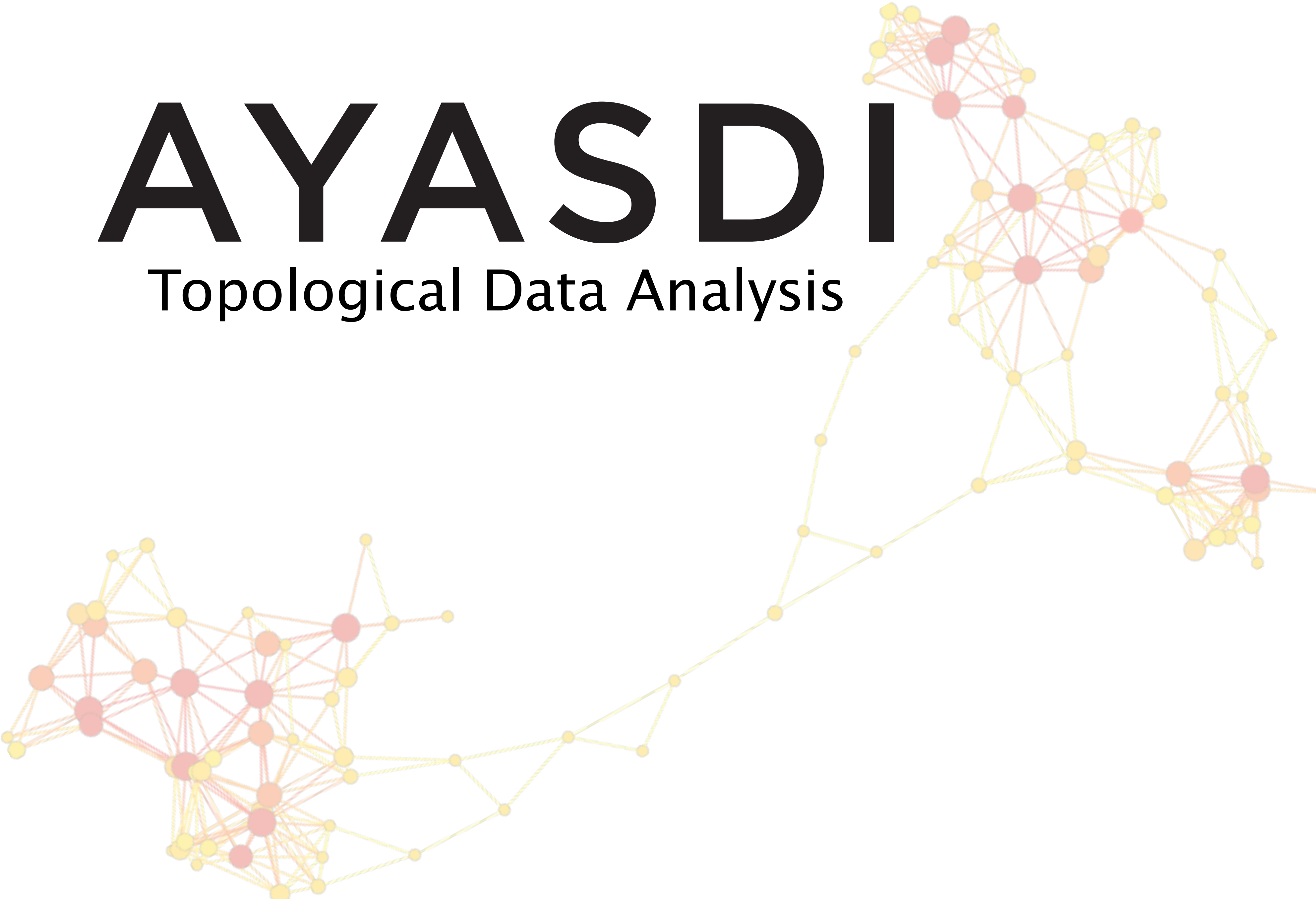
Topological Data Analysis



Data has **Shape**, Shape has **Meaning**, Meaning drives **Value**

Data Basics

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Data Basics

Q: What is the fundamental assumption when working with data?

Data Basics

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A: Distance between two data points

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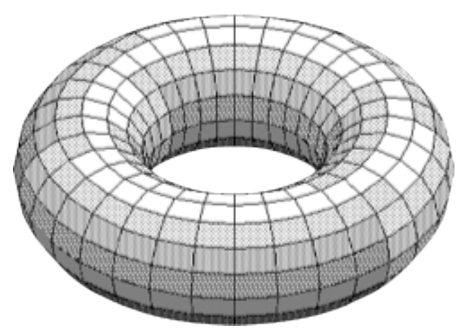
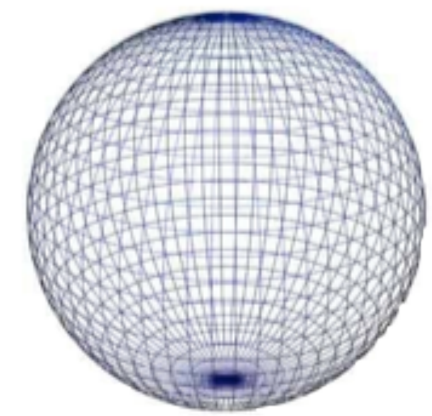
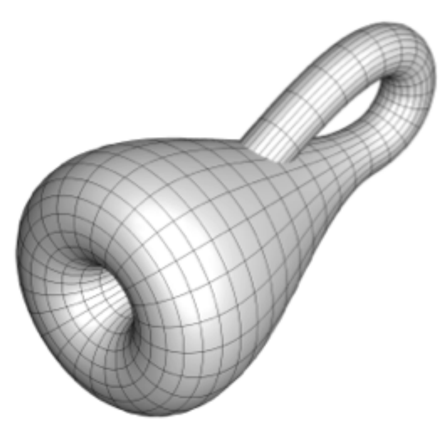
Why Topology?

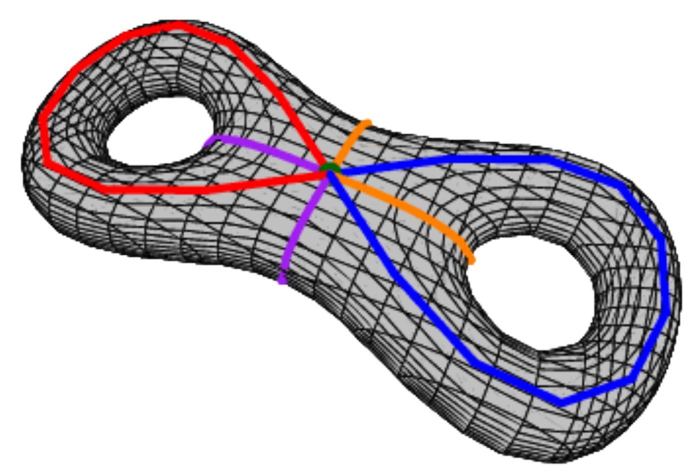
Topology

The branch of mathematics concerned with characterizing the geometric properties of shape









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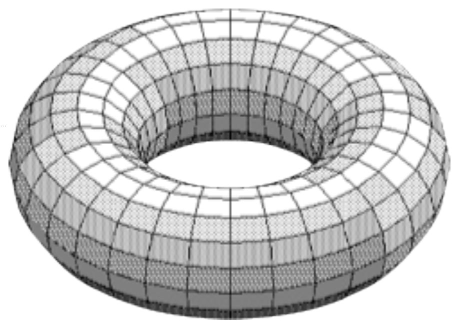
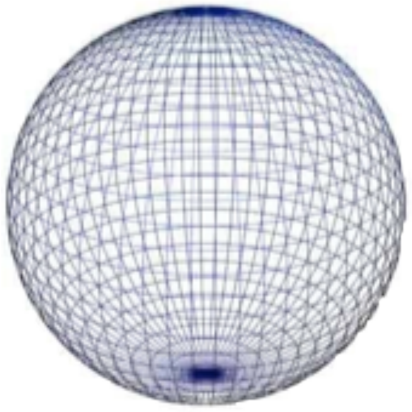
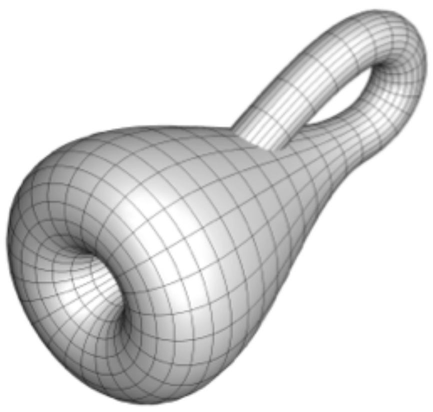
Why Topology?

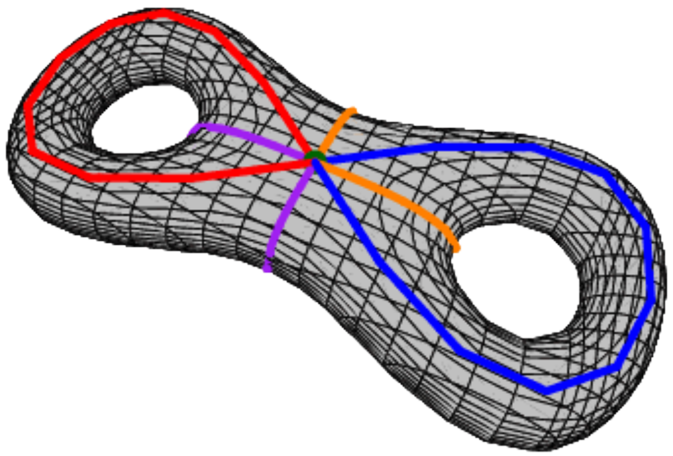
Topology
The branch of mathematics concerned with characterizing the geometric properties of shape

- Coordinate Invariant
- Deformation Invariant
- Compressed Representations









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Drop the Assumptions

Let the data tell you what information it holds

Traditional Analytics

- Assumes linearity or normal distributions
- Assume a model of behavior
- Low Dimensionality

Topological Data Analysis

- Assumes a measure of similarity
- Evaluate and correct models
- High Dimensionality

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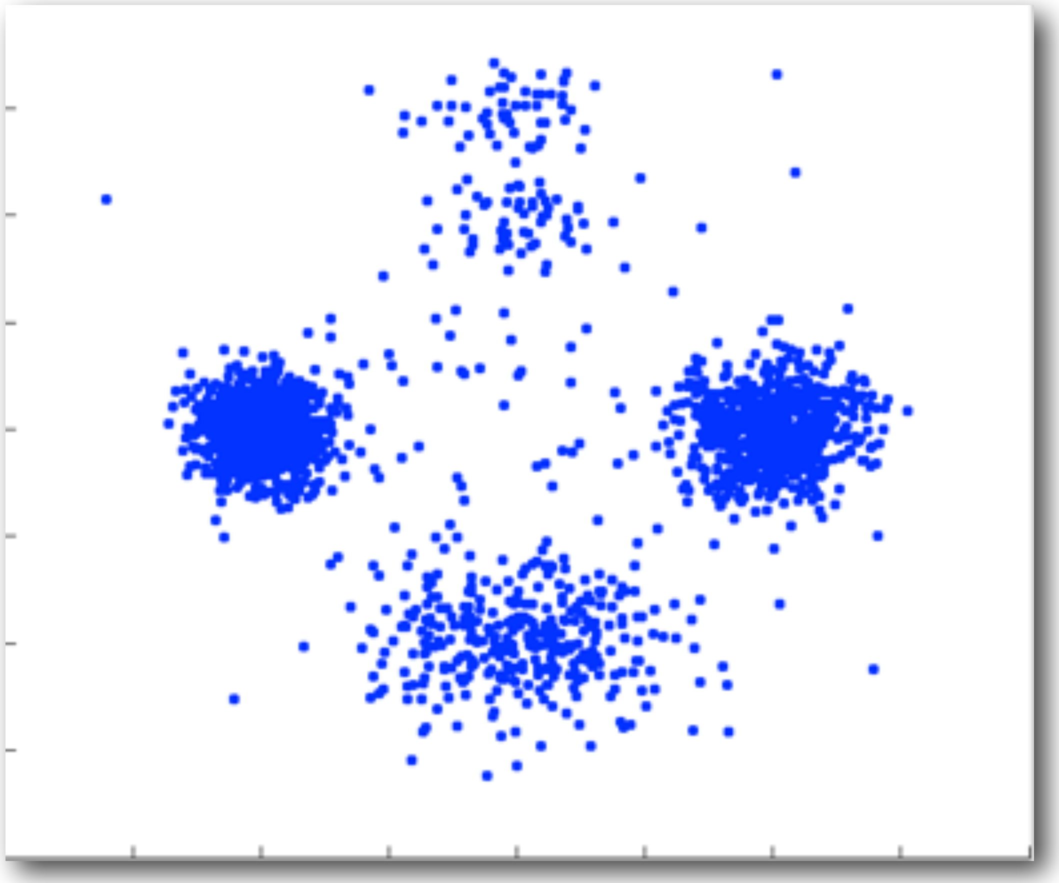
Topological Data Analysis

Using local information to gain global knowledge



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Topological Data Analysis

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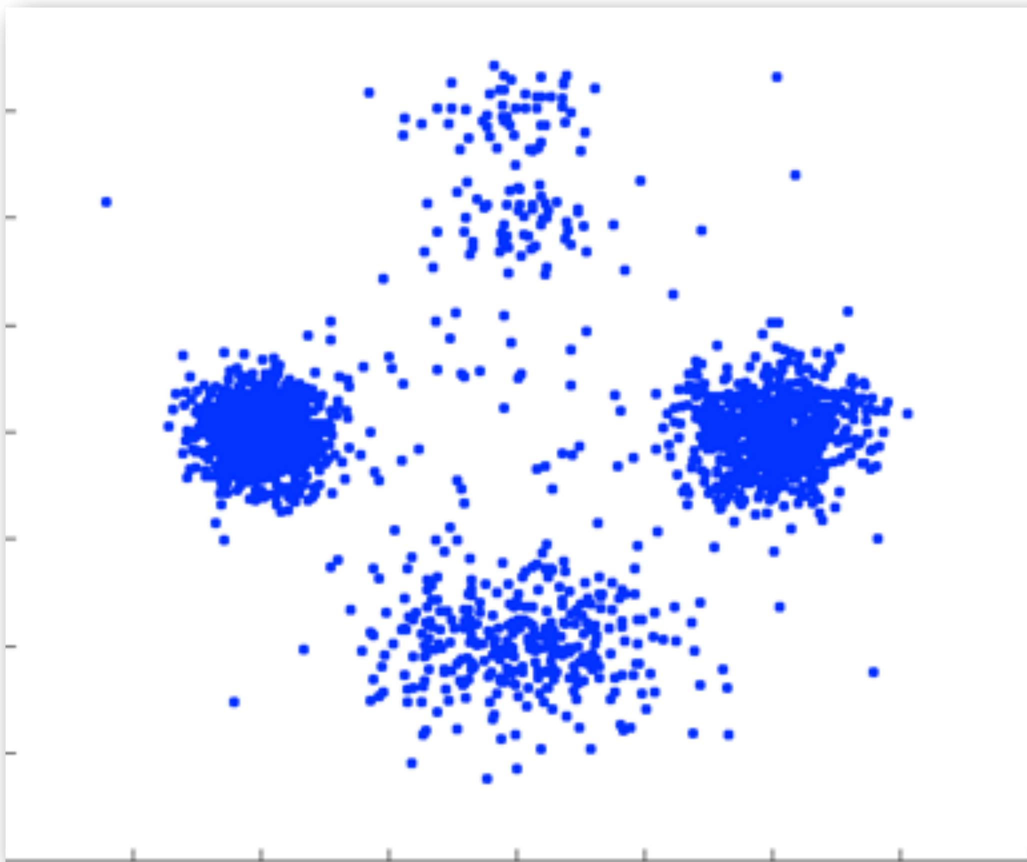
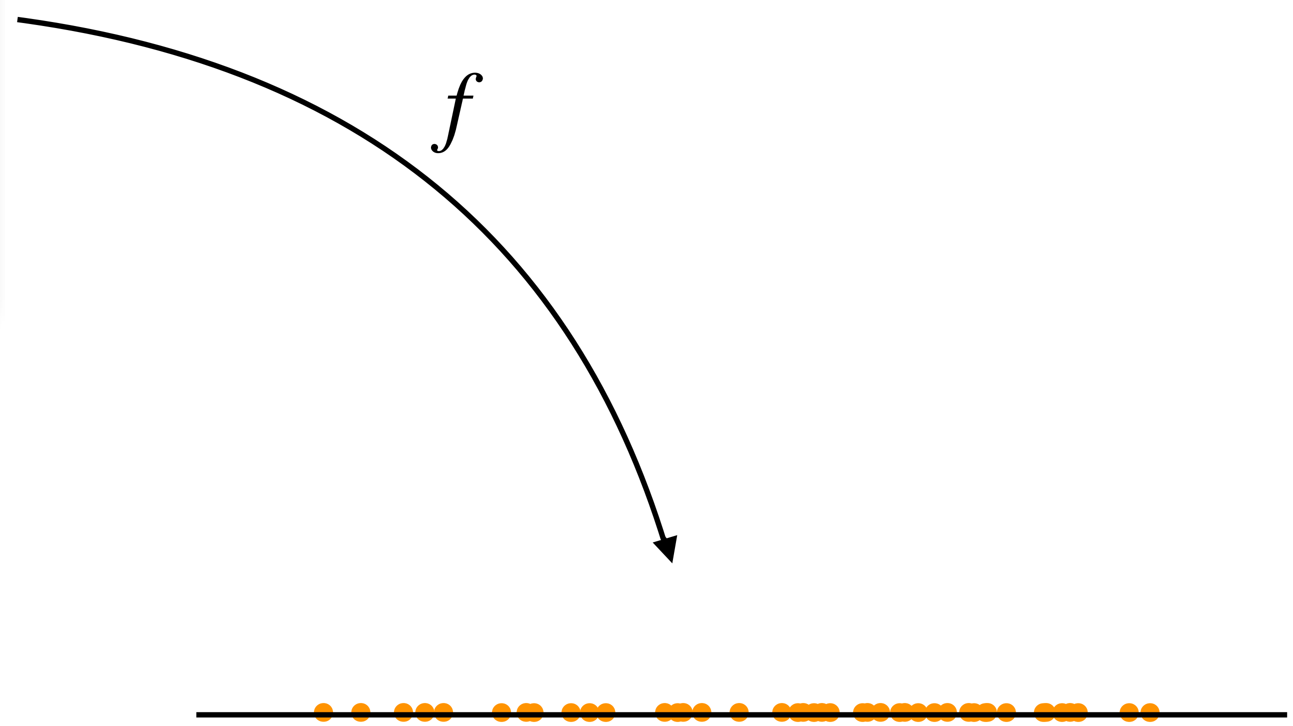


f is a function from the data to some other space (e.g. the real line)



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Topological Data Analysis

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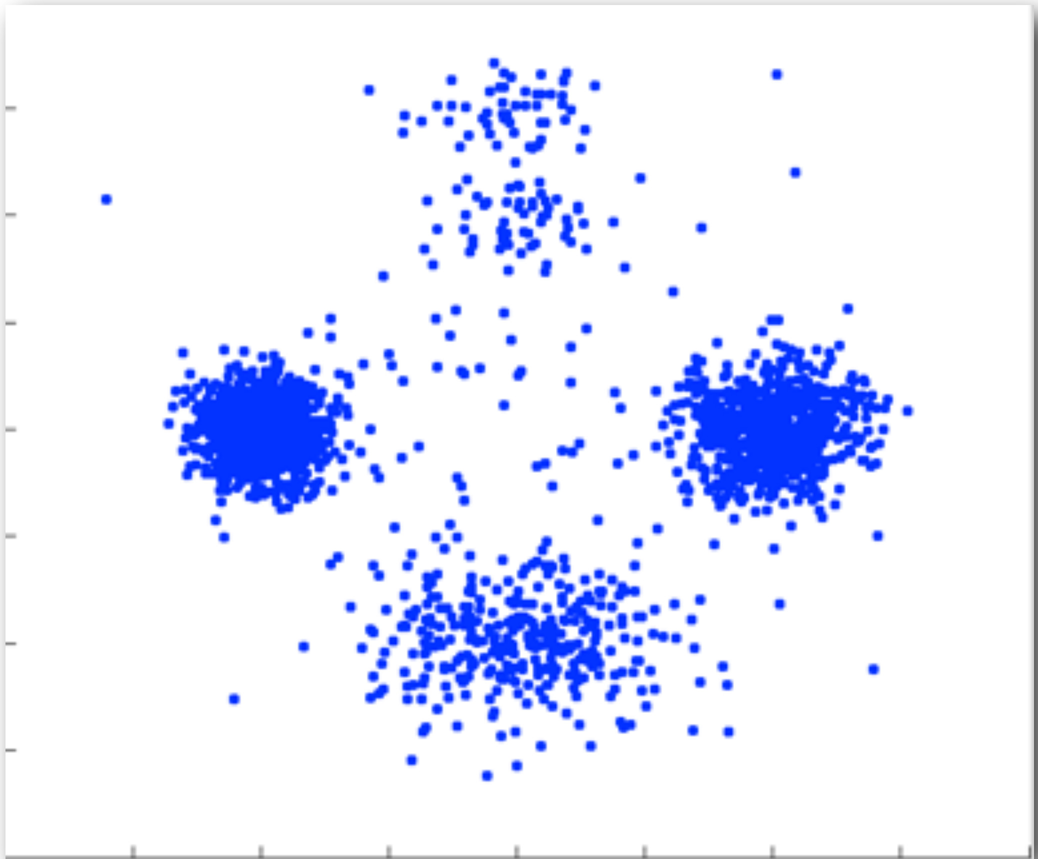
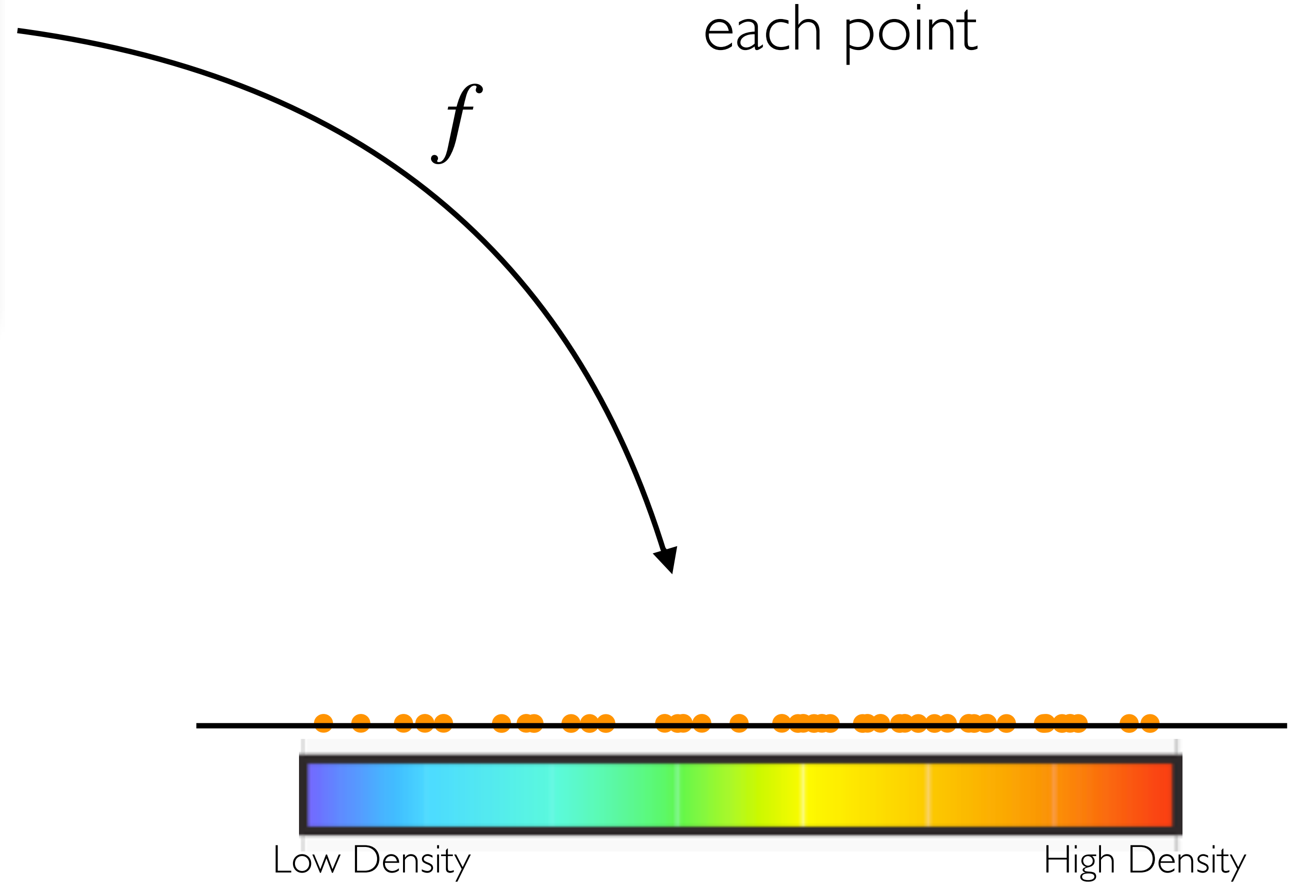


f is a function from the data to some other space (e.g. the real line)

In this example, f is a density estimator at each point



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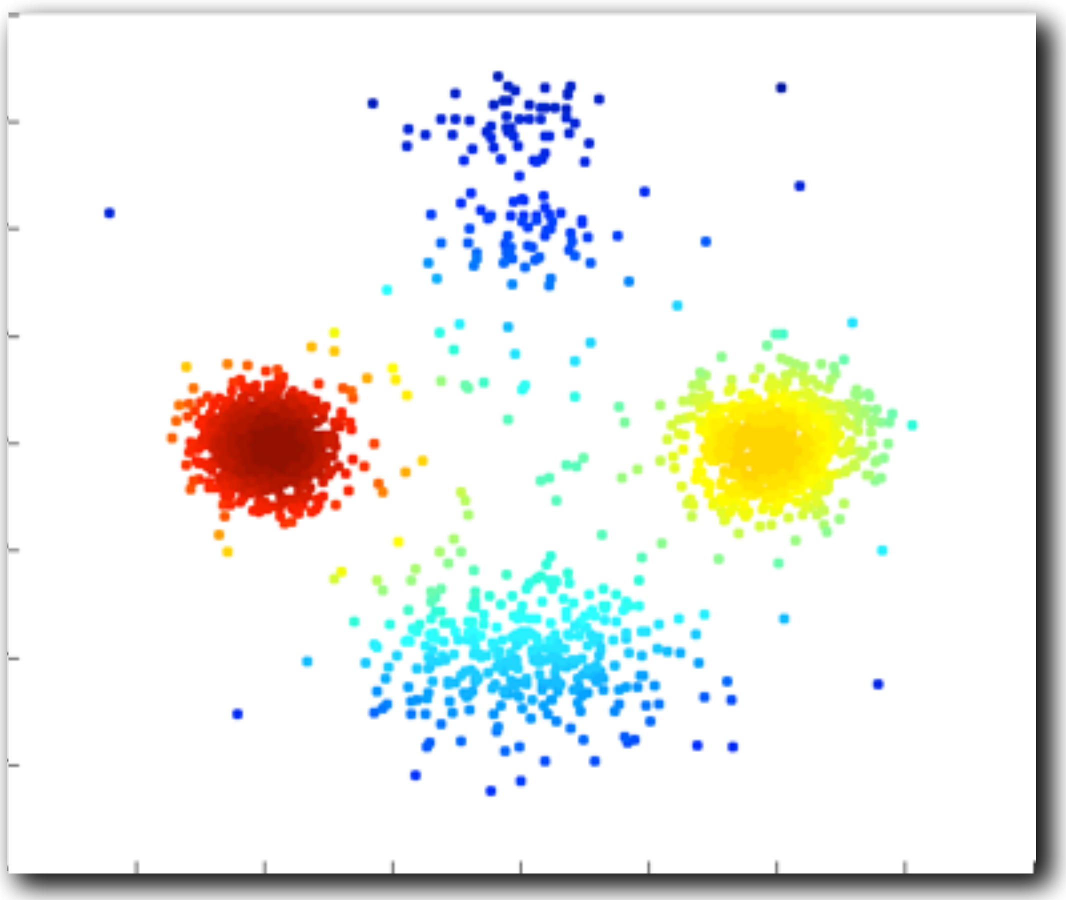
Topological Data Analysis

Using local information to gain global knowledge



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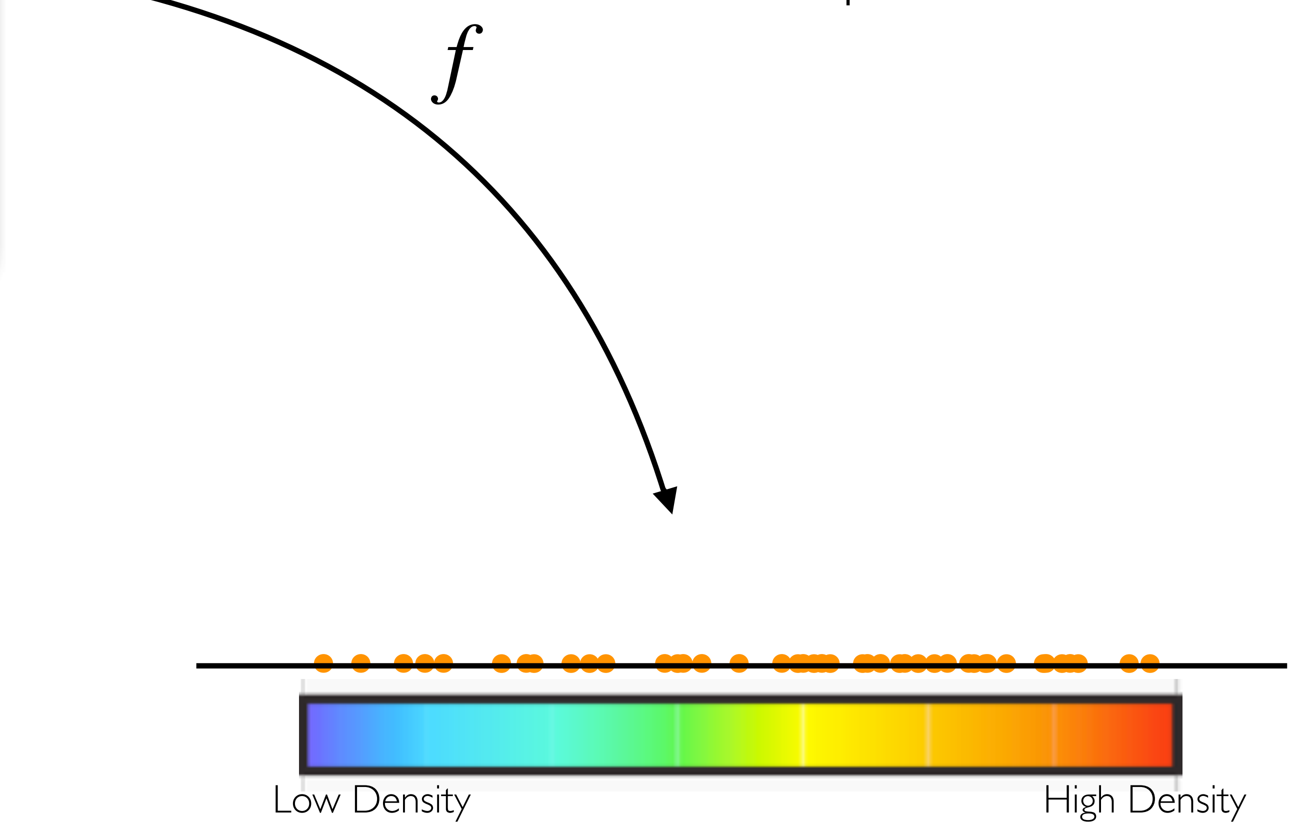
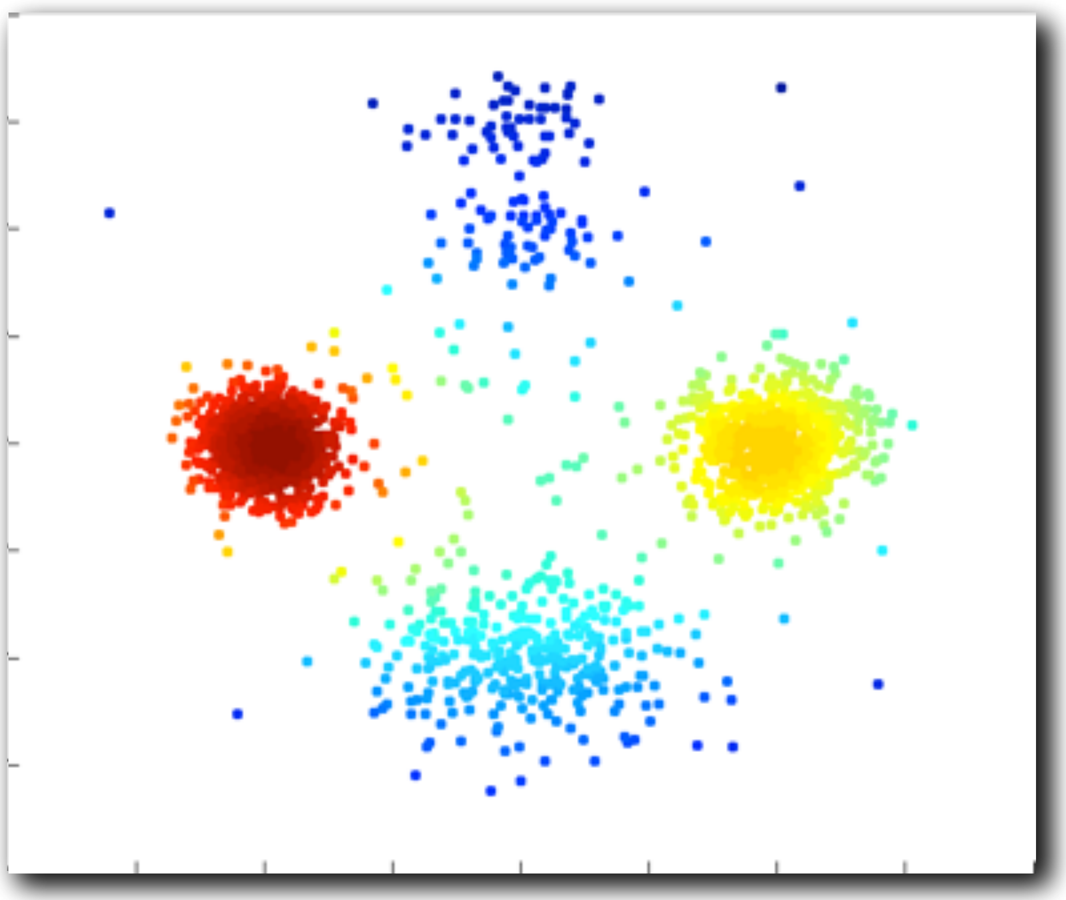
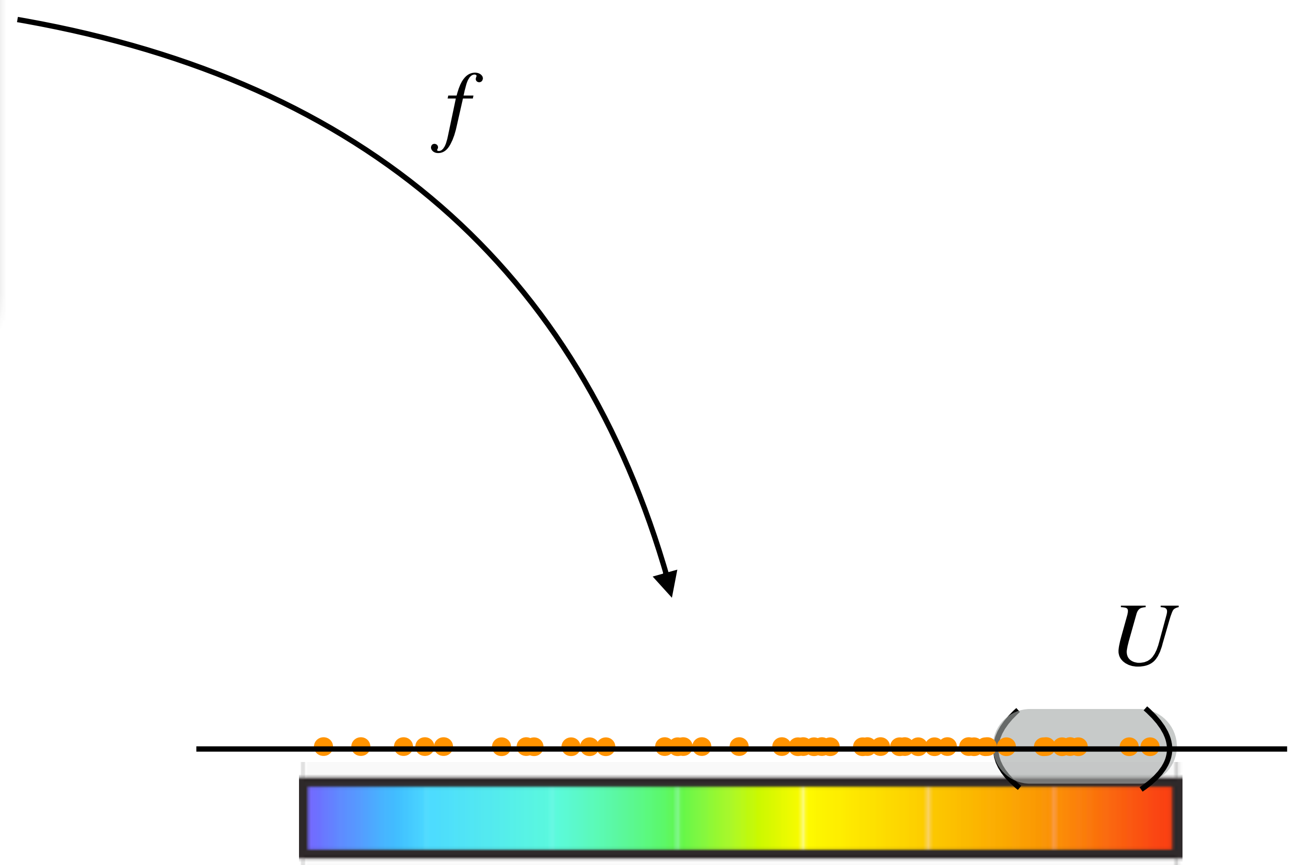


Topological Data Analysis

Using local information to gain global knowledge



U defines a set of similar points in the image of f



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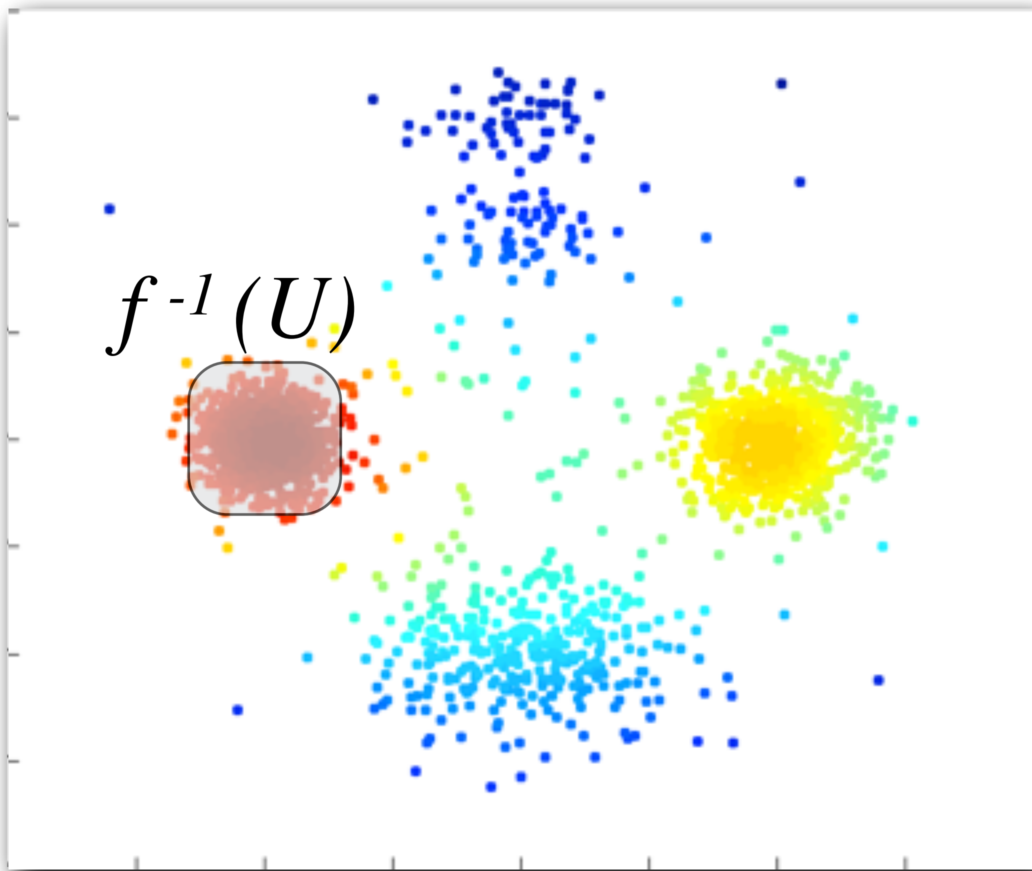
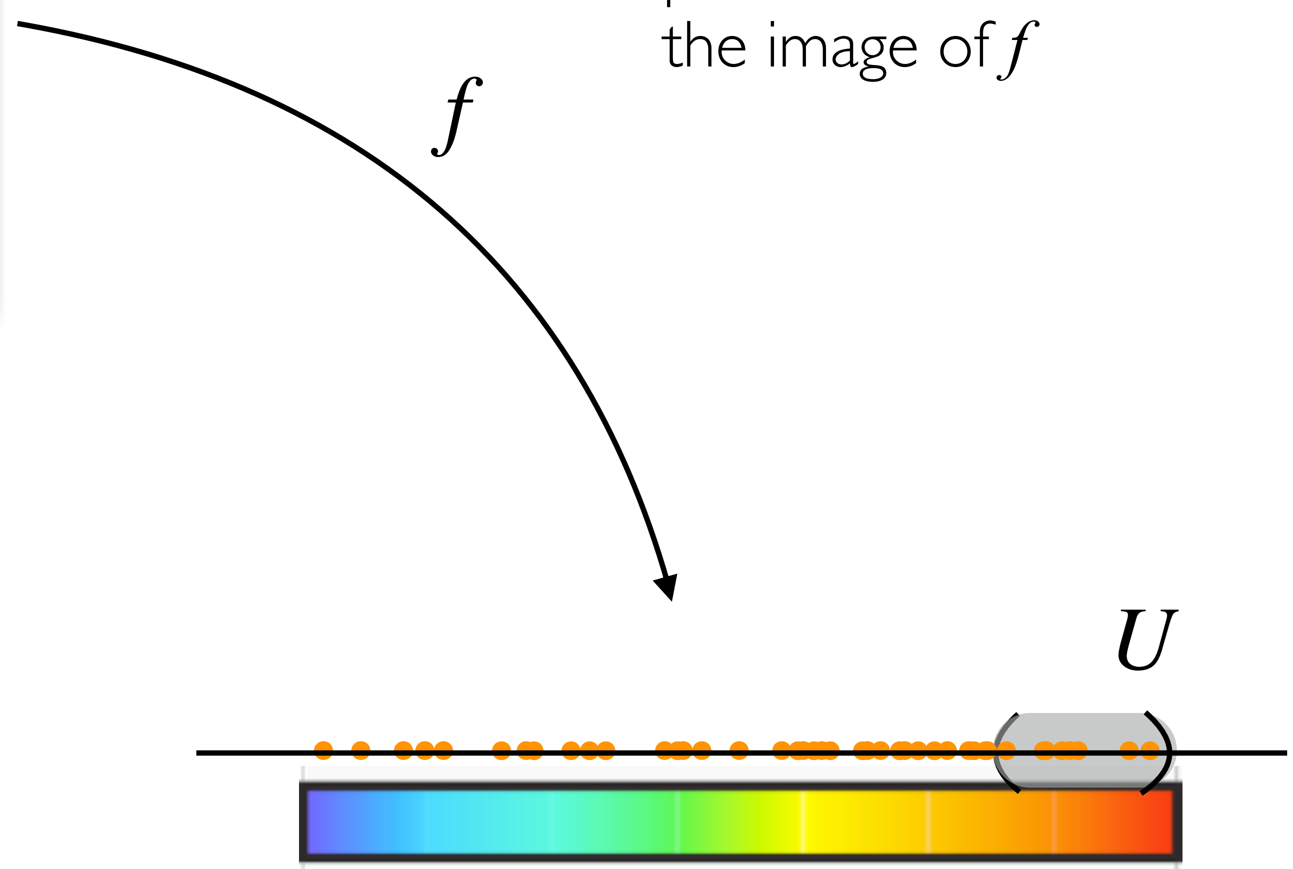
Topological Data Analysis

Using local information to gain global knowledge



U defines a set of similar points in the image of f

$f^{-1}(U)$ is a set of data points that are similar in the image of f



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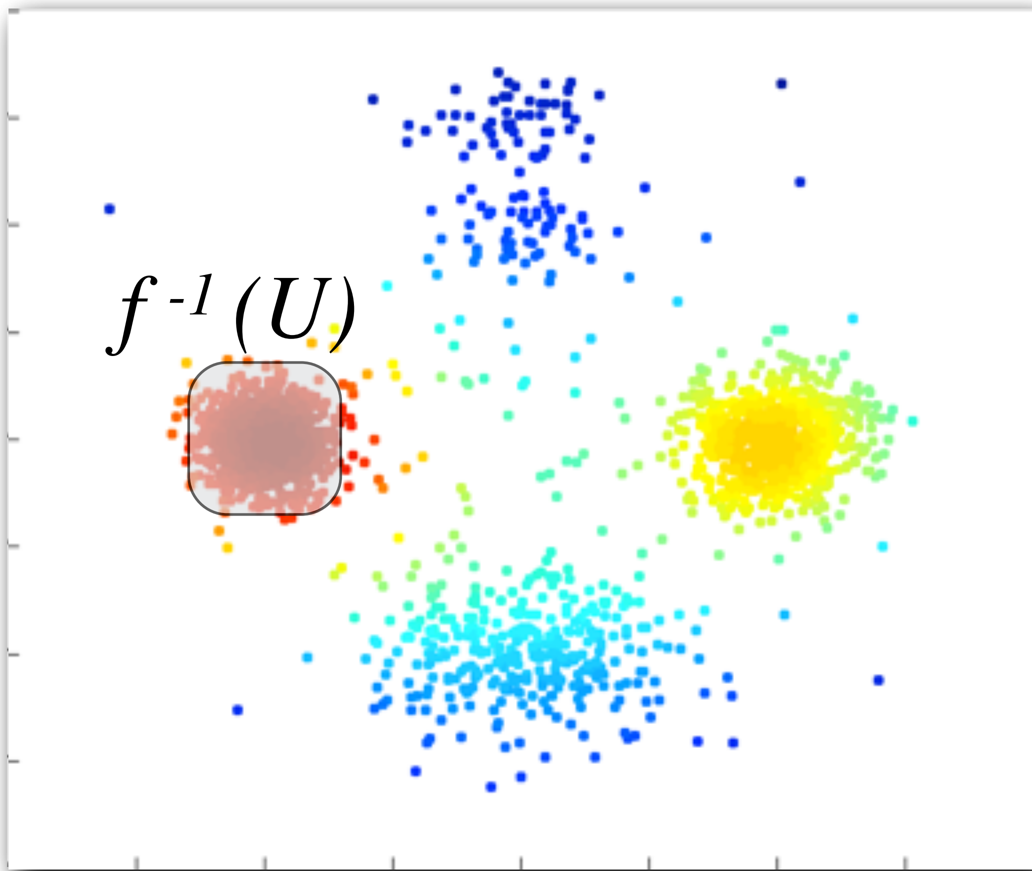
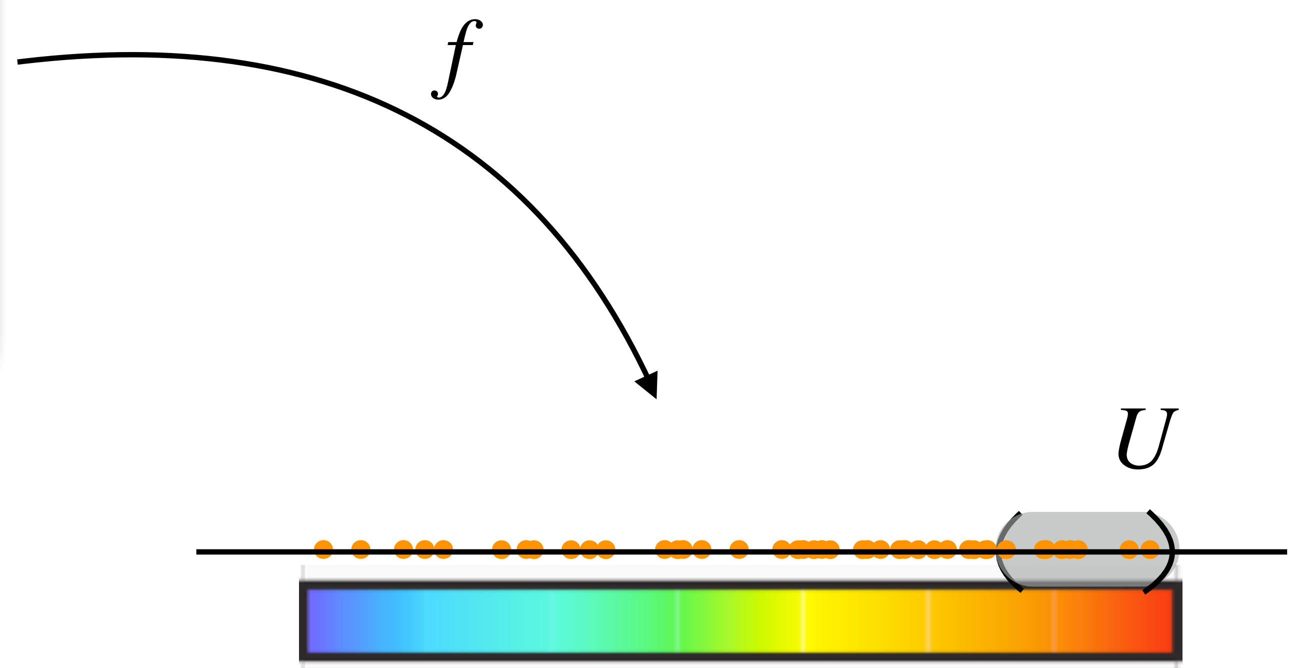
Topological Data Analysis

Using local information to gain global knowledge



Using the metric, perform clustering to determine the sets of similar points in $f^{-1}(U)$



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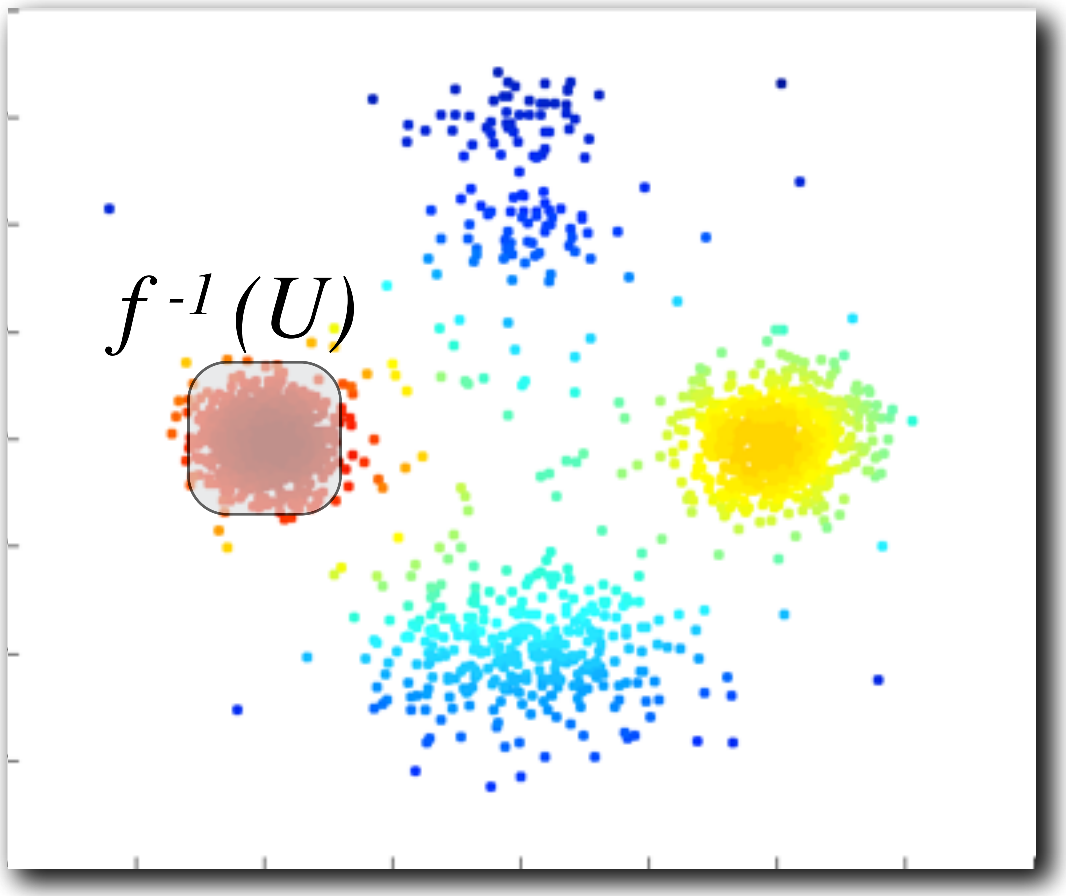
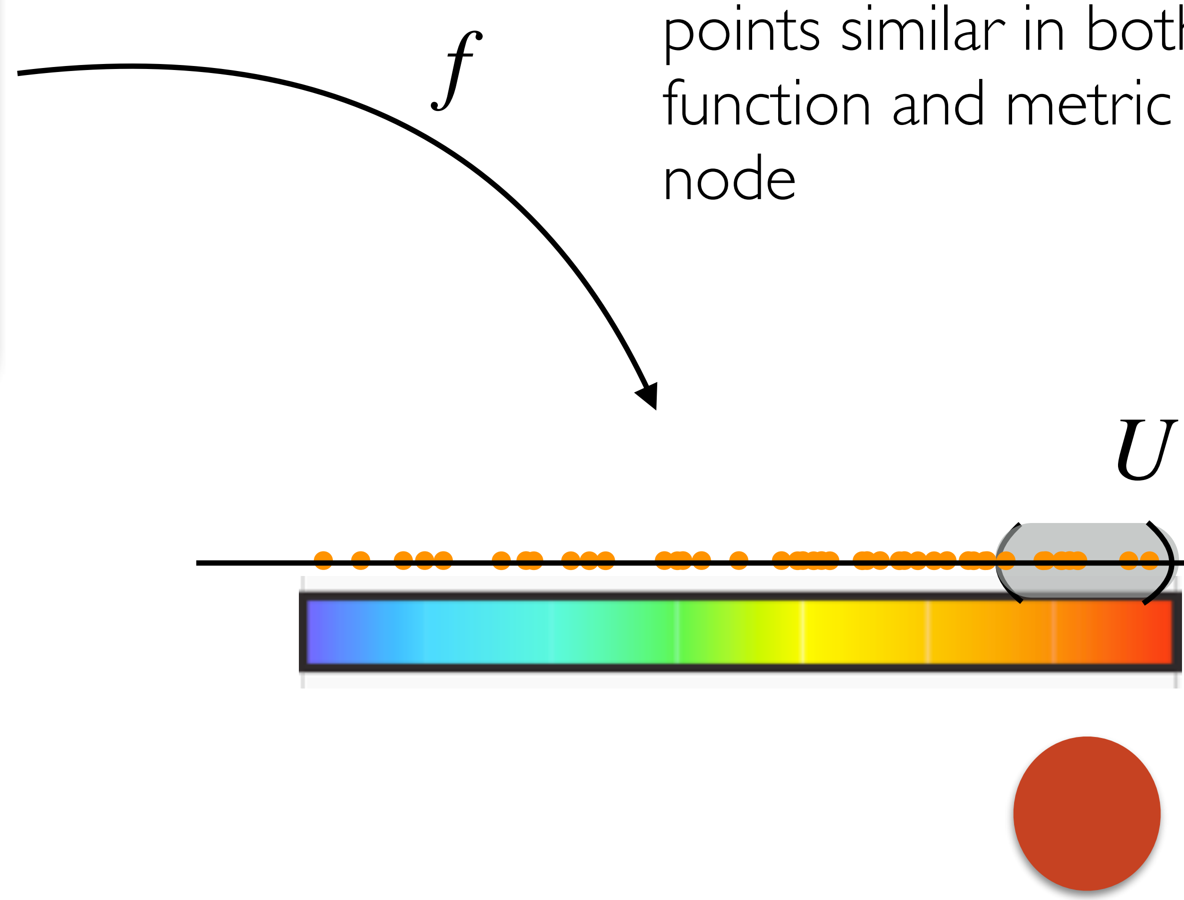
Topological Data Analysis

Using local information to gain global knowledge



Using the metric, perform clustering to determine the sets of similar points in $f^{-1}(U)$

Represent each set of points similar in both function and metric as node



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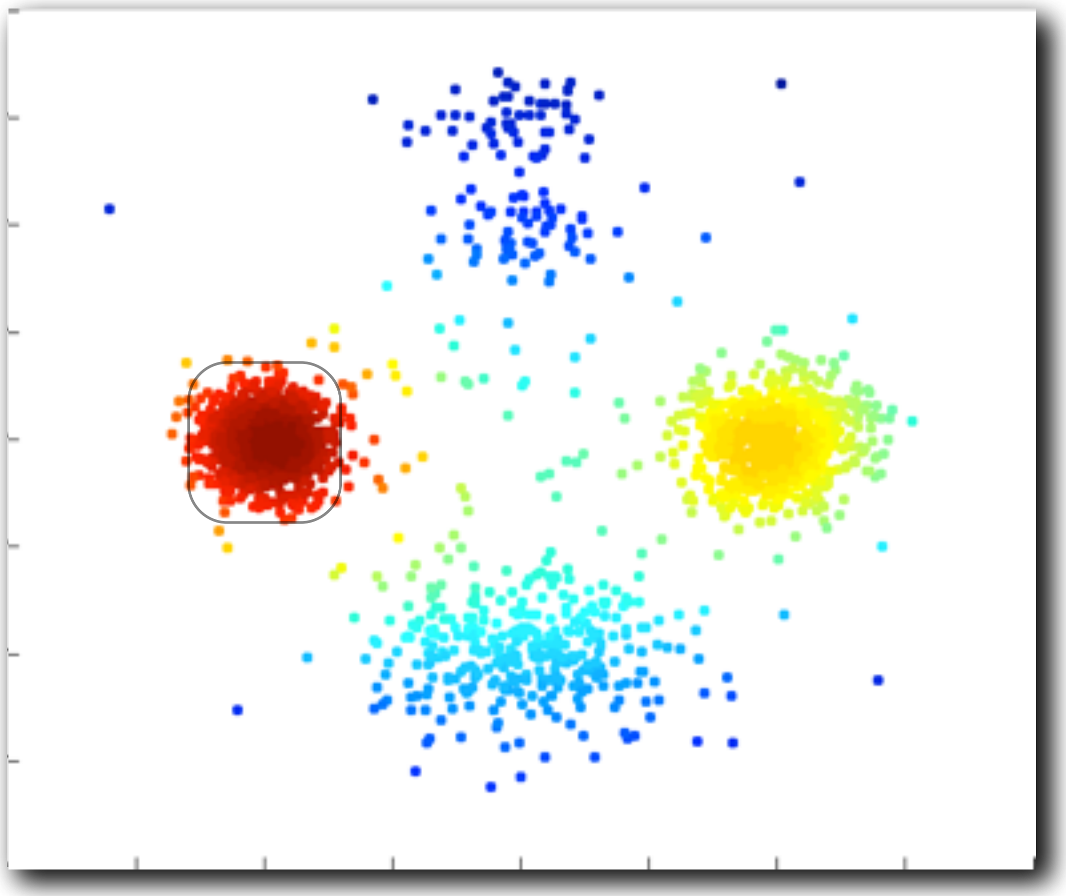
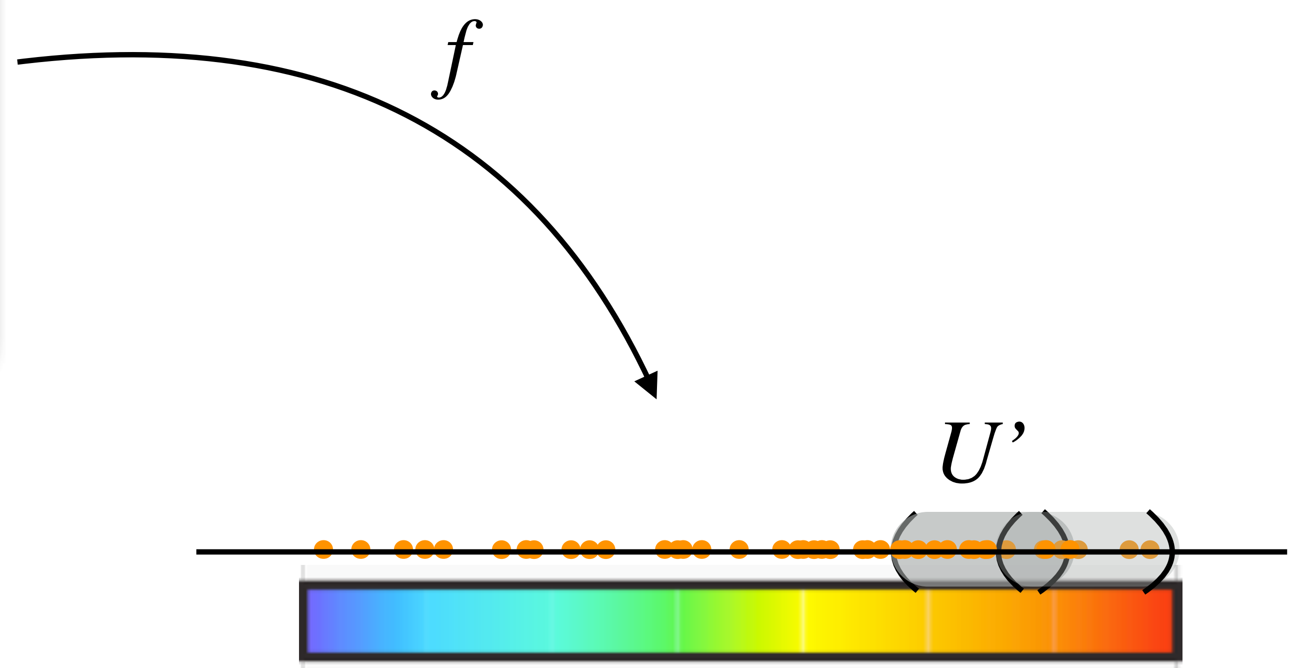


Repeat process with a different set of similar points in the image of the function



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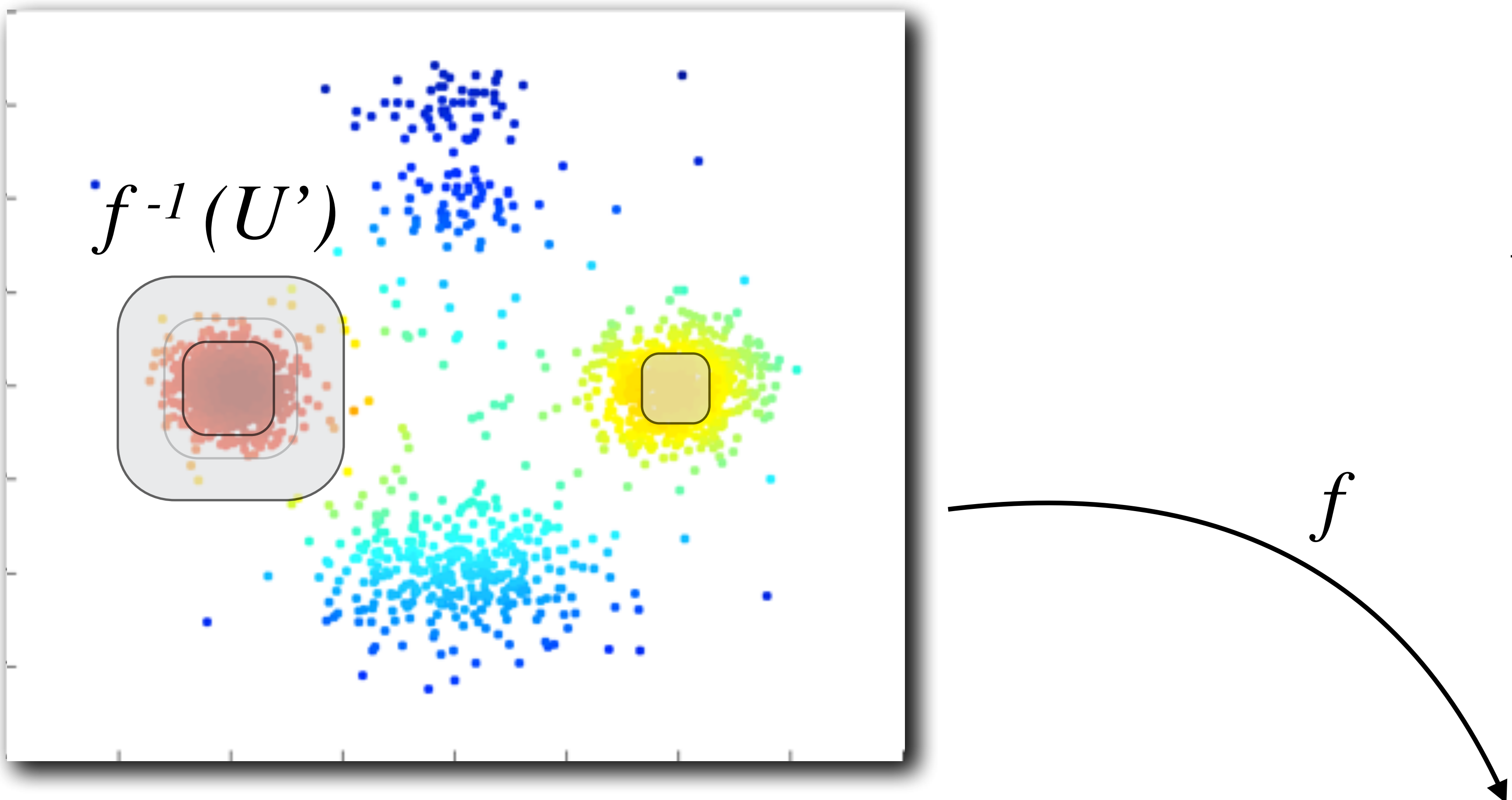
Topological Data Analysis

Using local information to gain global knowledge



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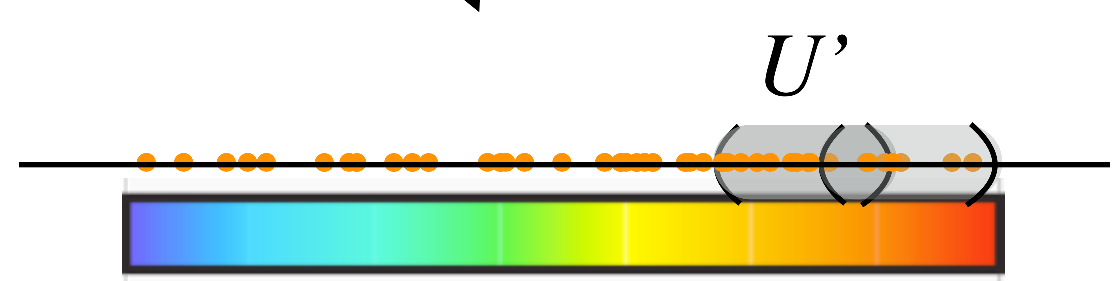

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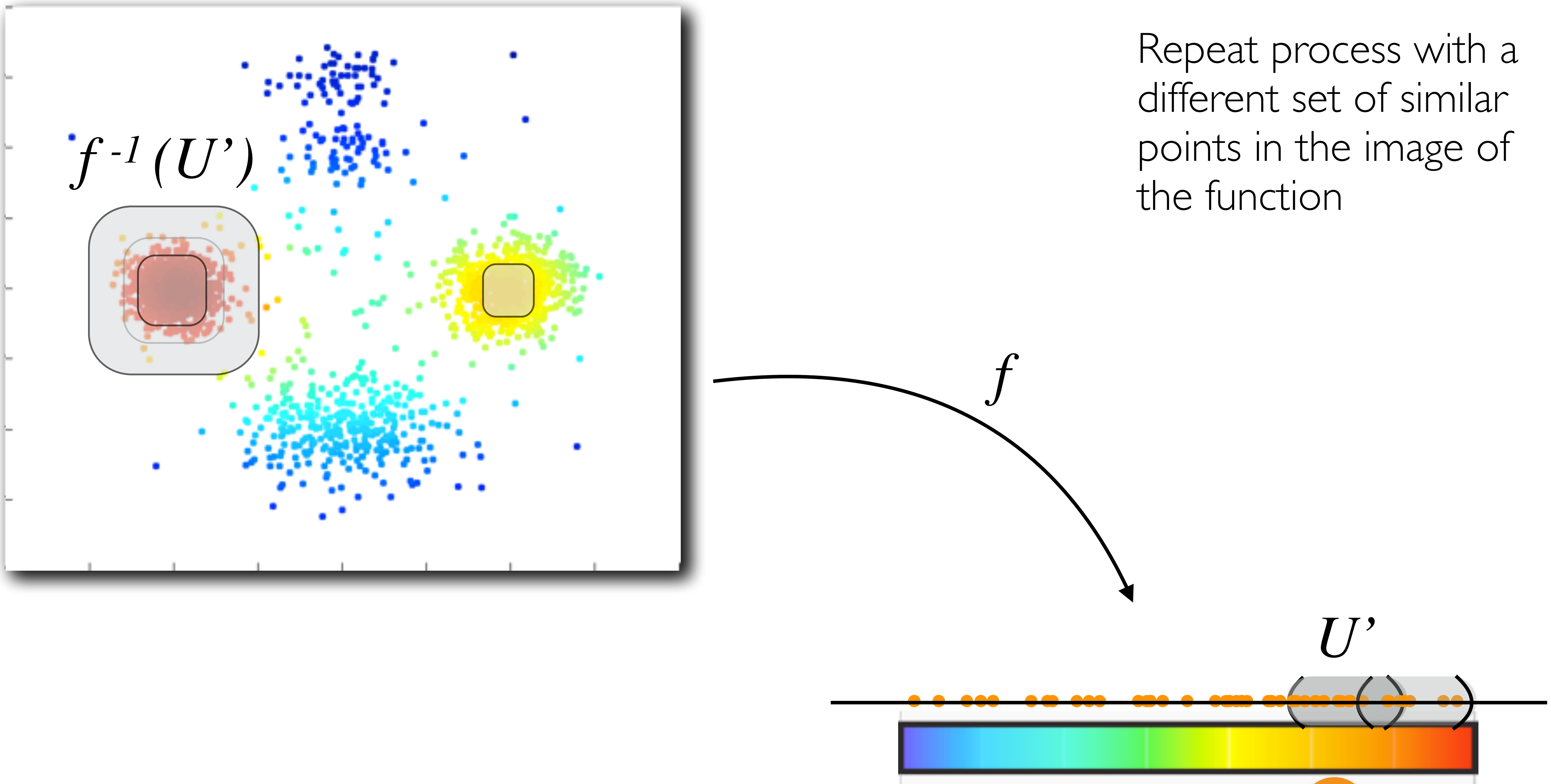
Using local information to gain global knowledge



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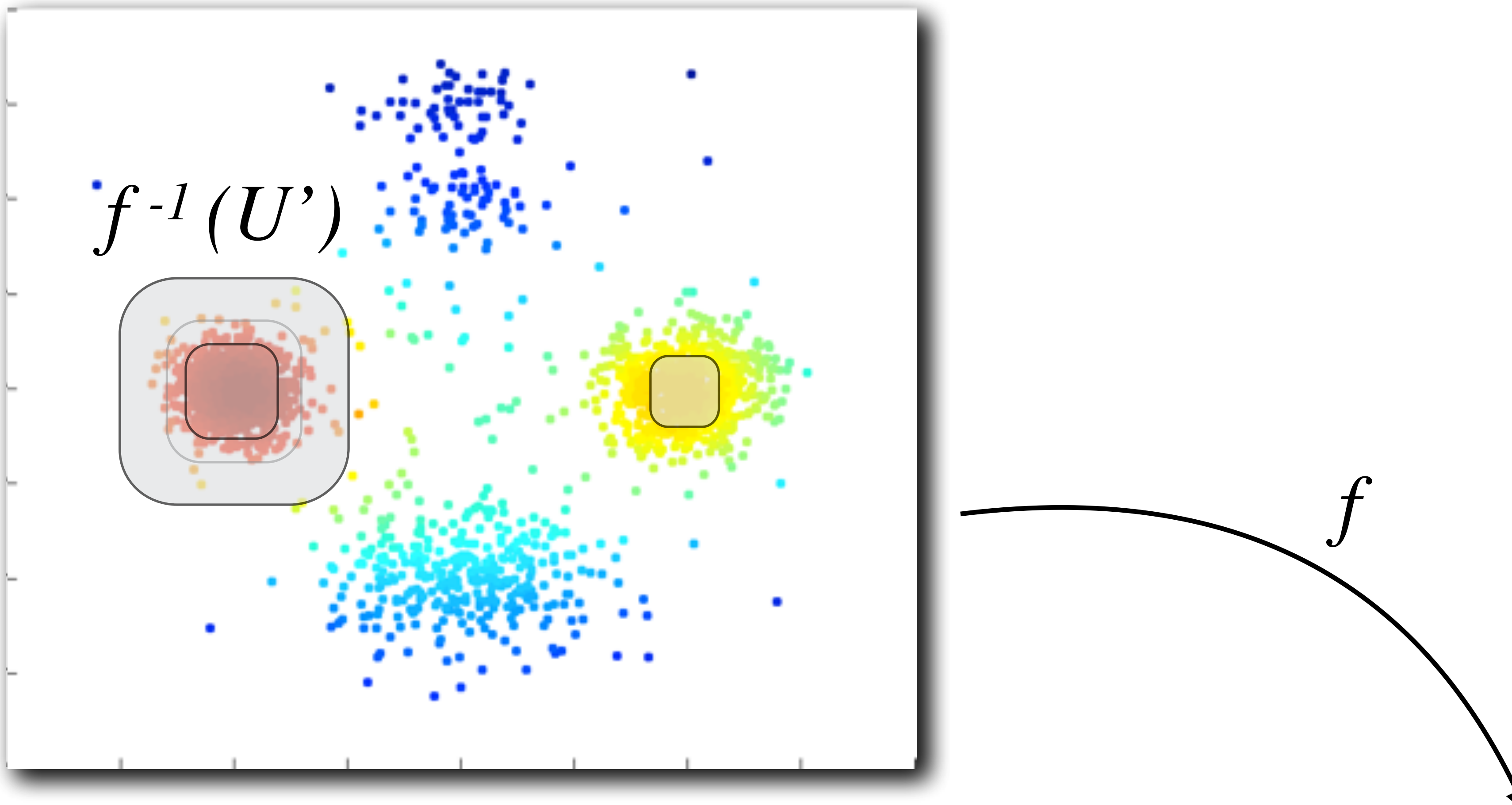

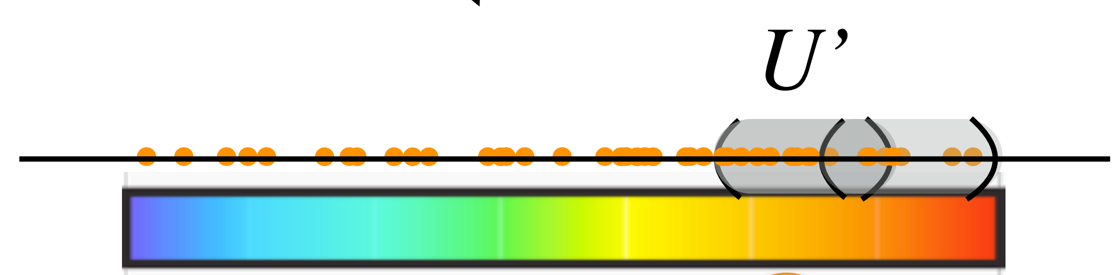

Repeat process with a different set of similar points in the image of the function

Edges between nodes indicate overlapping points. They capture the continuous nature of the data when viewed through the function

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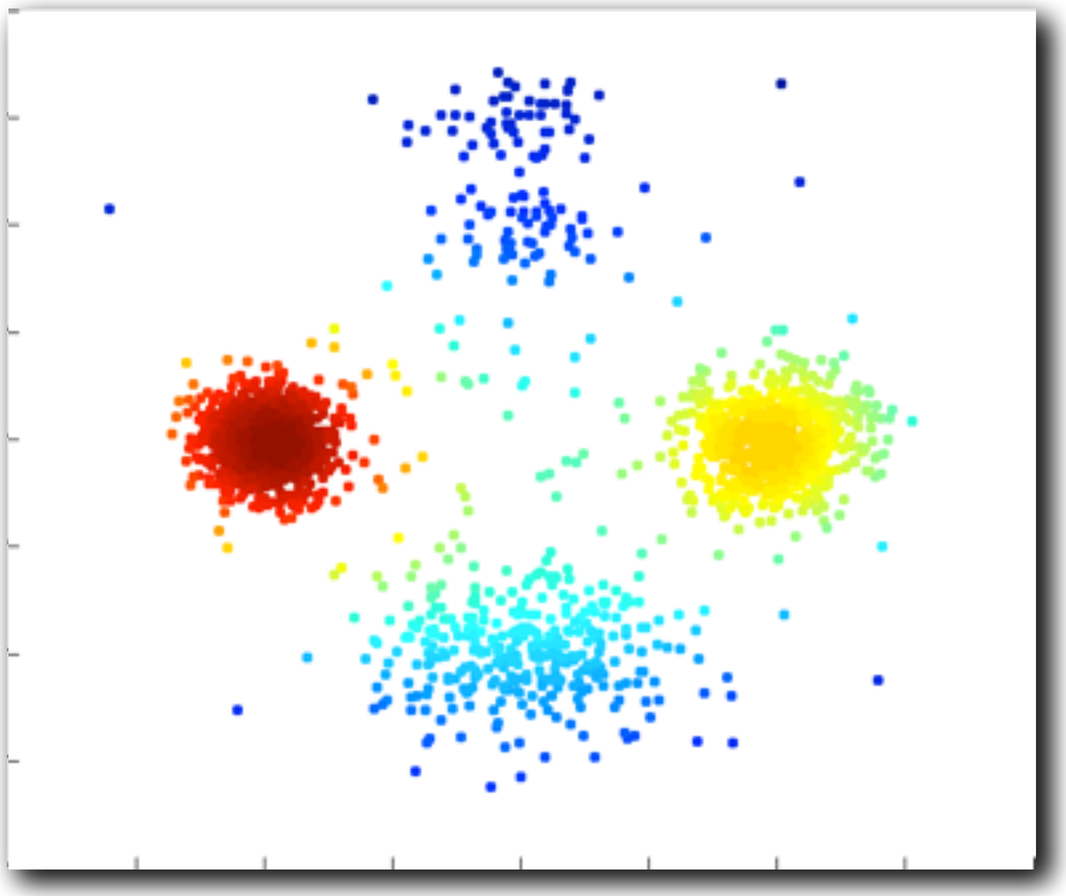
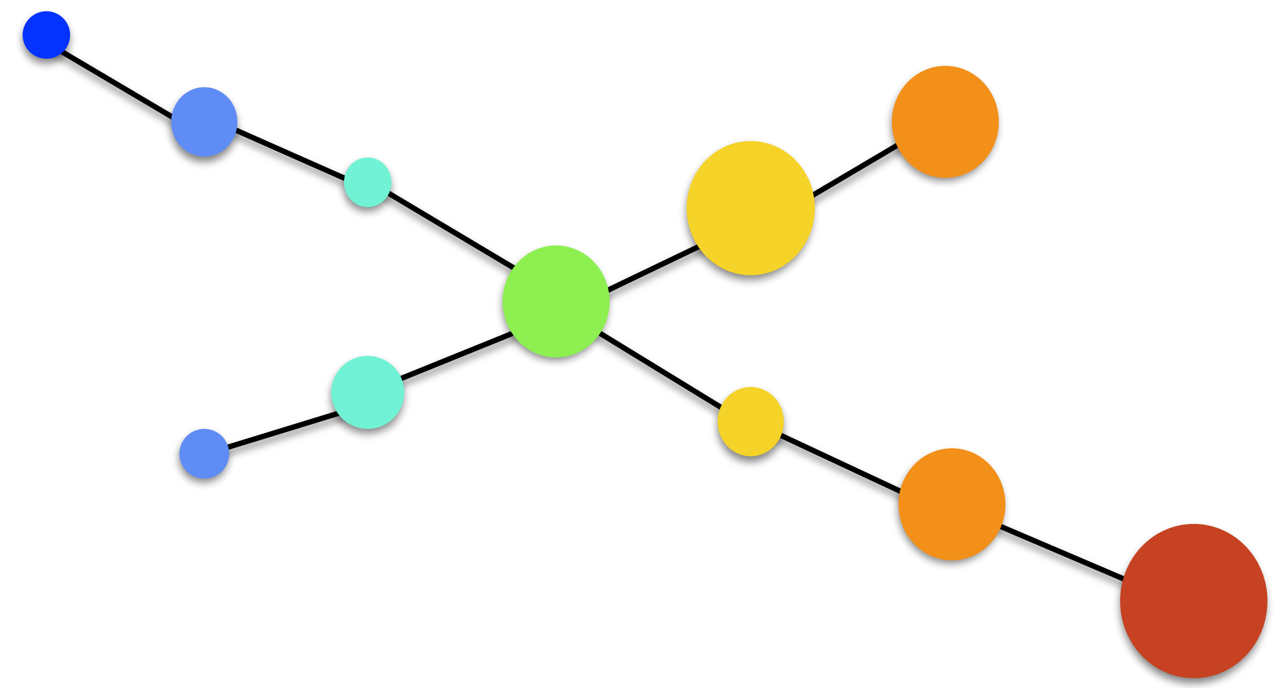
Topological Data Analysis

Powerful geometric summaries of your data



The resulting graph is a geometric summary of the data.



Nodes represent a set of points similar in both function and metric

Edges between nodes indicate overlapping points.

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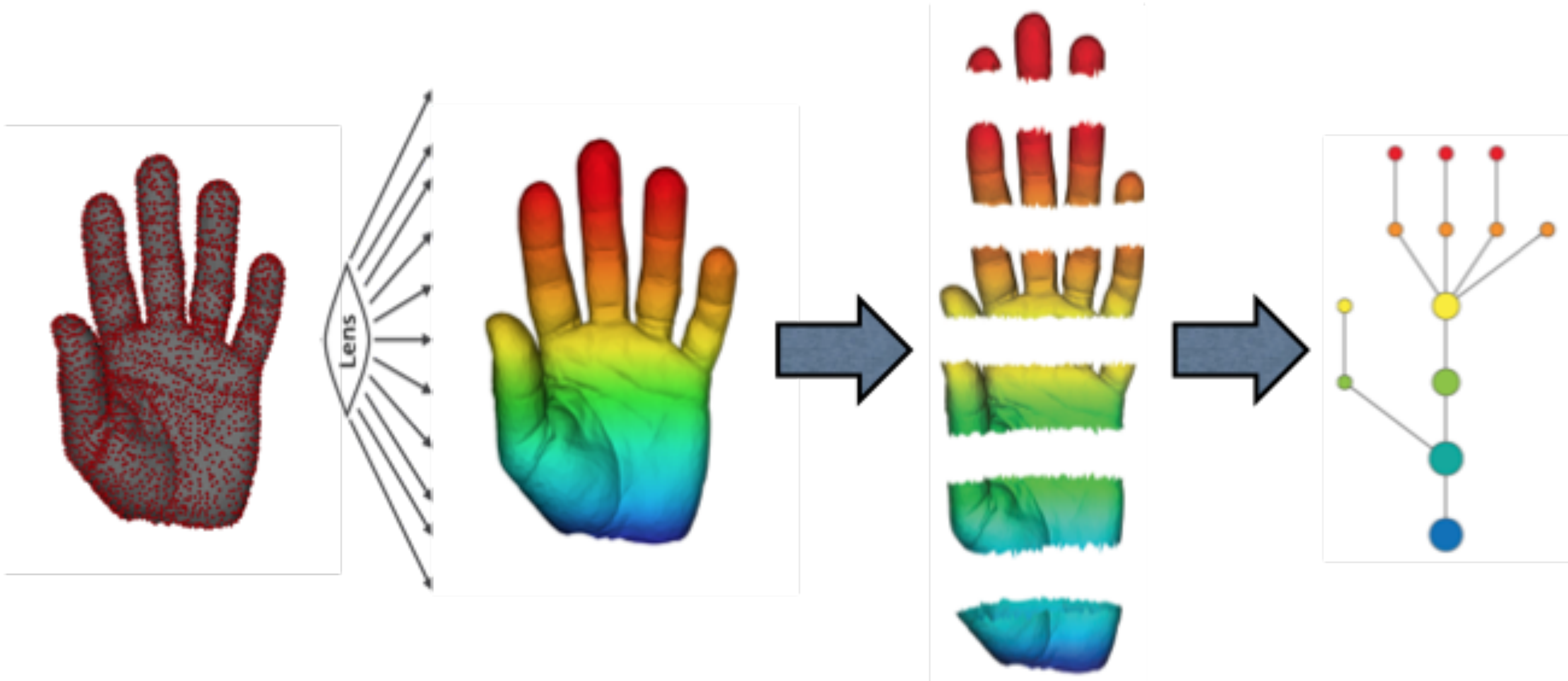
Basic Example

Characterizing shape in 3 dimensions



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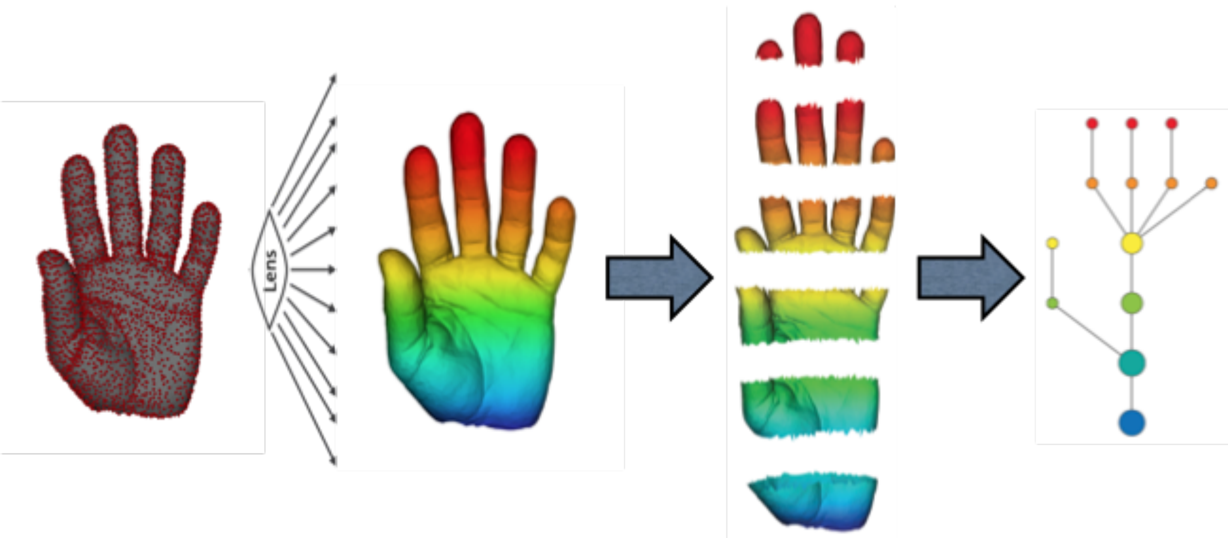
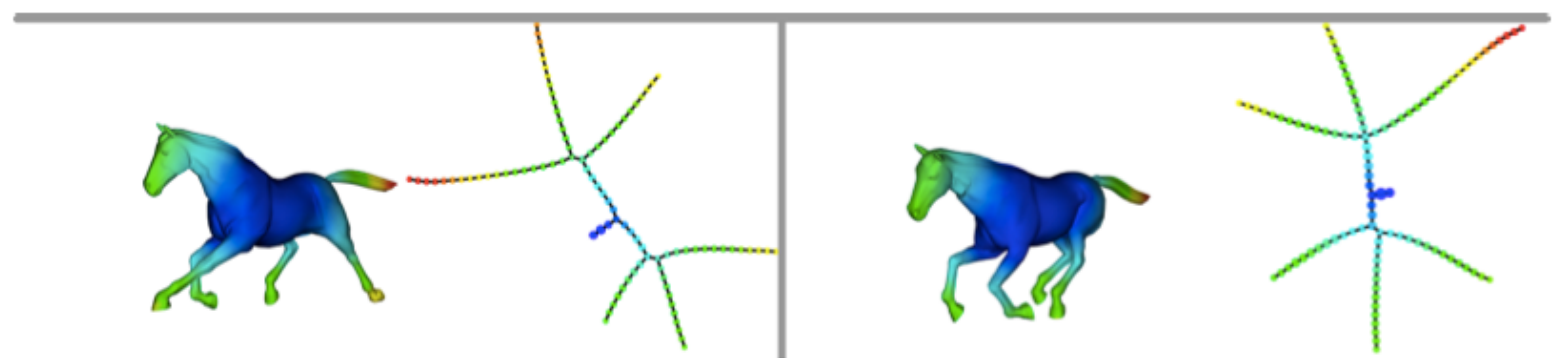
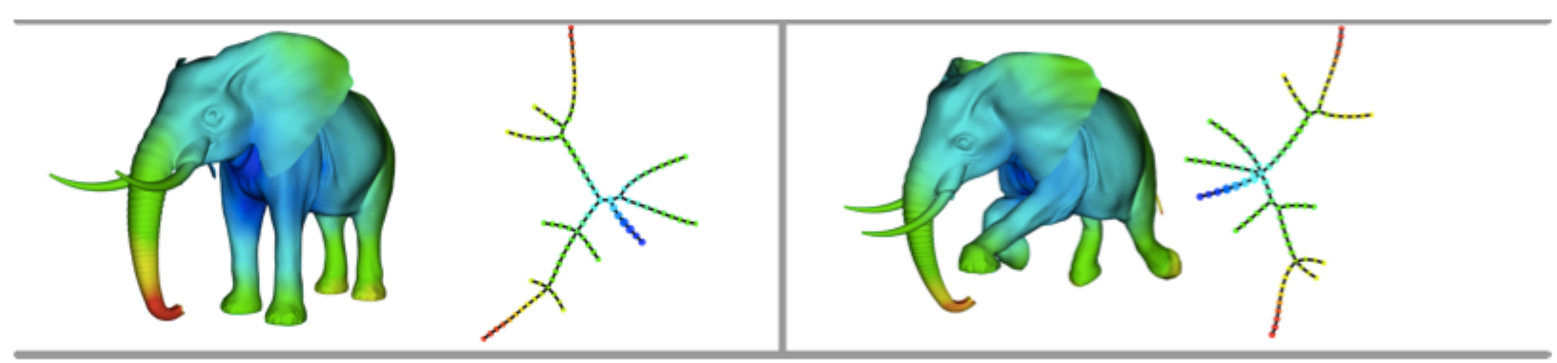
Basic Example

Characterizing shape in 3 dimensions







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Machine Learning and TDA

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Machine Learning and TDA

Incorporate traditional analytics through the function f

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Machine Learning and TDA

Incorporate traditional analytics through the function f

Statistics	Geometry/ Topology	Machine Learning	Data Driven
Mean/Max/Min/ Variance	Centrality	PCA/SVD	Age
n-Moment	Curvature	Autoencoders	Dates
Density	Harmonic Cycles	Isomap/MDS/TSNE	User Models
…	…	SVM Distance from Hyperplane	
		Error/Debugging Info	

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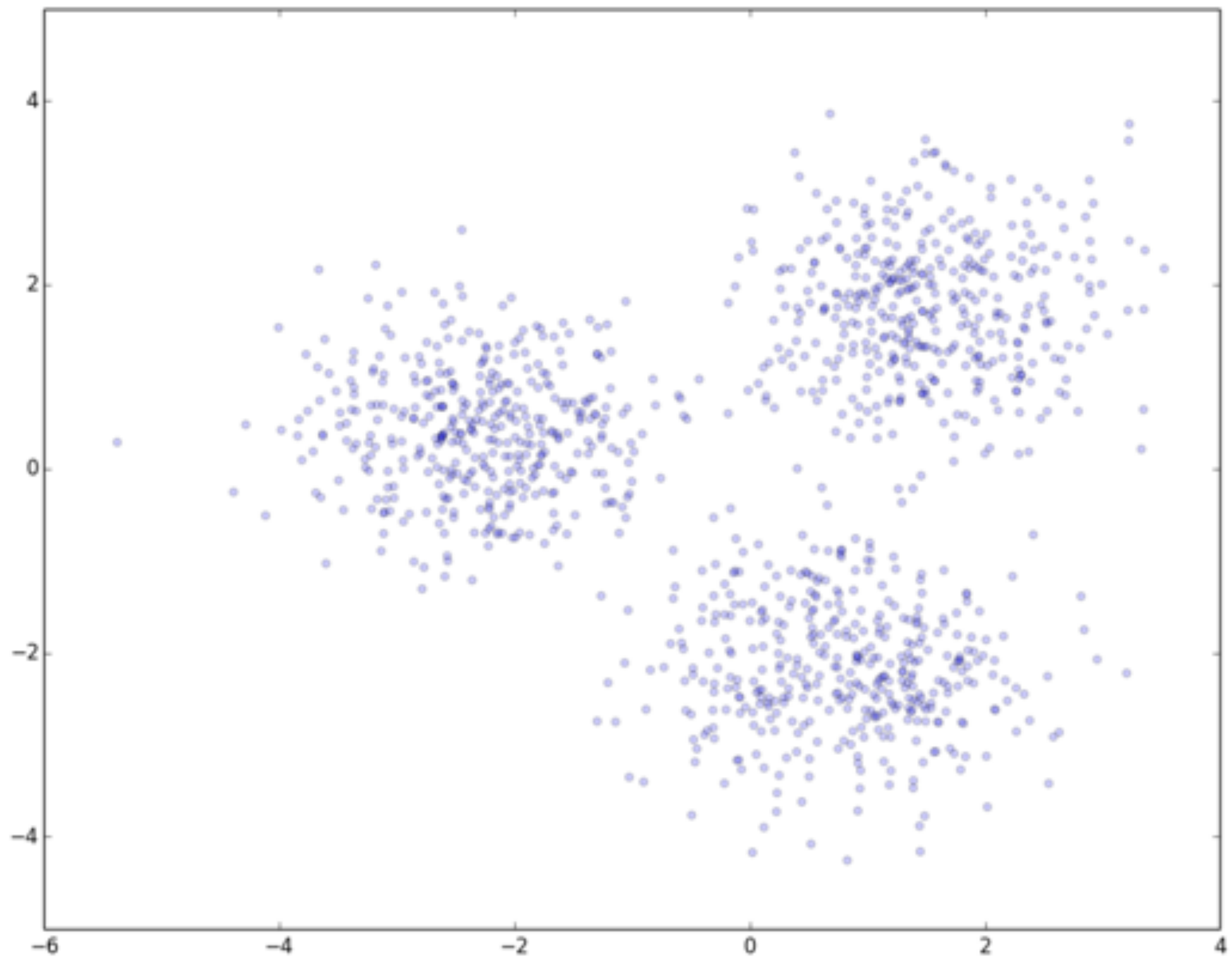
Machine Learning and TDA
Example: PCA

Provides unsupervised dimensionality reduction.
Easy to interpret.



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Machine Learning and TDA

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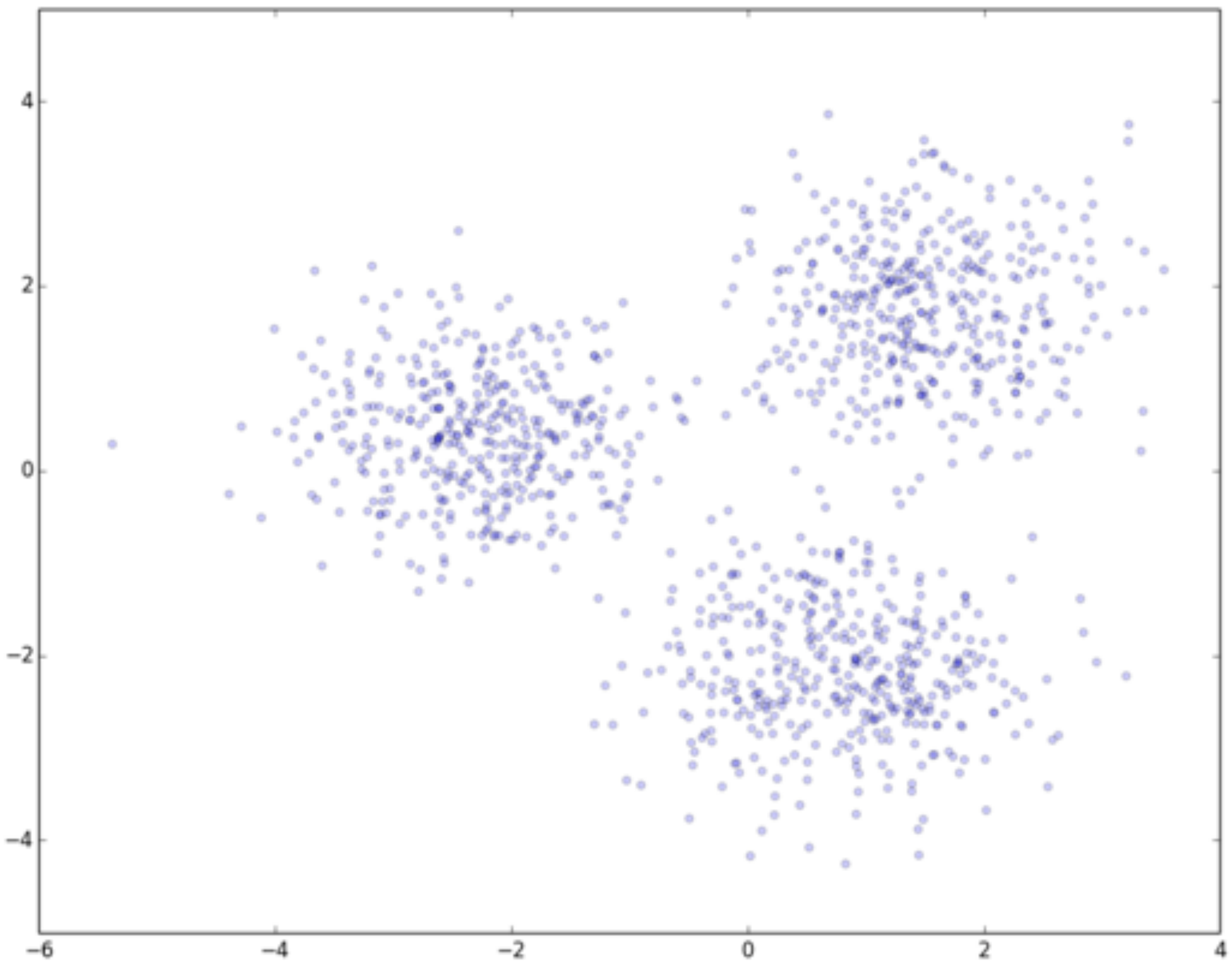

PCA captured 98.4% of the variance

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Unsupervised Learning: PCA

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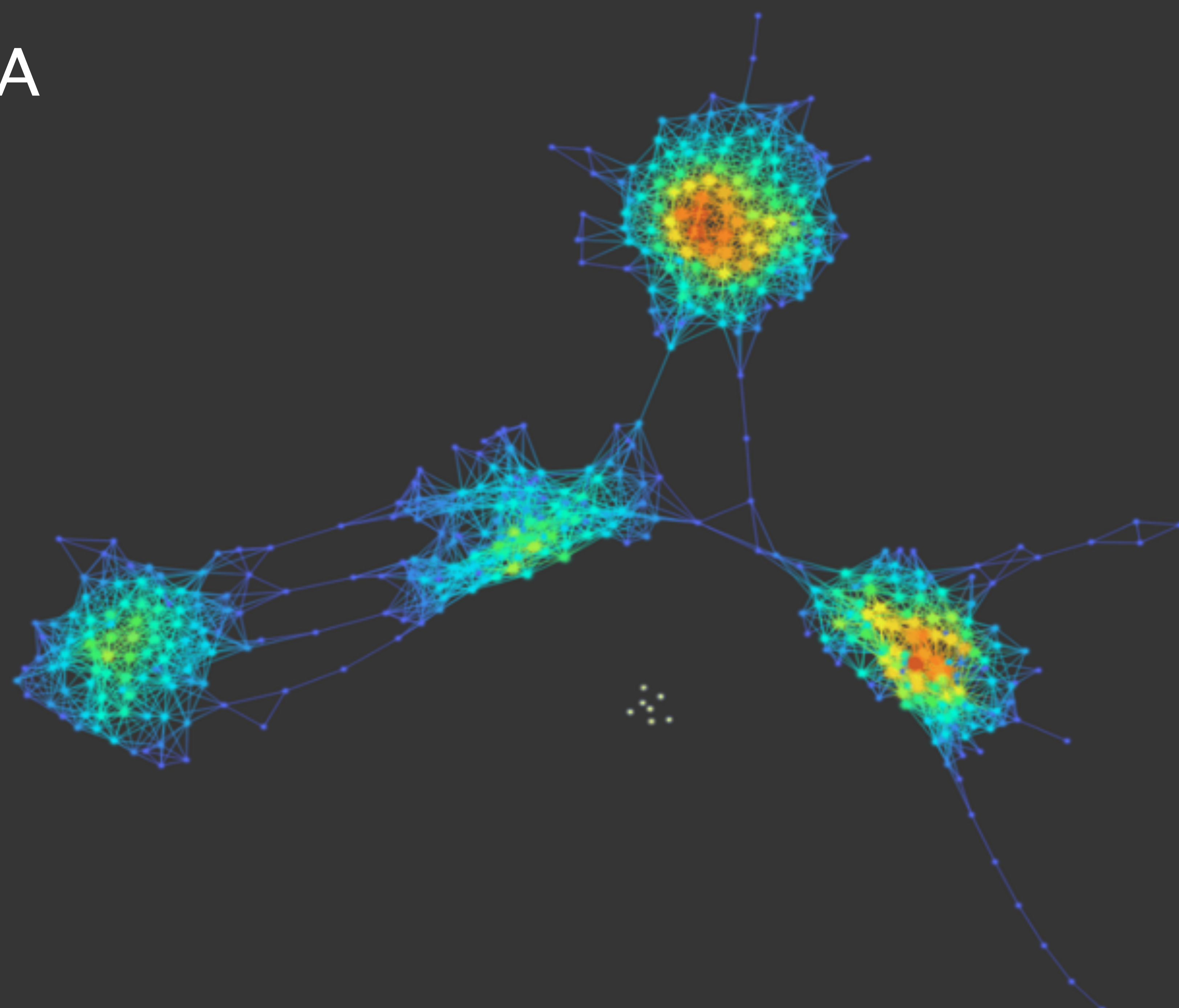
TDA + PCA



Unsupervised Learning: PCA

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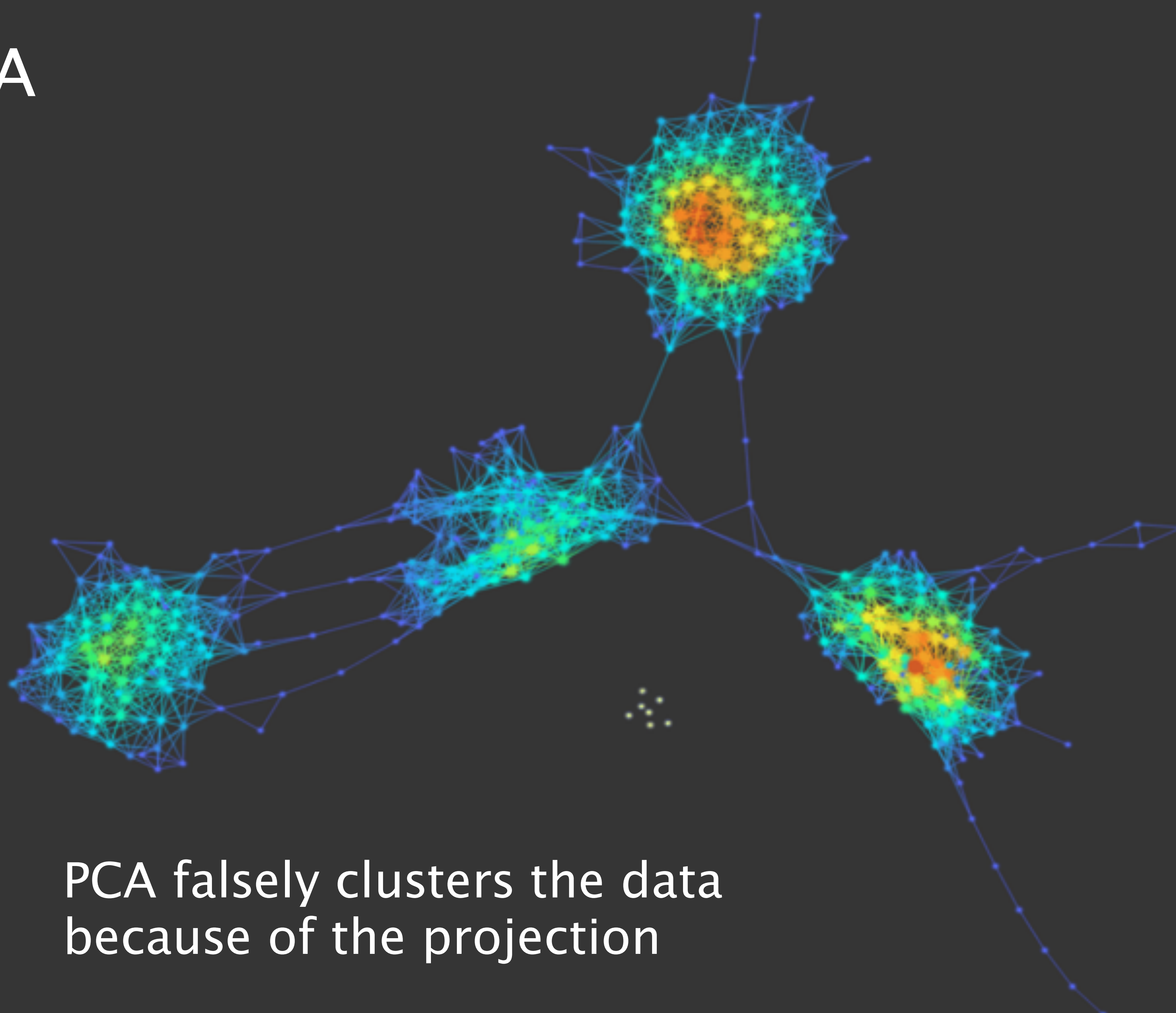
TDA + PCA



PCA falsely clusters the data
because of the projection

TDA clusters in the inverse image

Emergency room triage model

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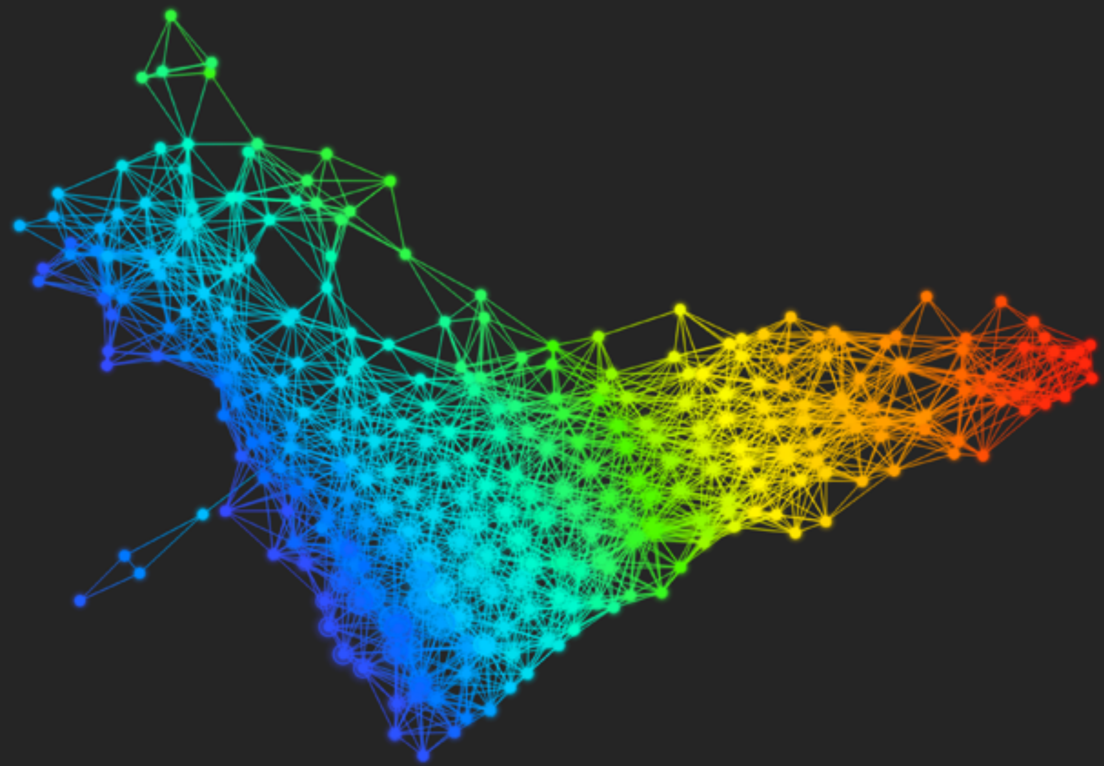
Predicted mortality

Low High



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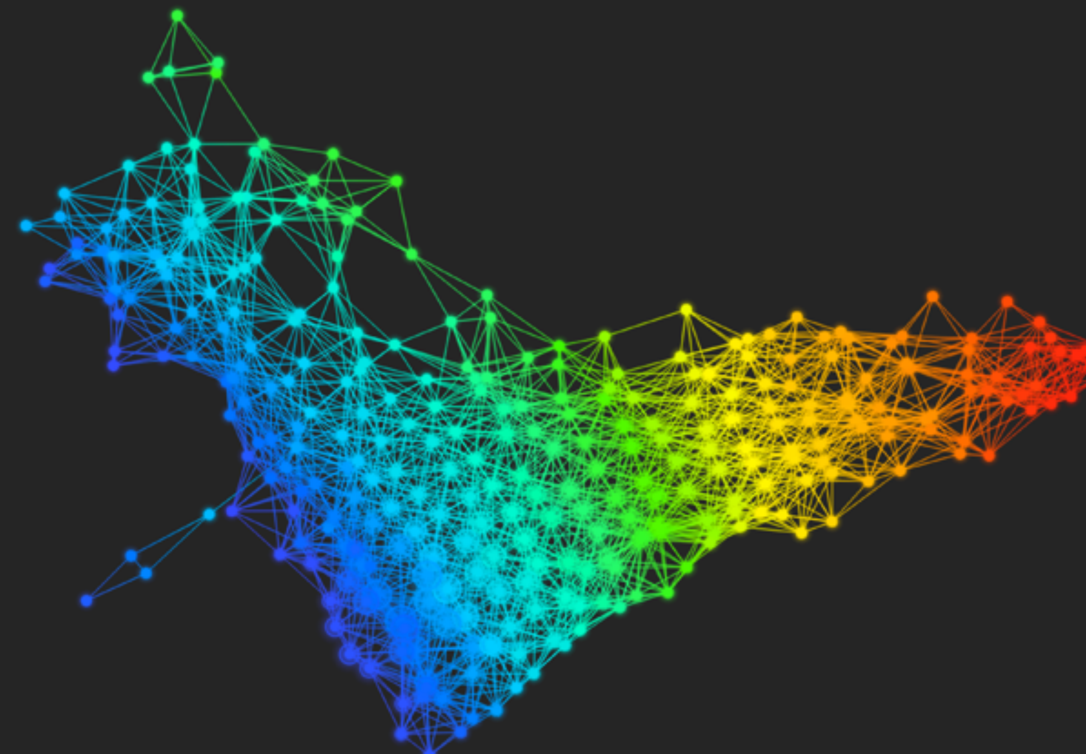
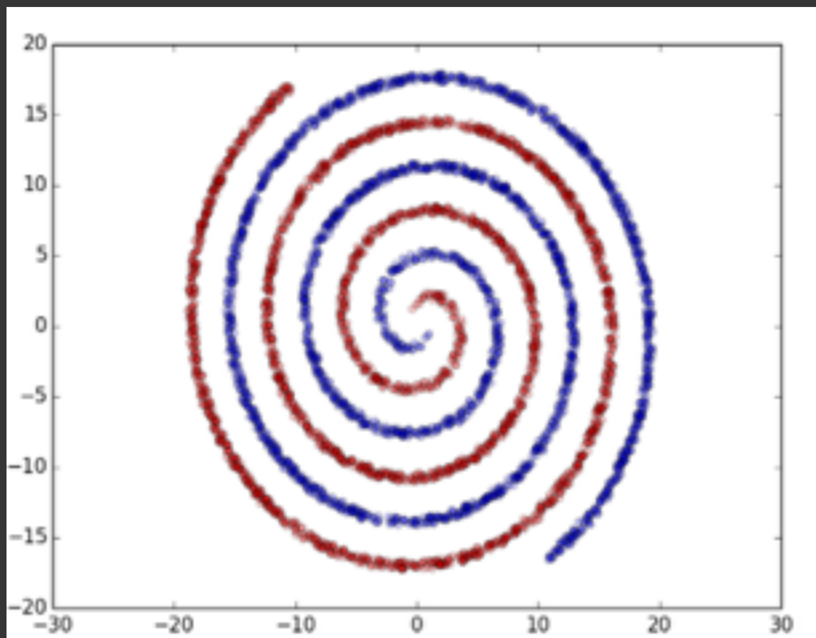


Actual mortality Low High

Missing responses to particular questions caused model to fail for these patients

TDA tells us where to look for problems and questions

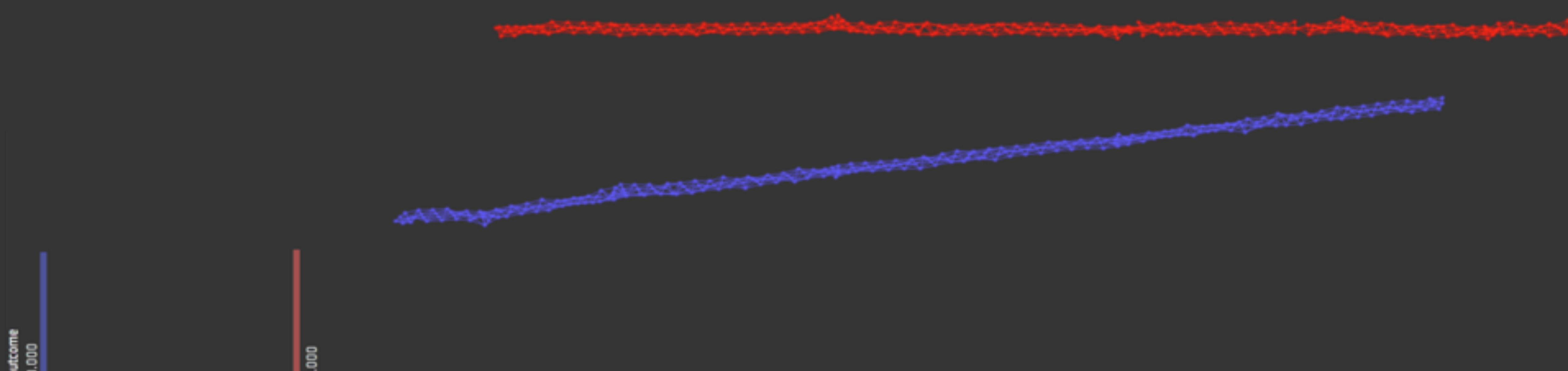
TDA: Beyond Machine Learning



Working locally means features don't change when stretched or distorted.

TDA is

- resistant to noise
- requires less preprocessing of data
- robust/stable in its answers



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Customer Use Cases

Predictive Maintenance & Machine Uptime

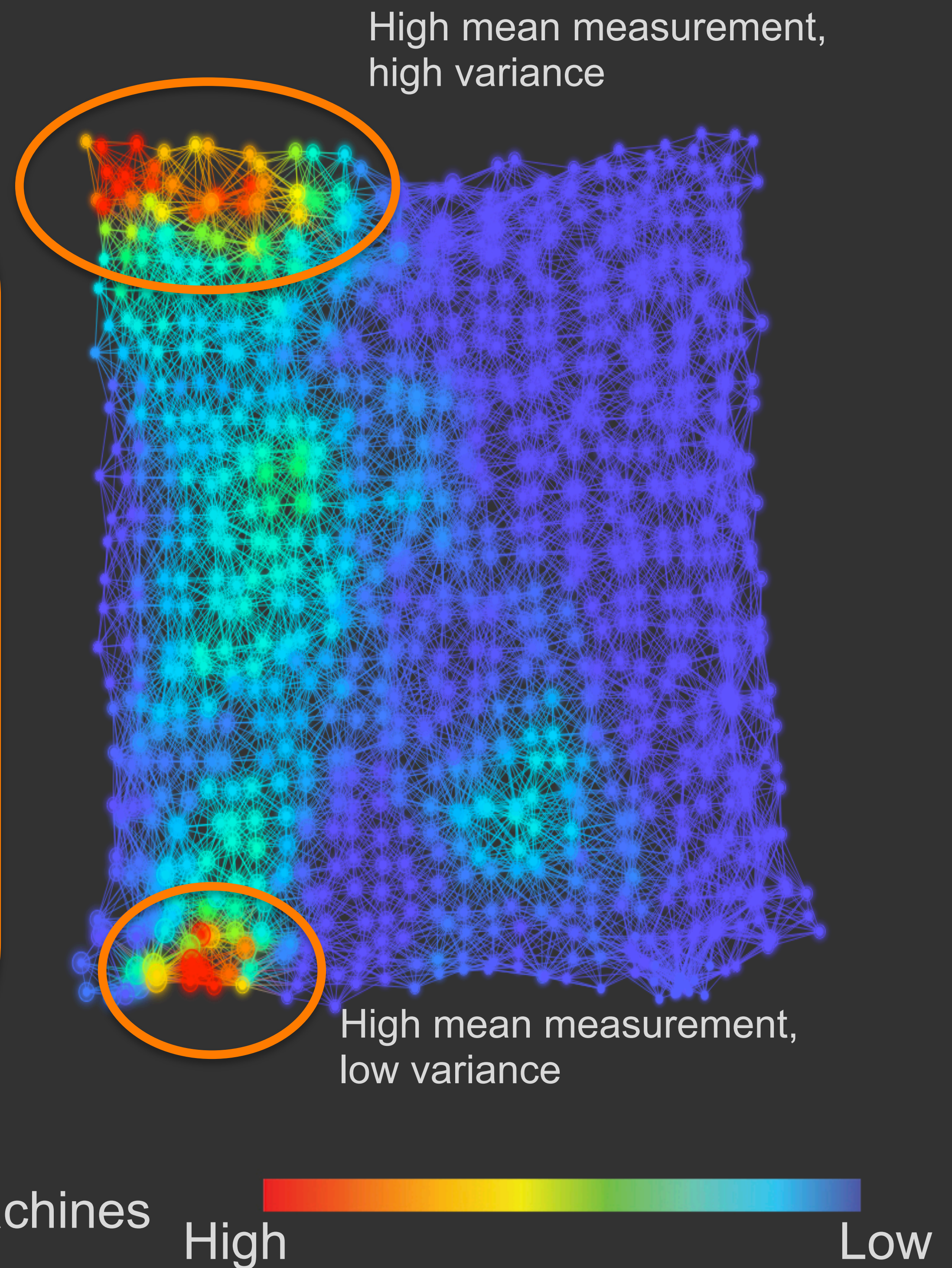
Challenge: identify indicators in sensor data that help indicate machinery failure

Data: system measurements capturing machine characteristics

Result: identification of the key machine attribute that reveals impending failure

- High mean, high variance – failure
- High mean, low variance – failure
- High mean, medium variance – no failure

The key attribute could be identified using standard methods, but that information was insufficient to predicting failure.



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Carbon Capture: Searching Zeolite Structures

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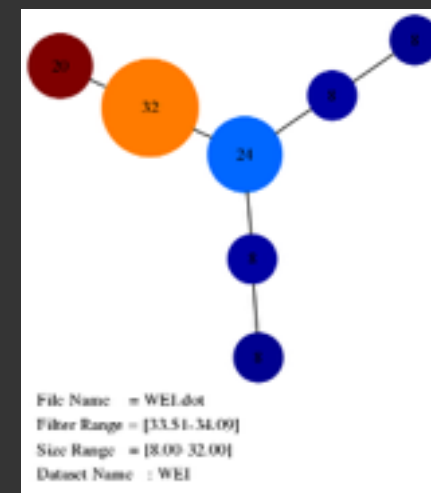
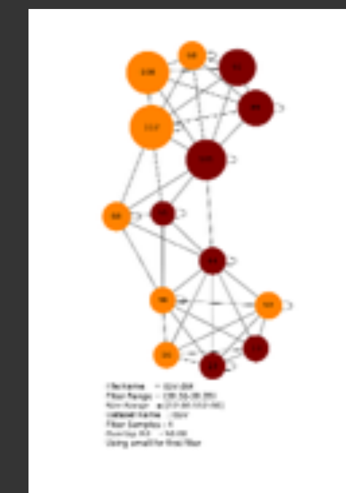
Problem: Search database of compounds to find structures with good carbon capture properties

Data: 30,000 3D crystalline structures of theoretic zeolite compounds

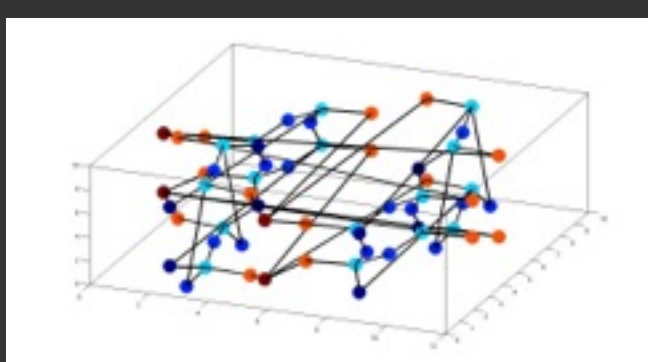
Result: Identified compound that had 10x selectivity for CO_2 over CH_4

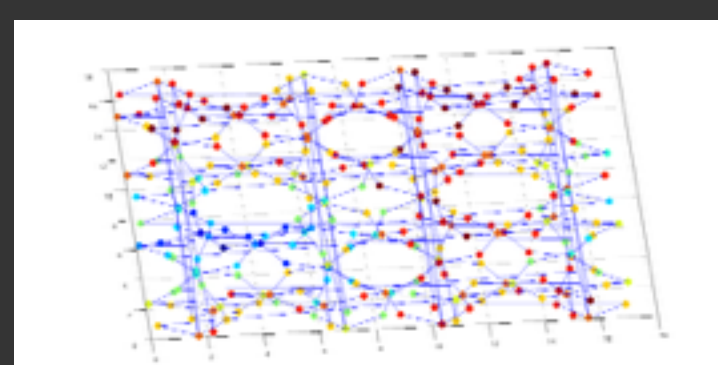
Example geometric summaries





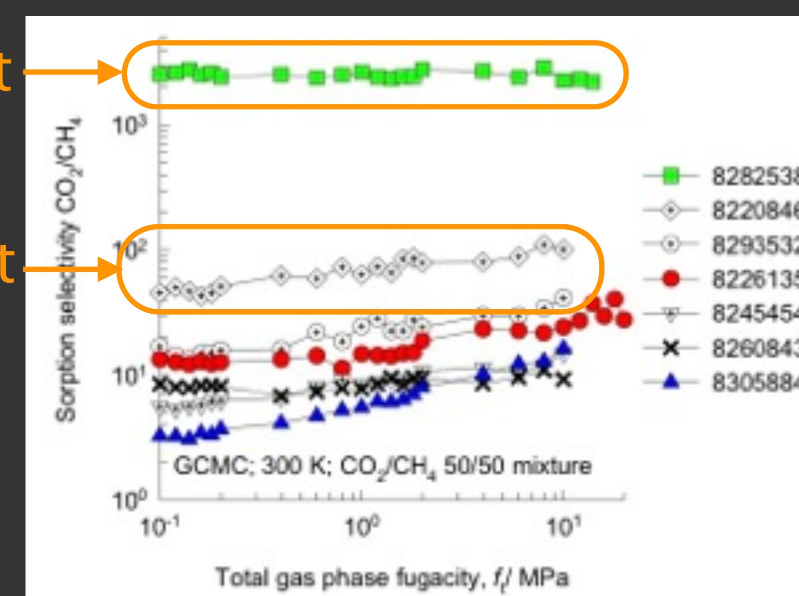
Example data





Newly discovered best

Previous best



TDA + Random Forest: Credit Card Fraud

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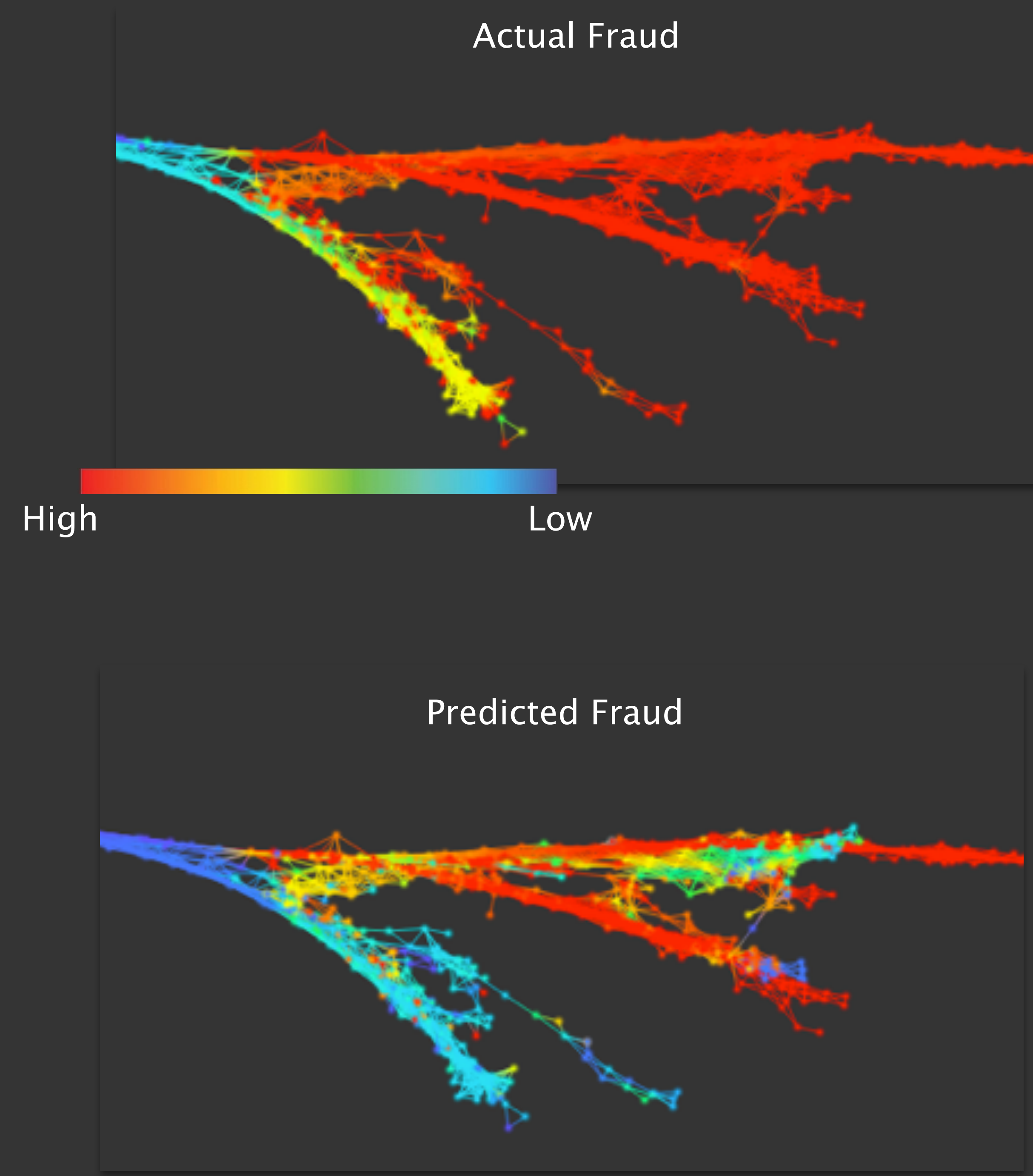
<u>Problem</u>: Identify credit card fraud

<u>Data</u>: Predictions from 200 random forest trees on several hundred features on credit card transactions

<u>Result</u>: Identified large subset of mis-categorized fraud. Uniquely identify the characteristics of this group and improved accuracy from 28% to 99.3%

Geometric Summary built with Random Forest Metric



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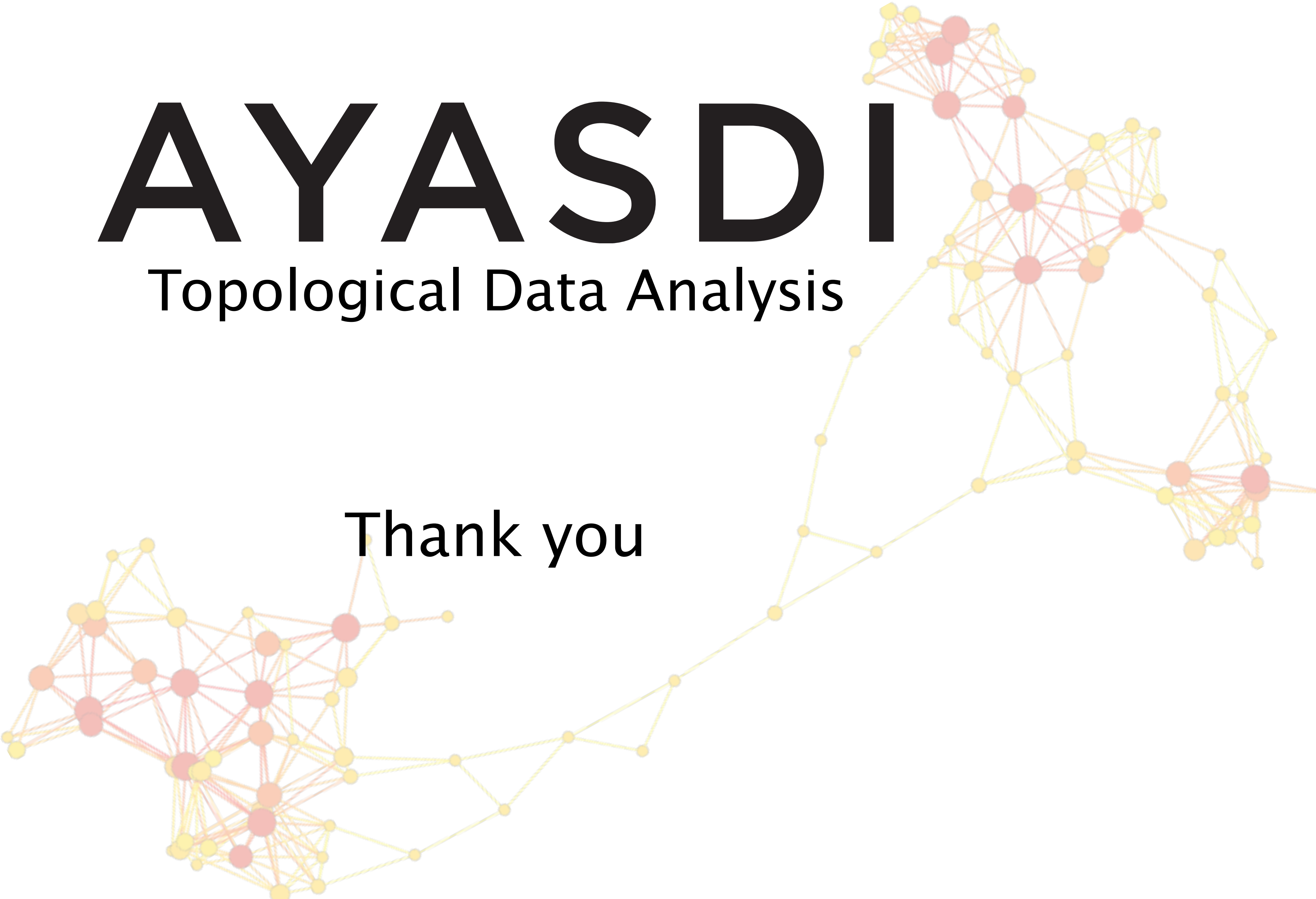
Topological Data Analysis



Thank you

Data has **Shape**, Shape has **Meaning**, Meaning drives **Value**