Shape and Meaning

An Introduction to Topological Data Analysis

Anthony Bak

AYASDI

Goals

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- Show you how TDA provides a framework for many machine learning/data analysis techniques

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Caveats: I am only talking about the strain of TDA done by Ayasdi

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TDA will be the tool that summarizes out the irrelevant stories to get at something interesting.

Data Has Shape

And Shape Has Meaning

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$\Rightarrow$ In this talk I will focus on how we extract meaning.

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The goal of TDA is to understand (for us, summarize) the shape with no preconceived model of what it should be.

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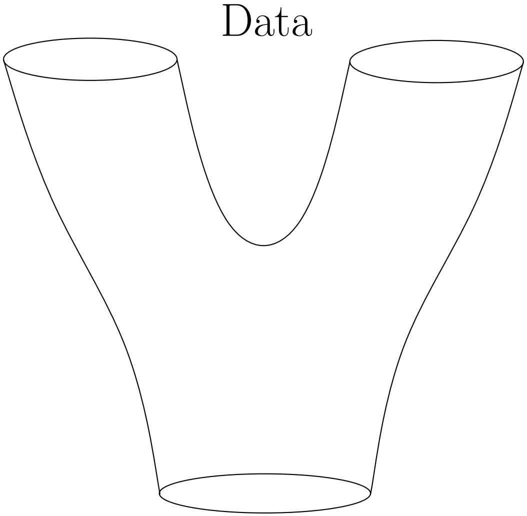
$\Rightarrow$ We will not need either of these assumptions once we're in "Data World".

$\Rightarrow$ Even more importantly, data in the real world is *never* like this

Math World



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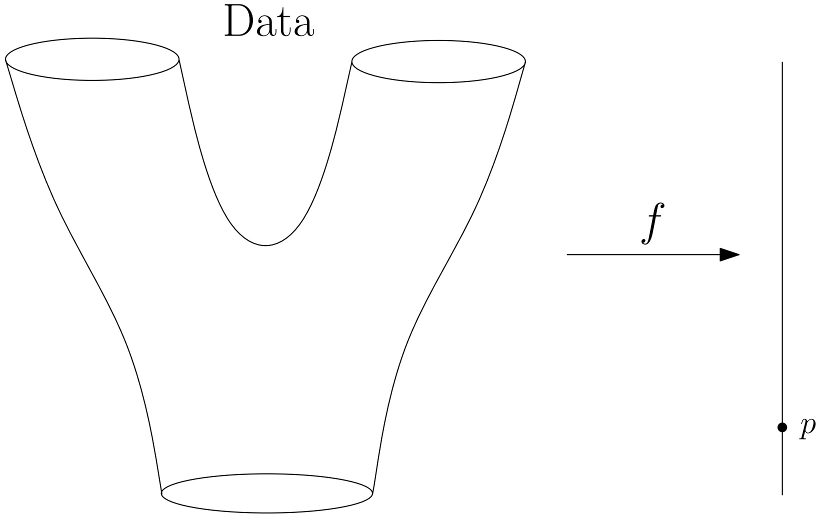

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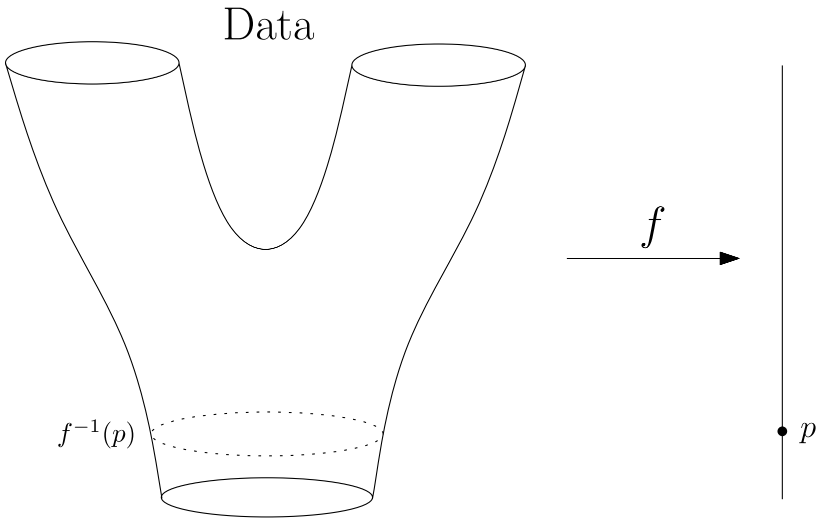

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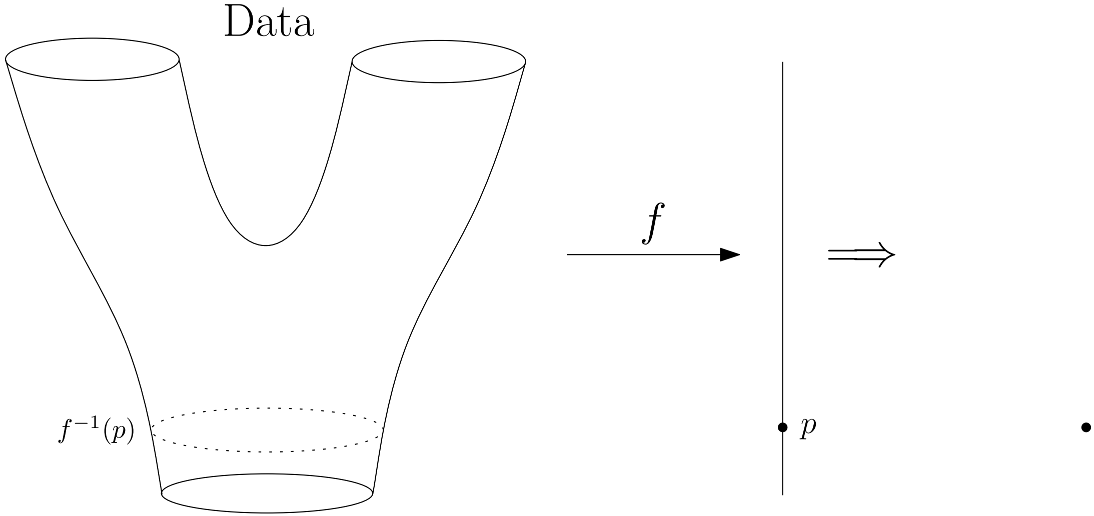

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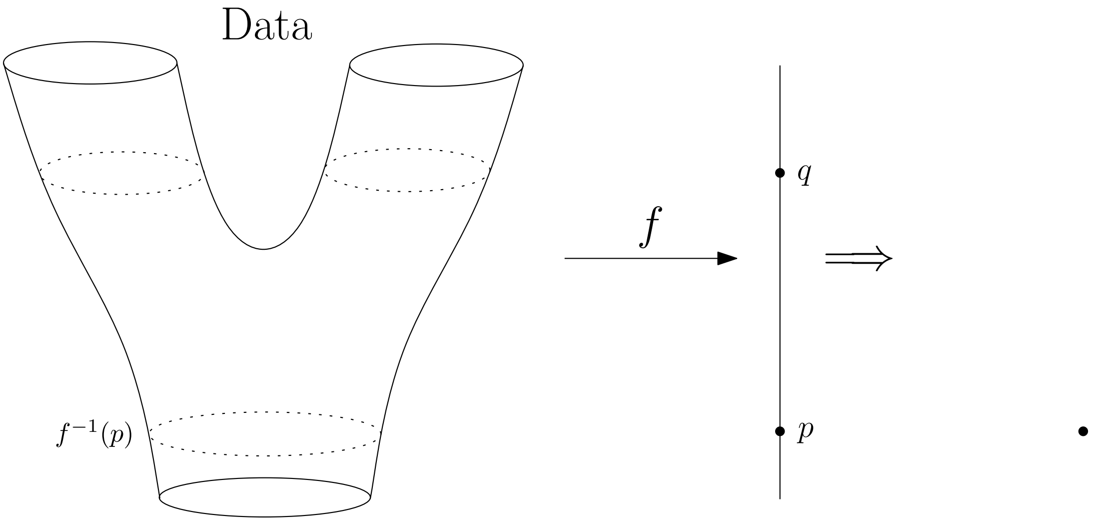

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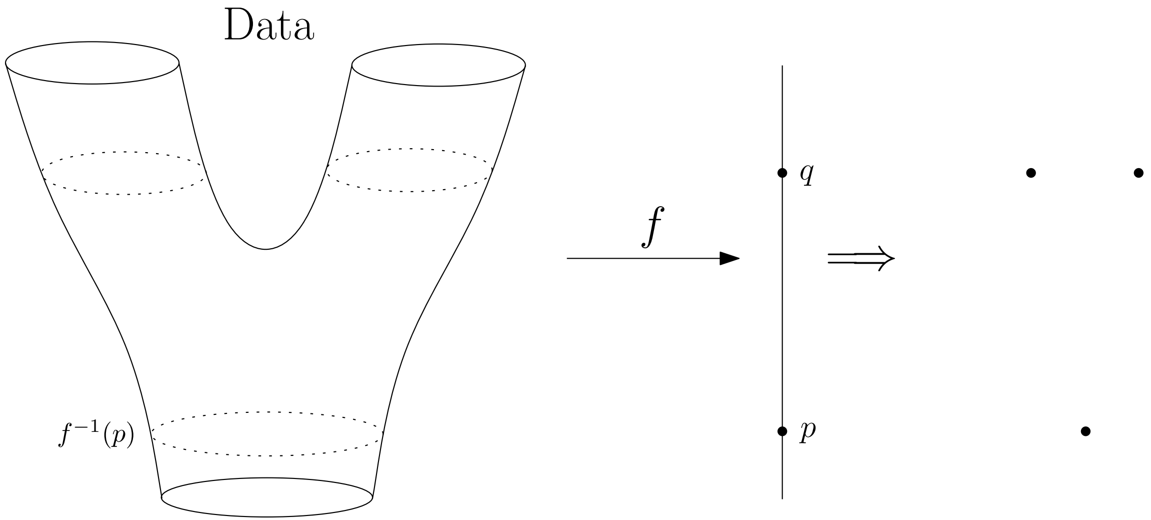

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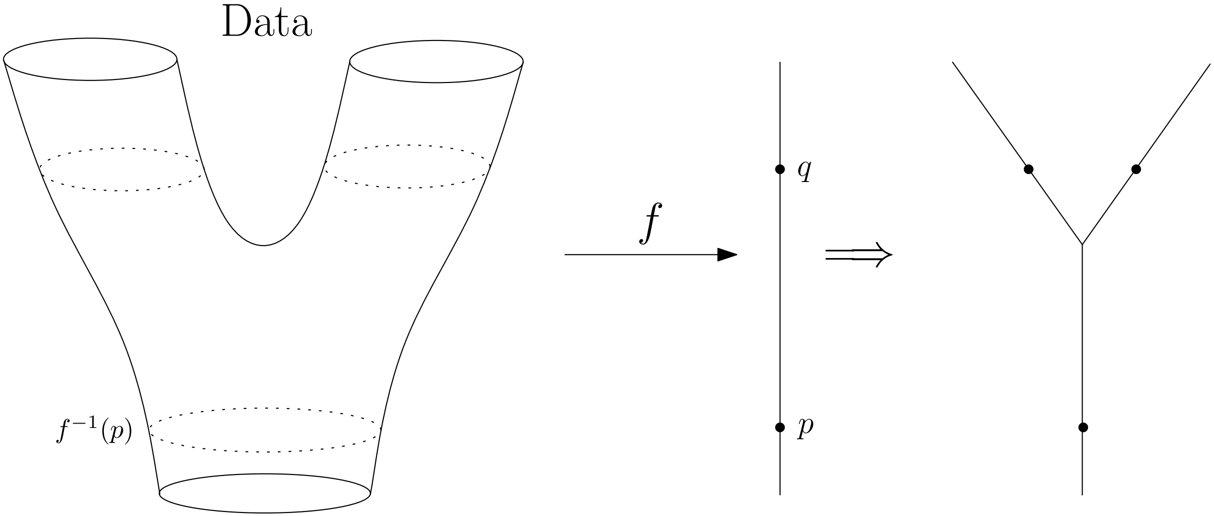

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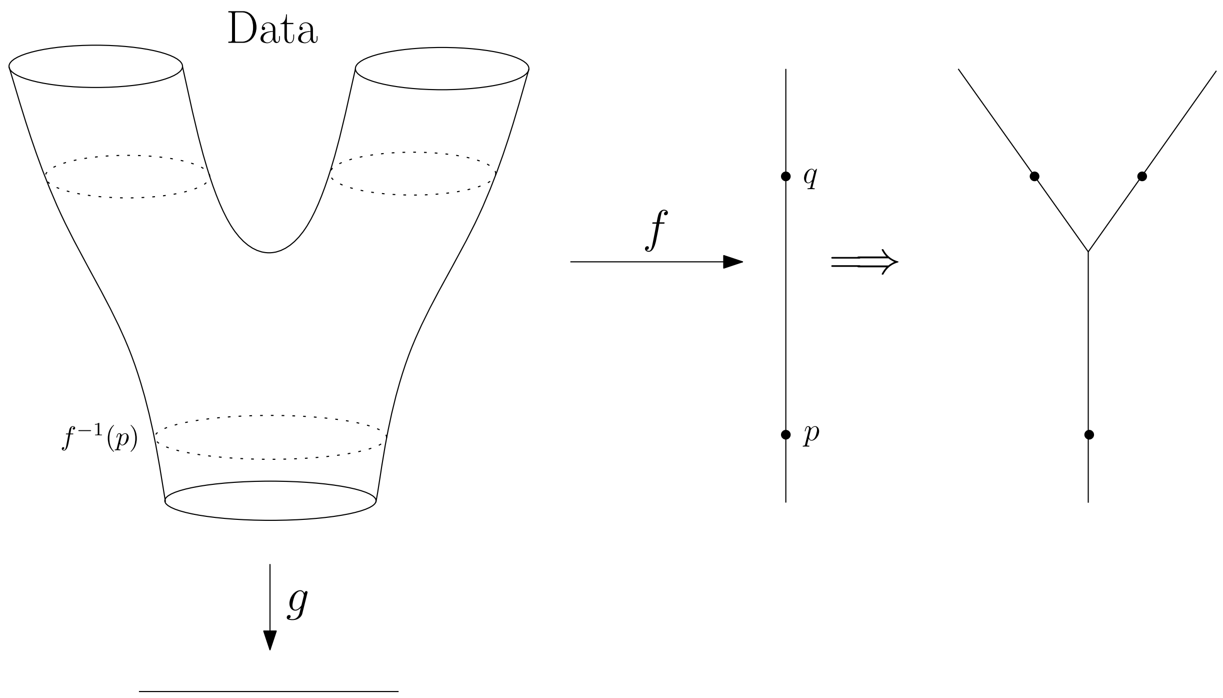

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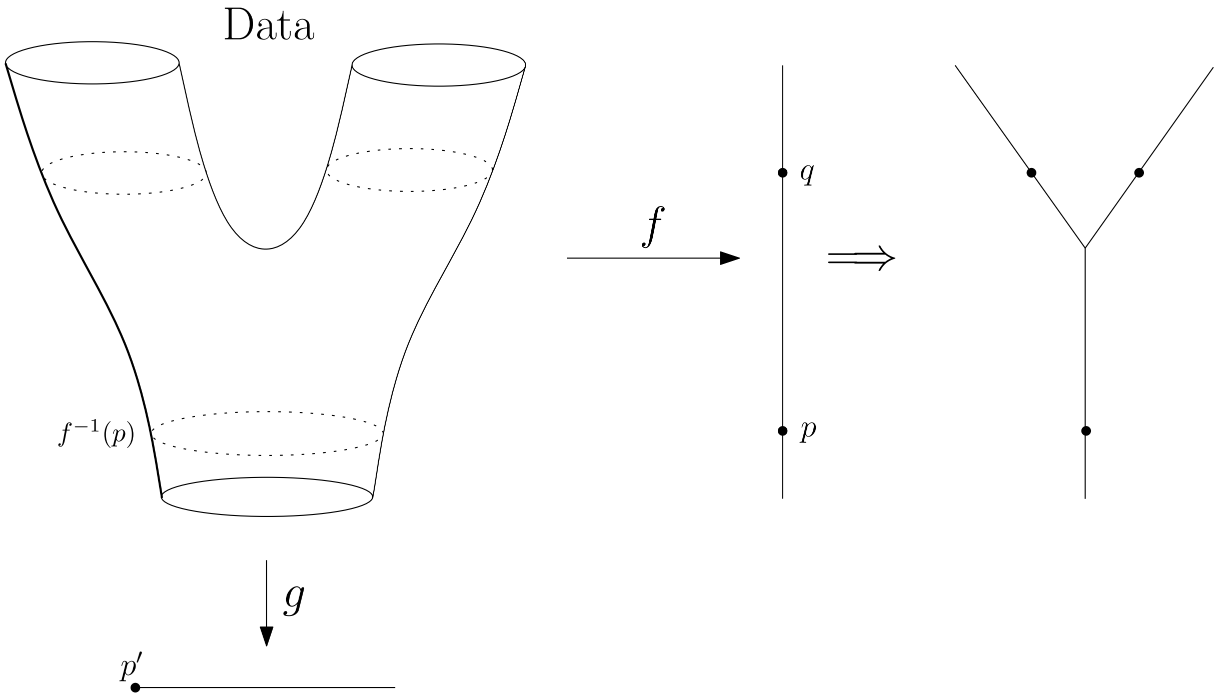

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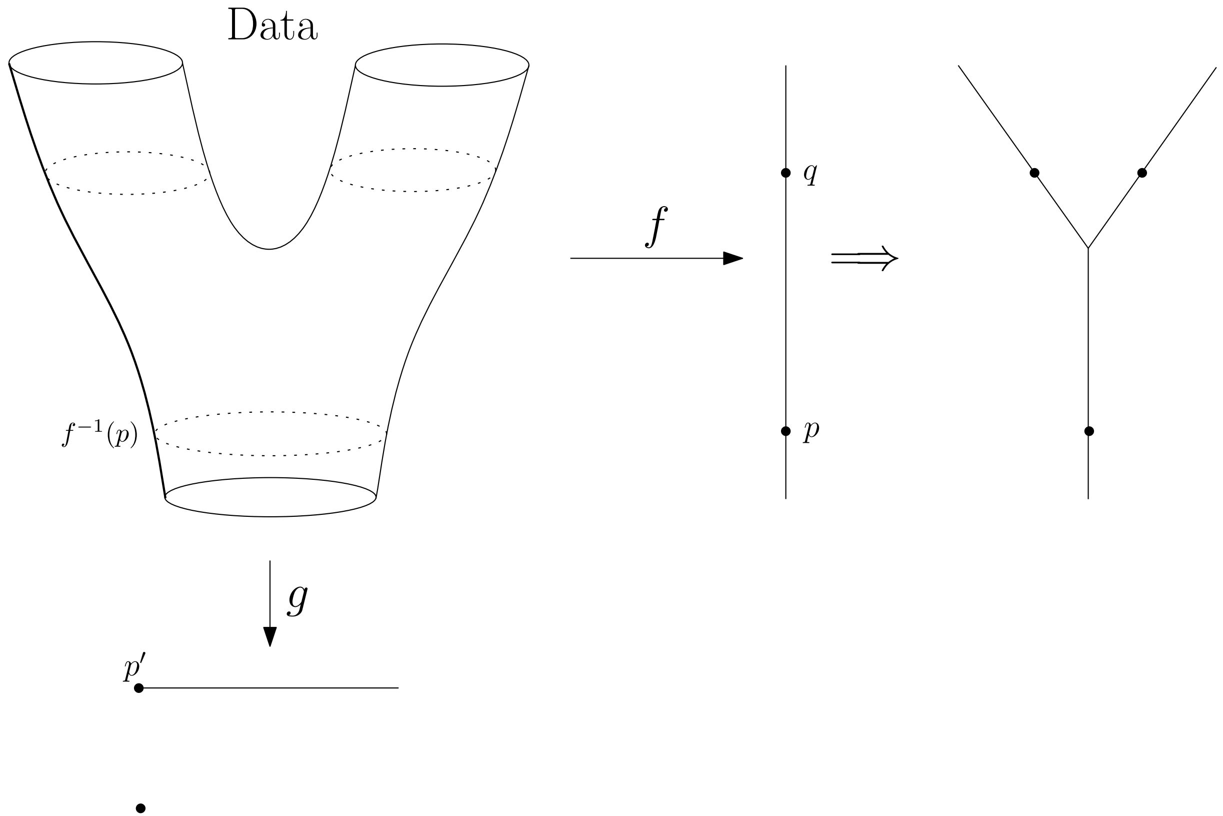

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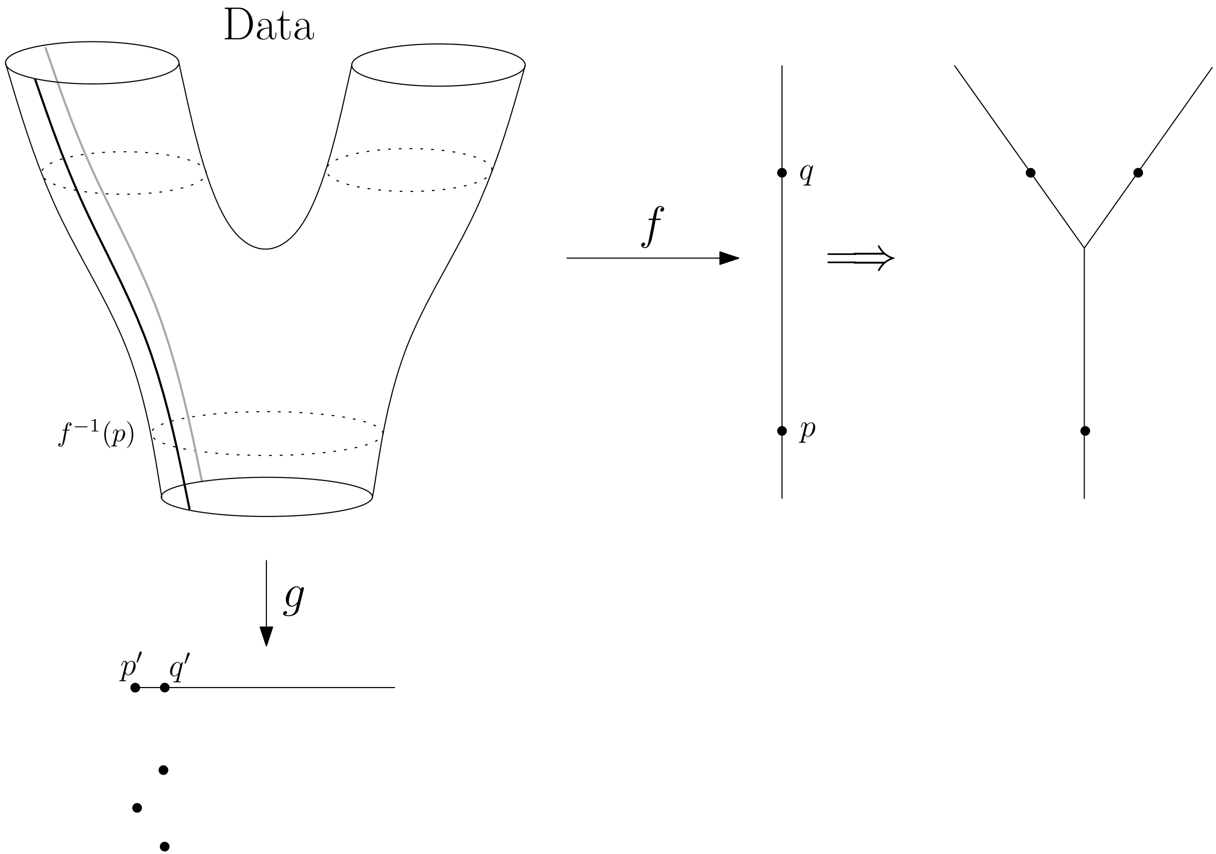

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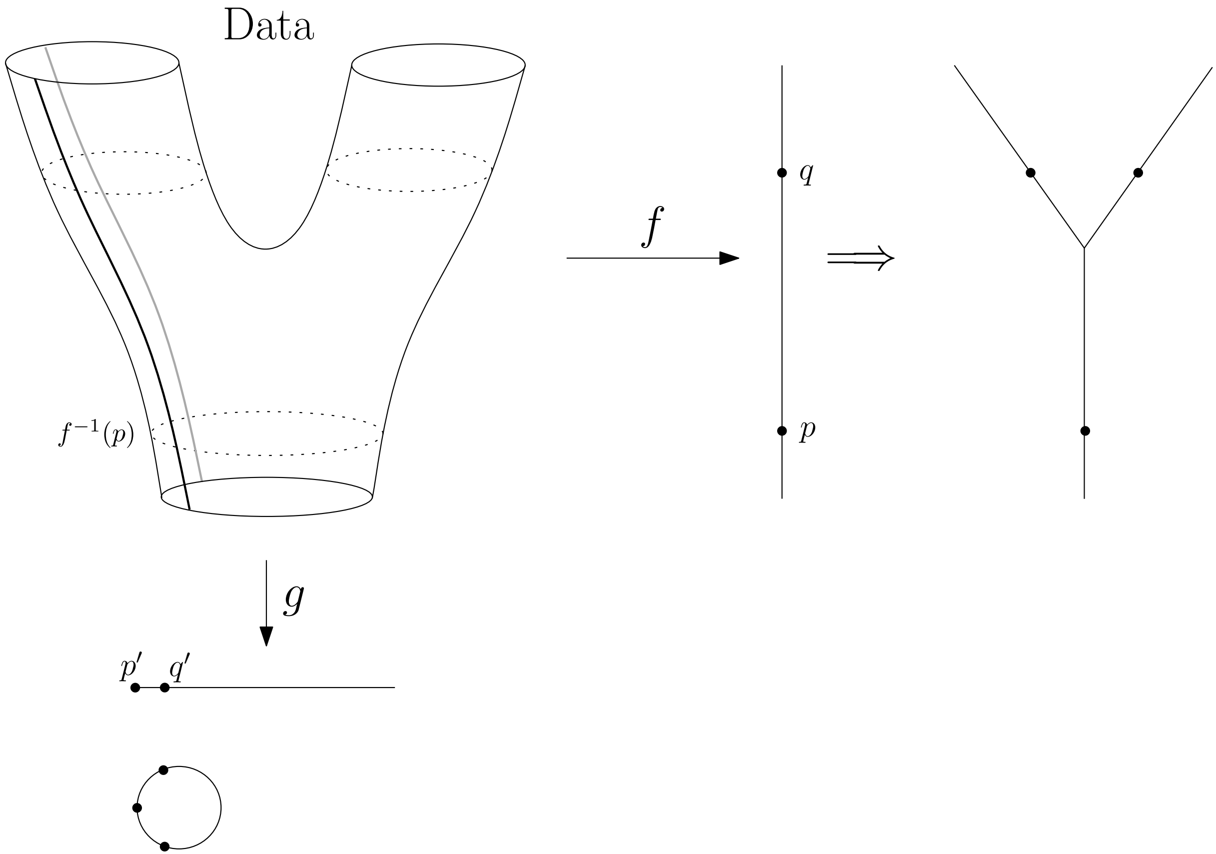

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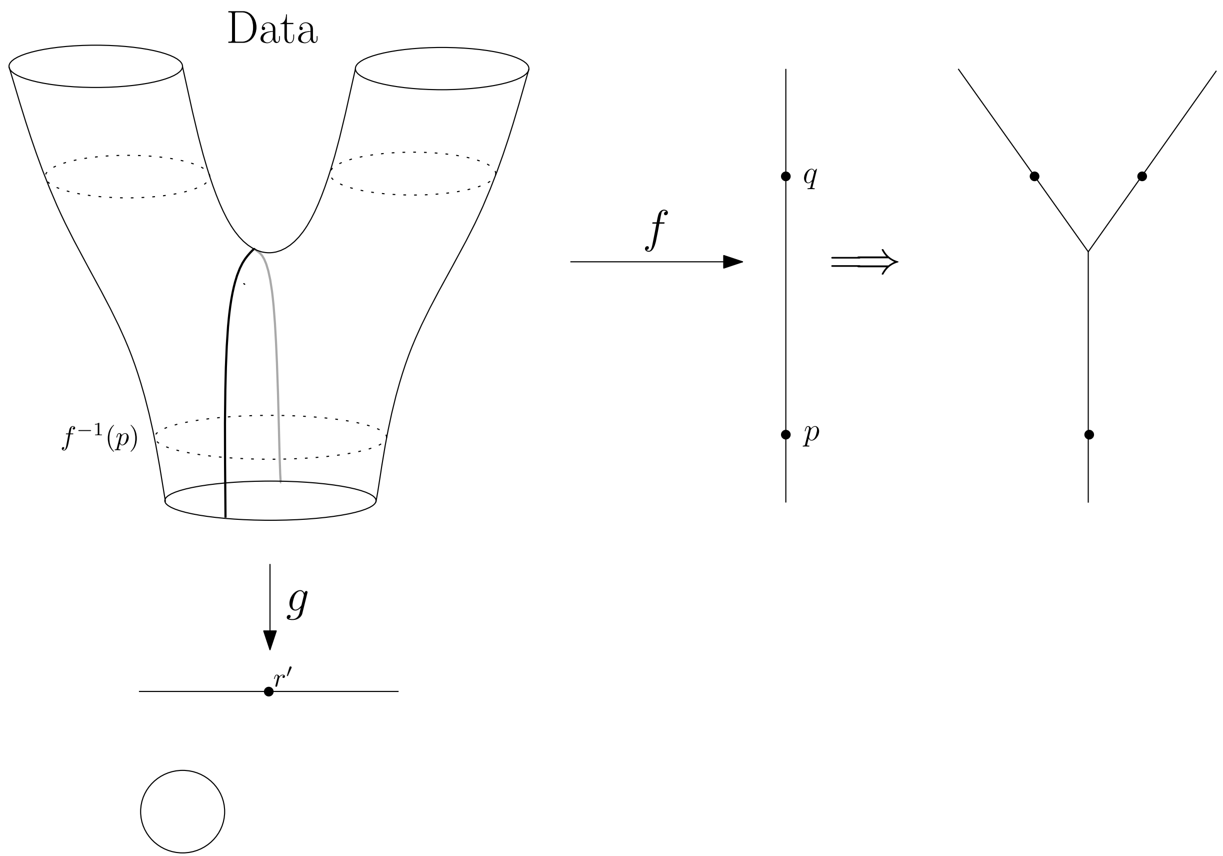

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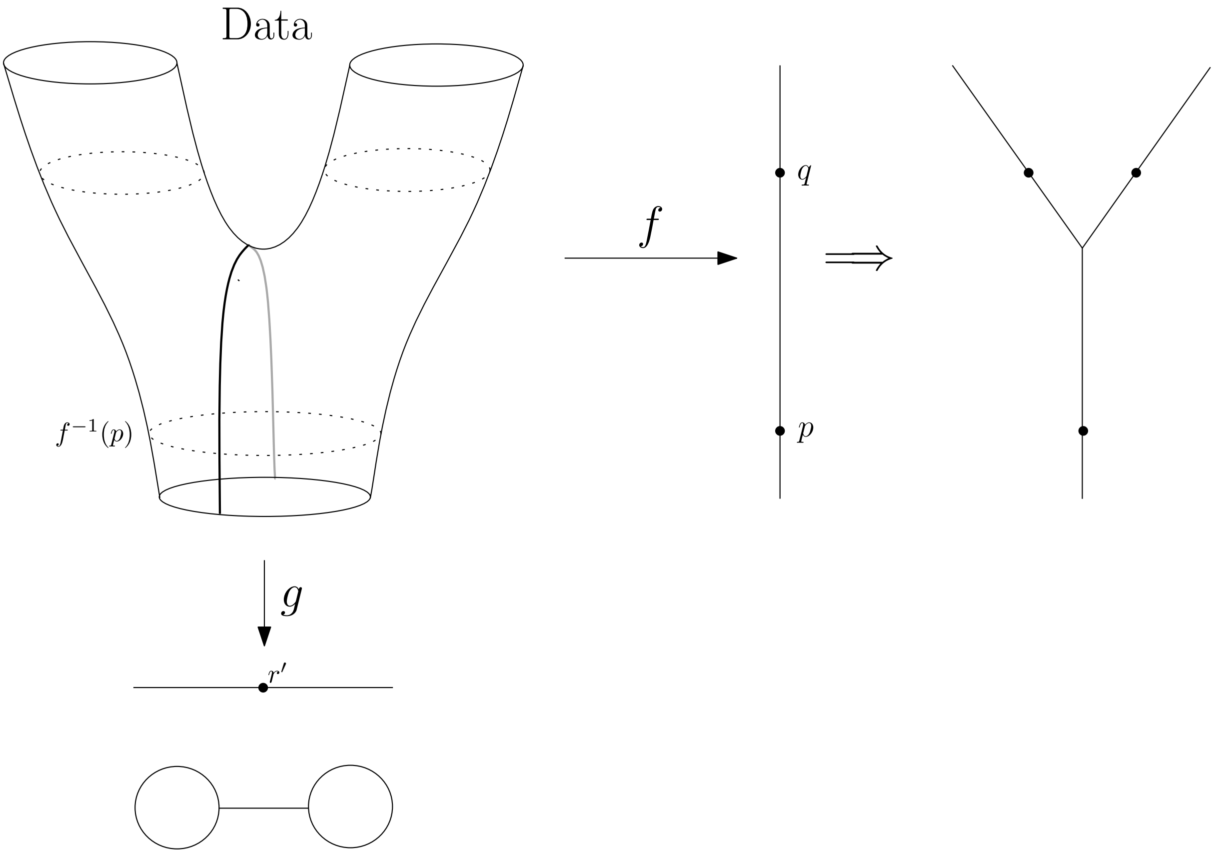

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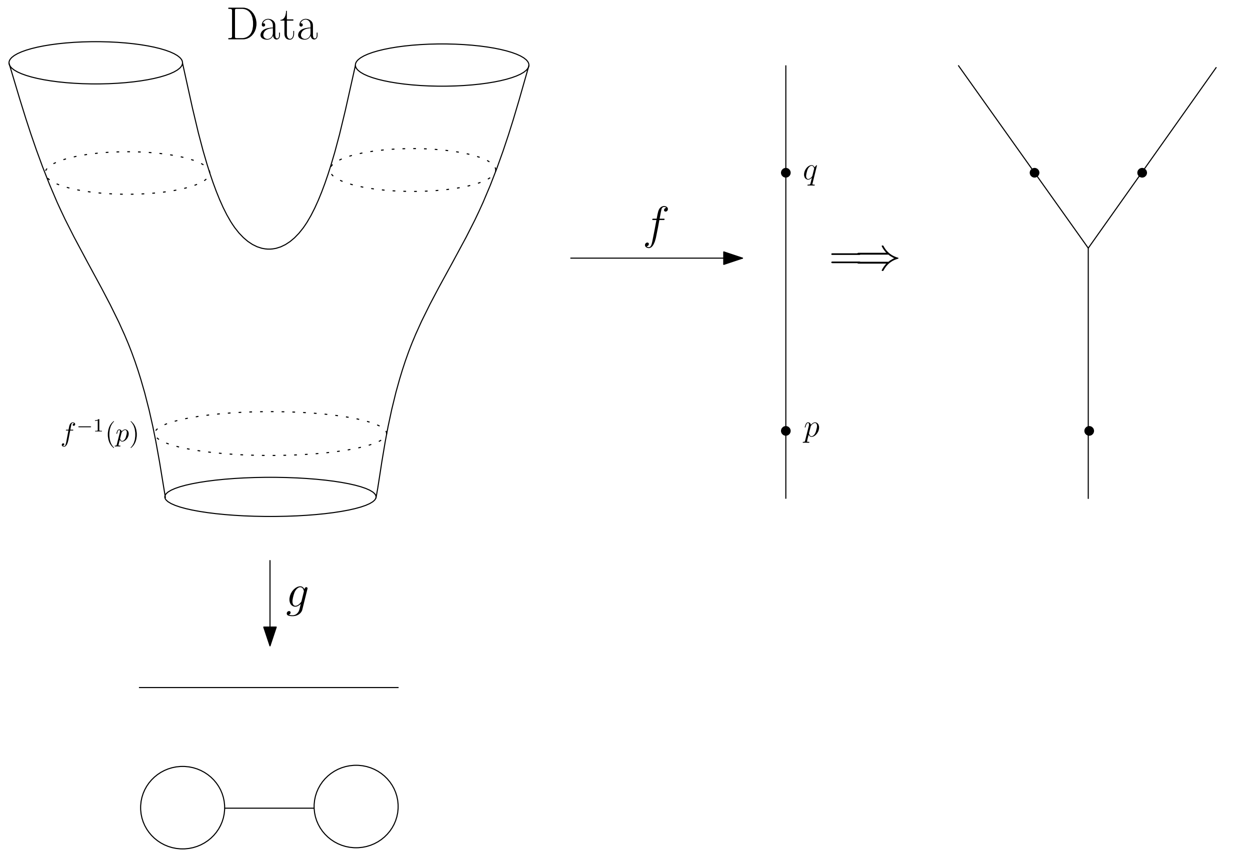

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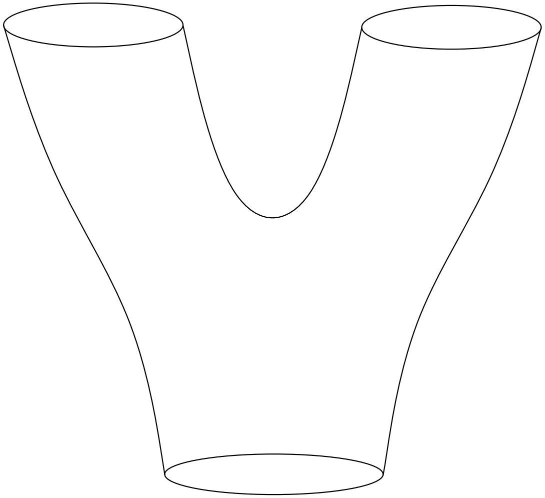
What is the summary if we use both lenses, *g* and *f* at the same time?



$$\xrightarrow{(g, f)}$$

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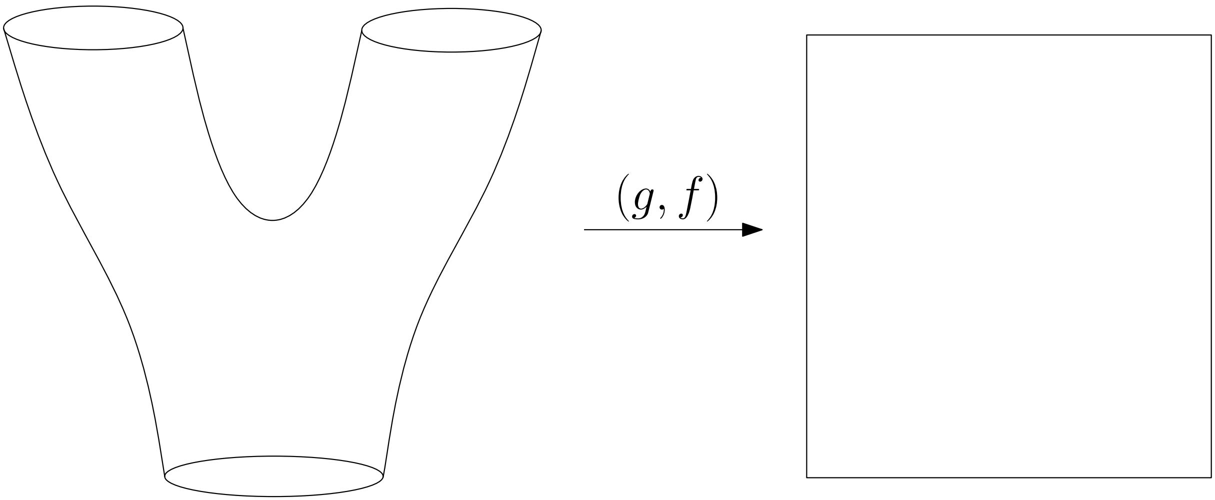

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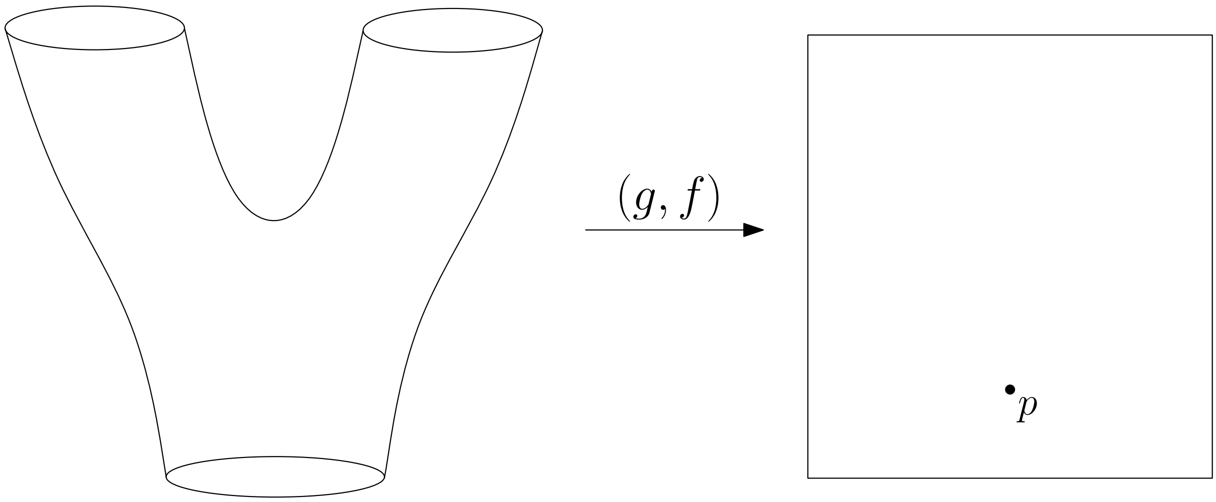

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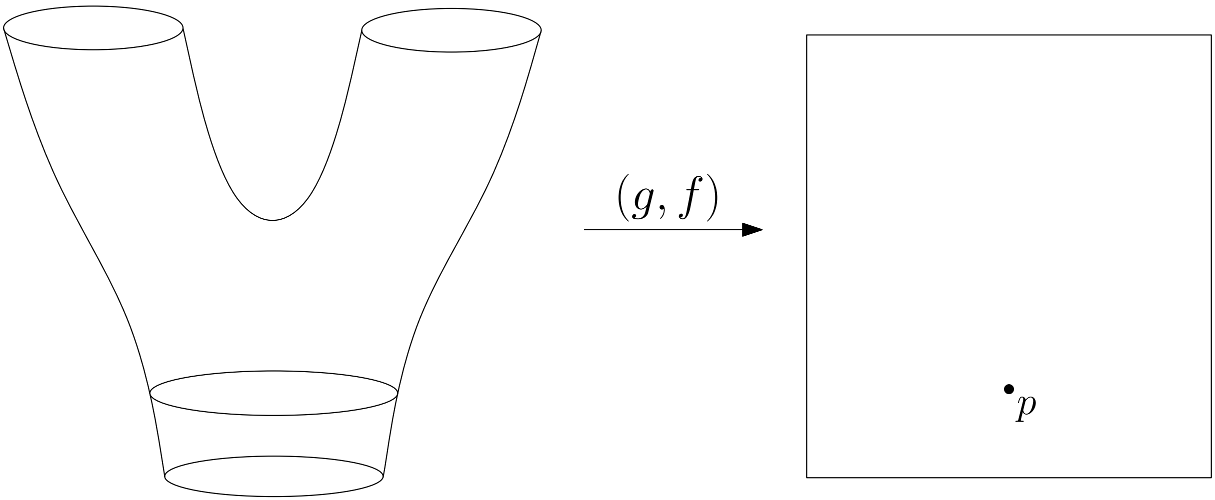

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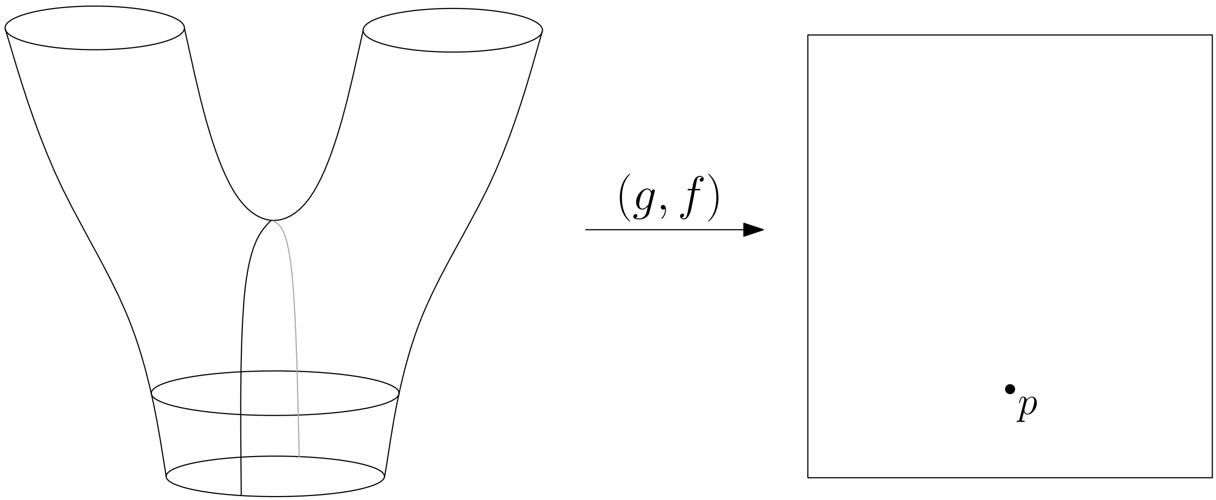

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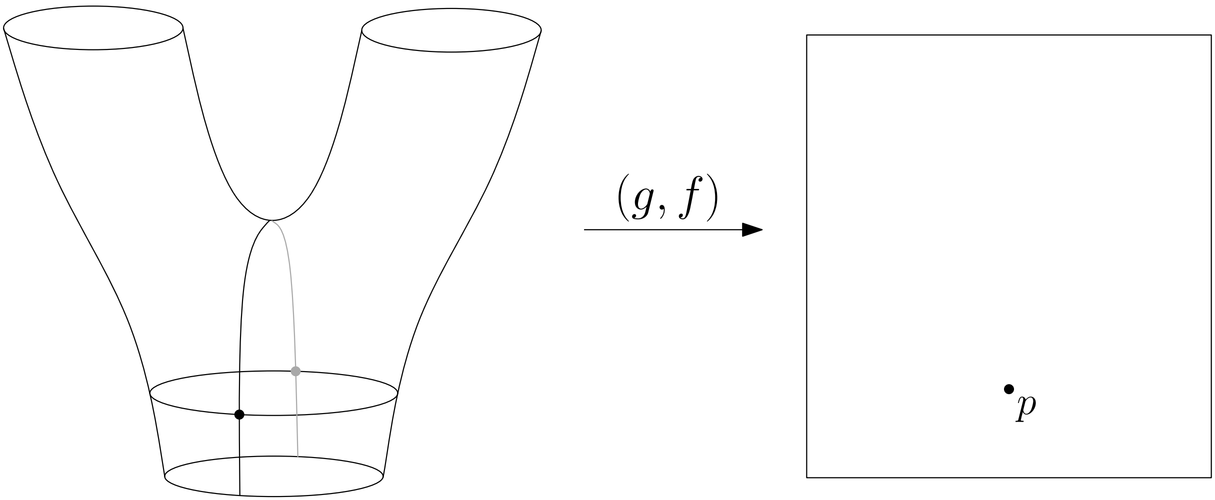

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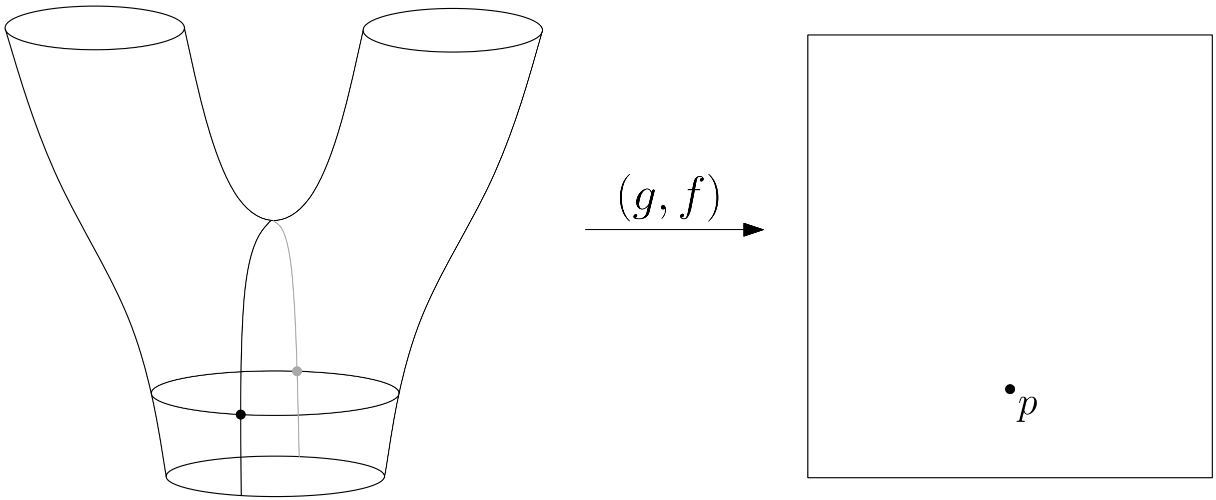

$\Longrightarrow$ We recover the original space

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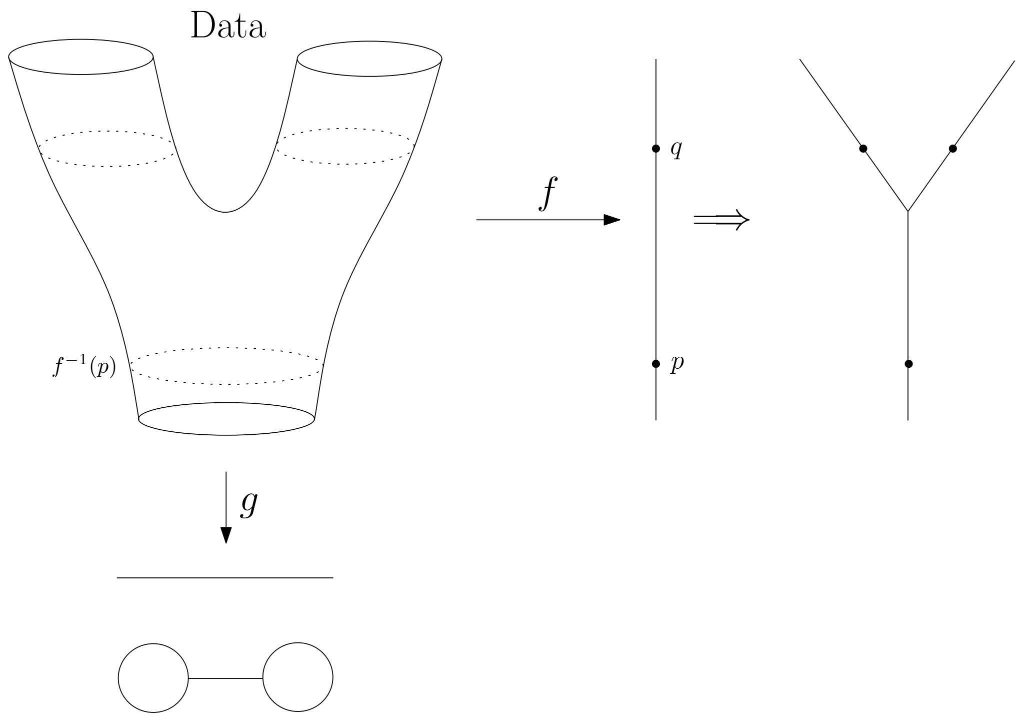
$\Rightarrow$ Instead we select a set of functions to *tune in* to the signal we want.

This is what Ayasdi does:



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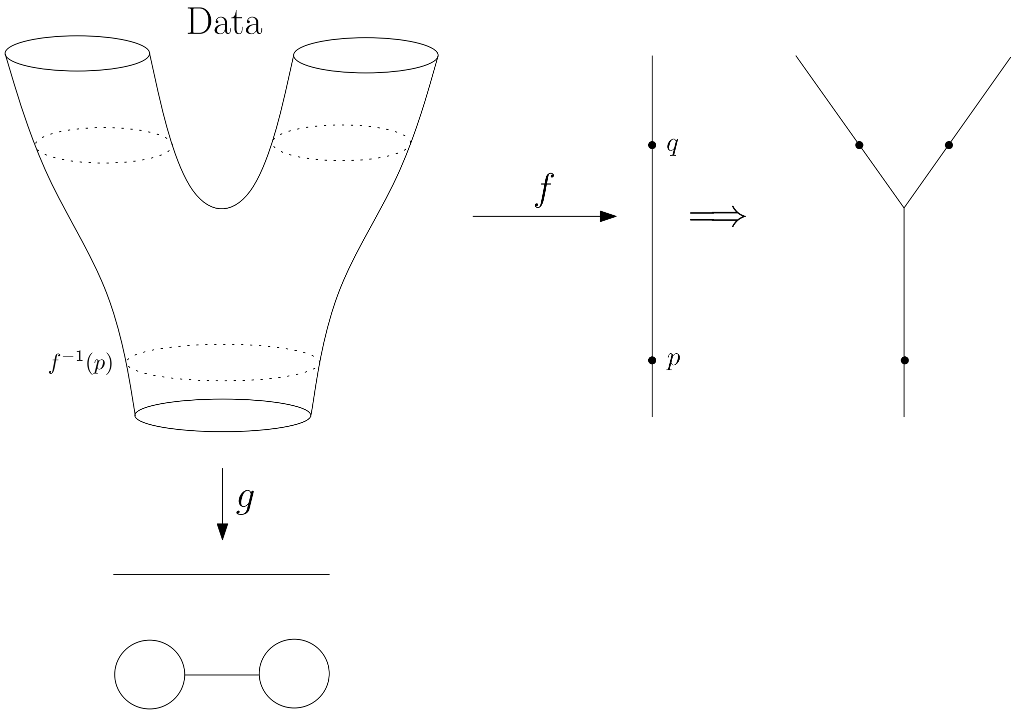

Modulo some details....

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$\Rightarrow$ We get "easy" understanding of the localizations of quantities of interest.

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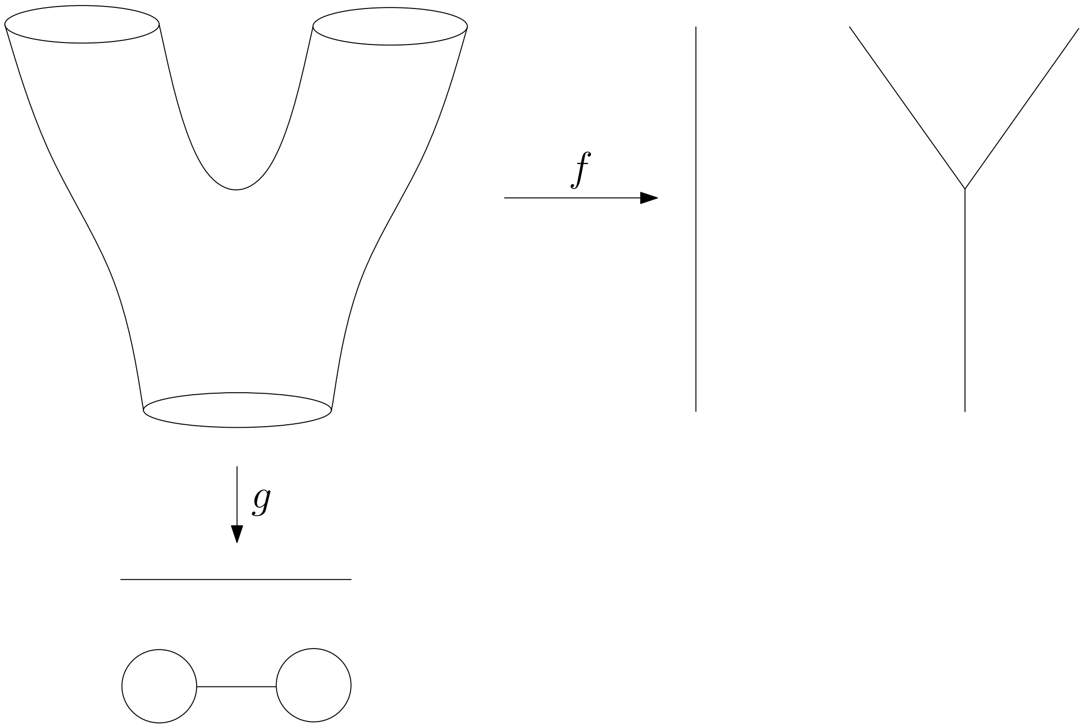

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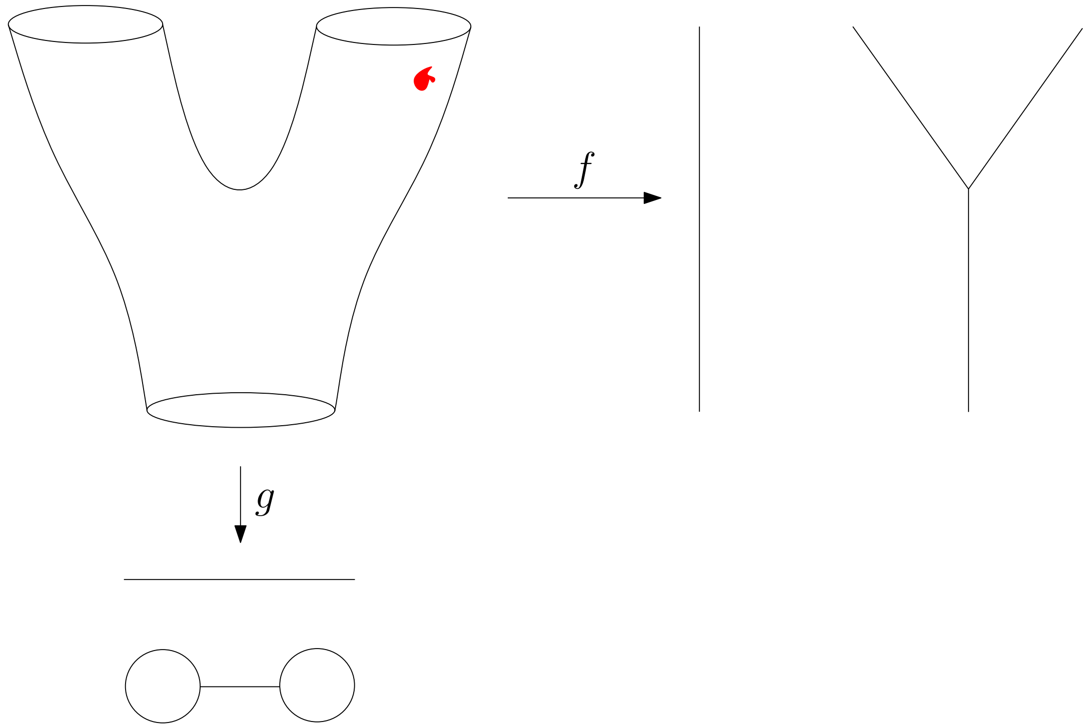

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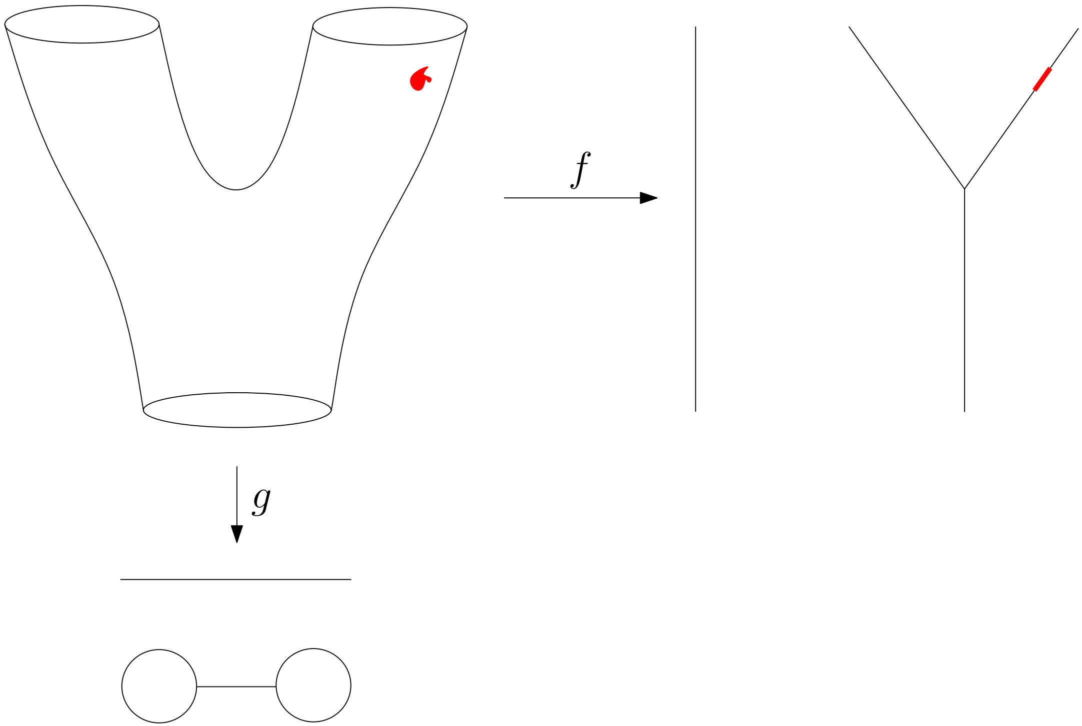

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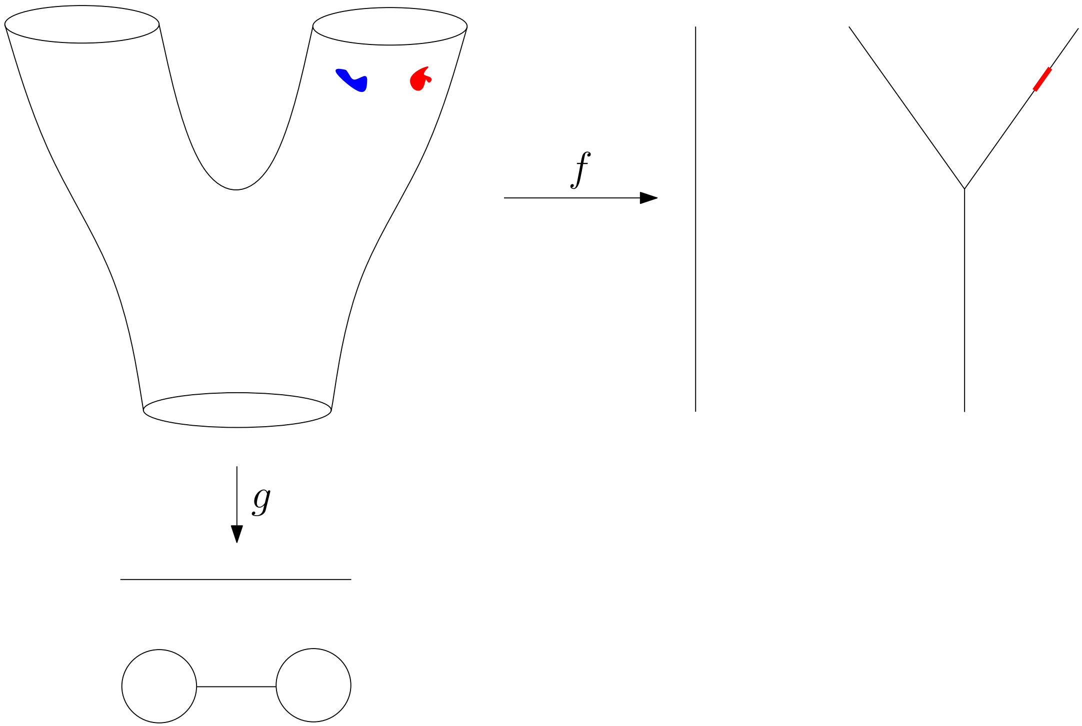

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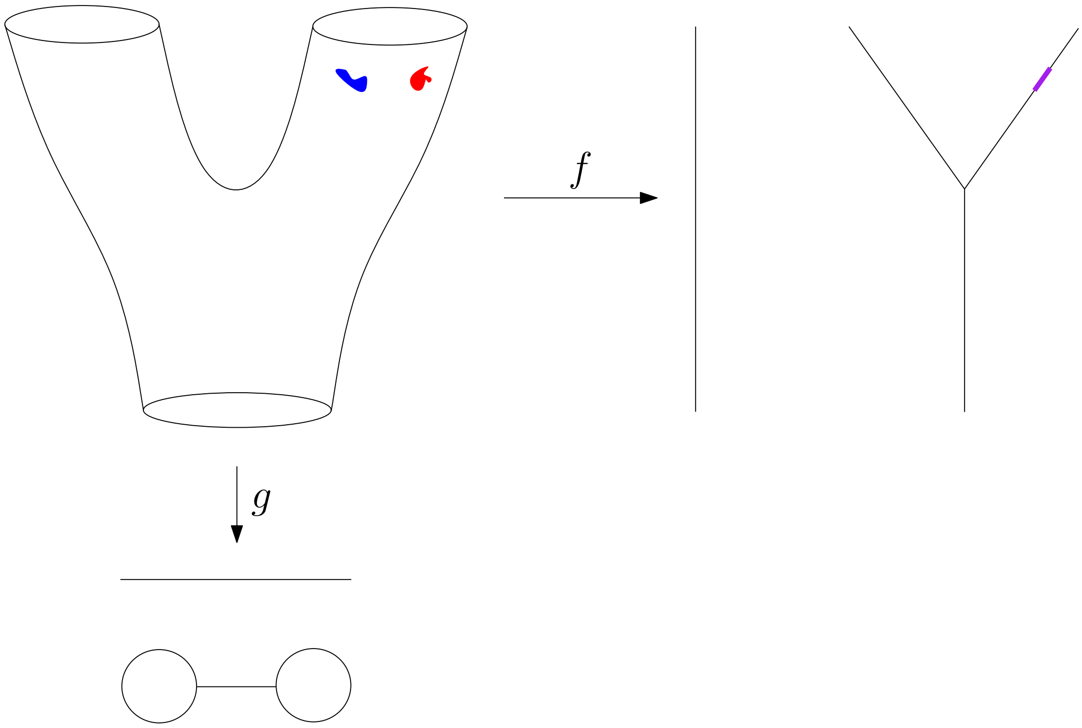

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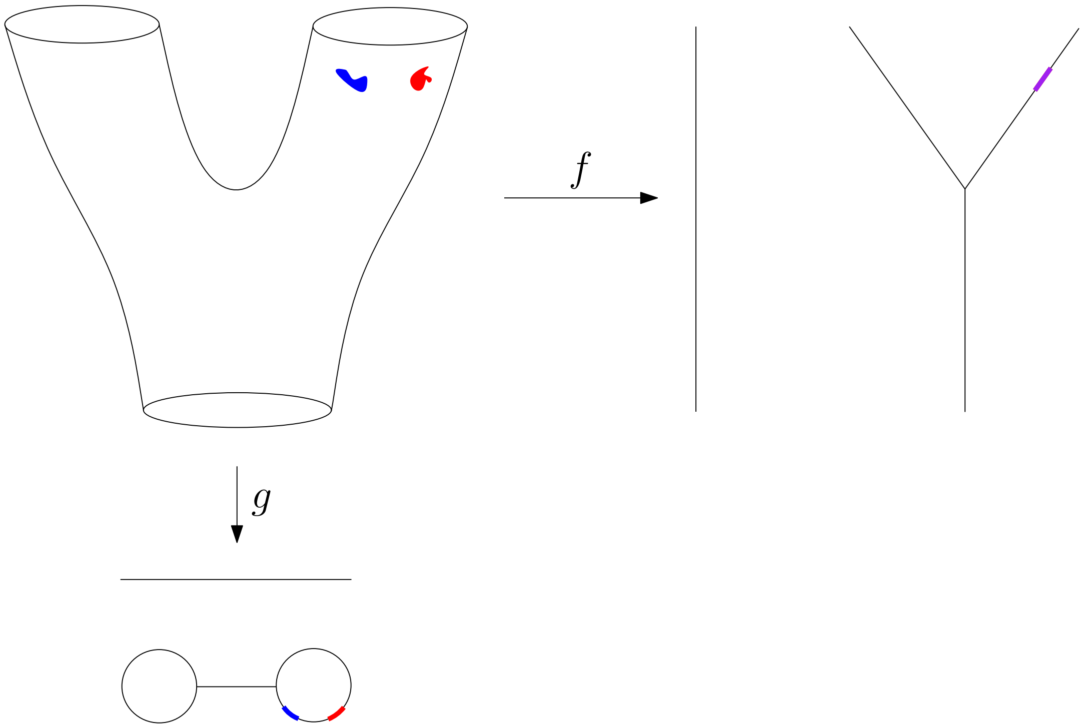

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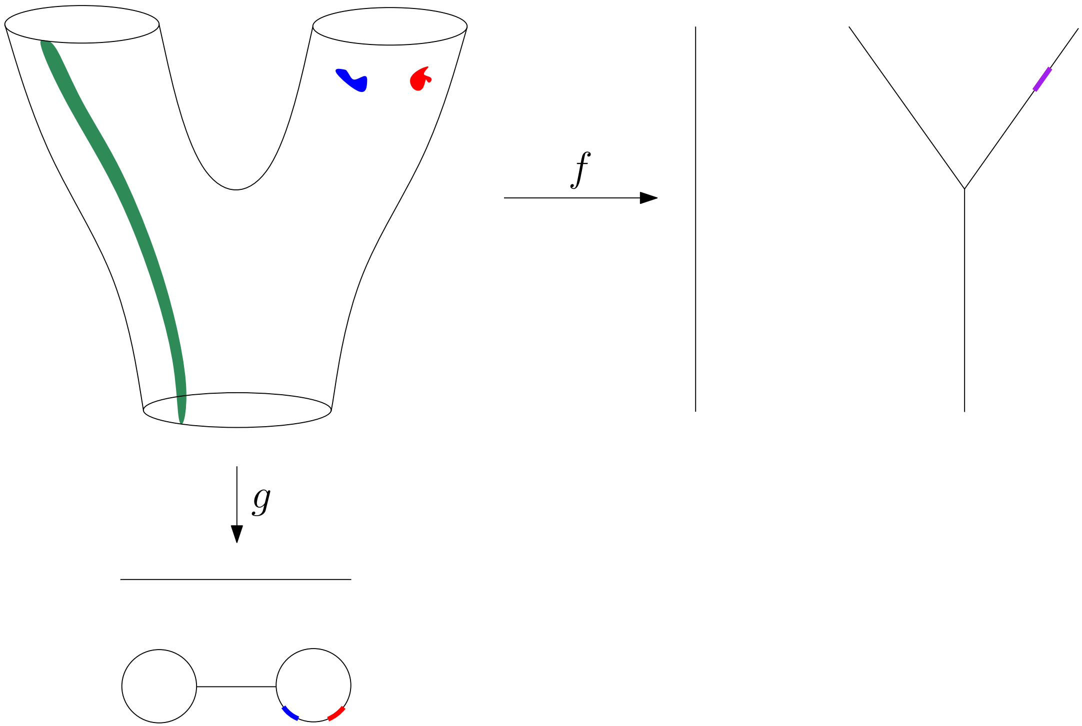

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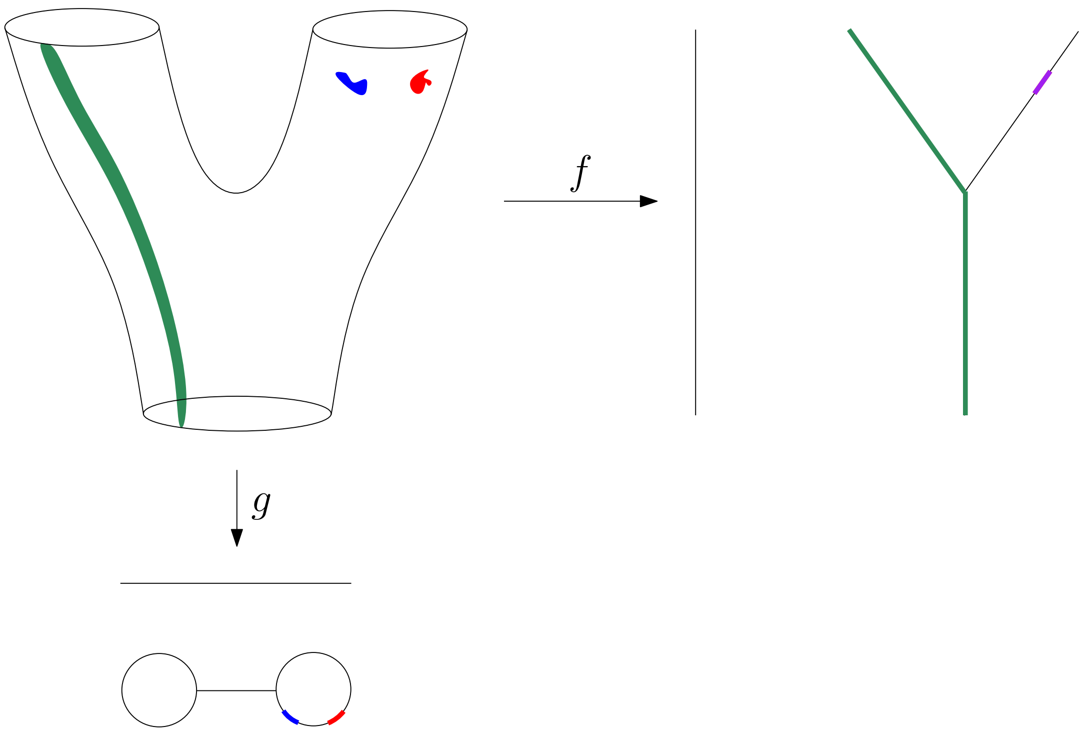

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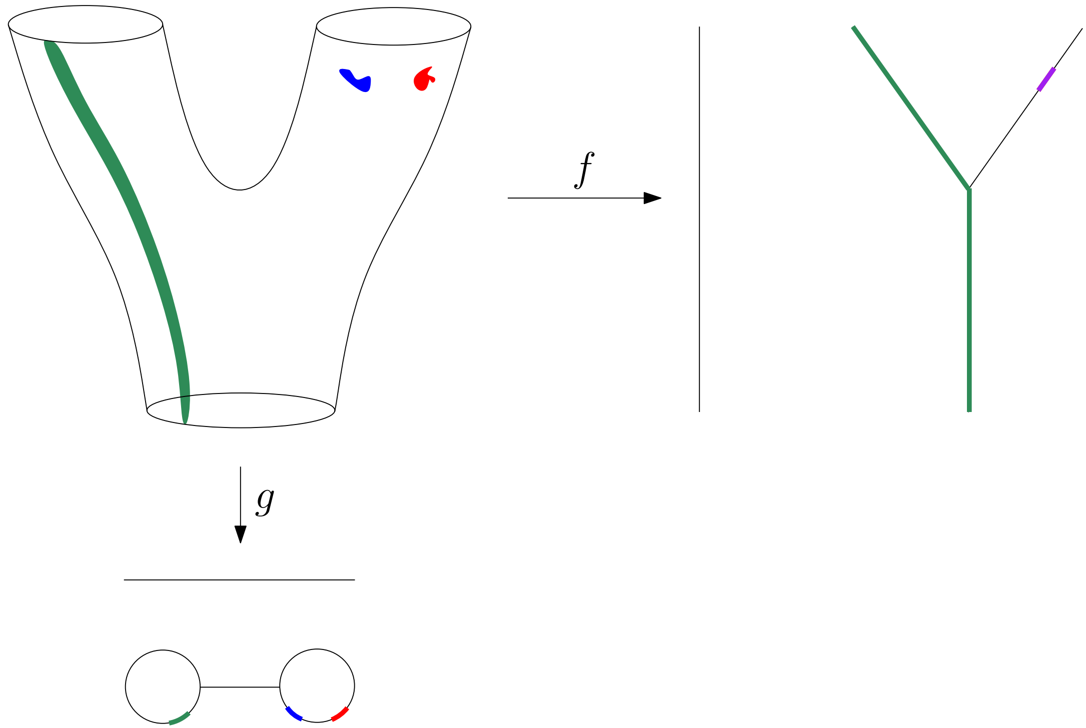

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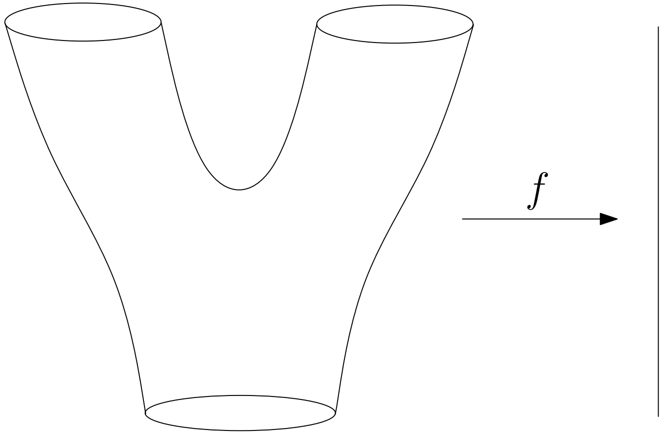
- For easy localizations many different lenses will be informative.
- For hard (= geometrically distributed) localizations we have to be more careful. But even then, we frequently get incremental knowledge even from a poorly chosen lens.

Modulo Details....

We want to move from this mathematical model to a data driven setup.

Step 1



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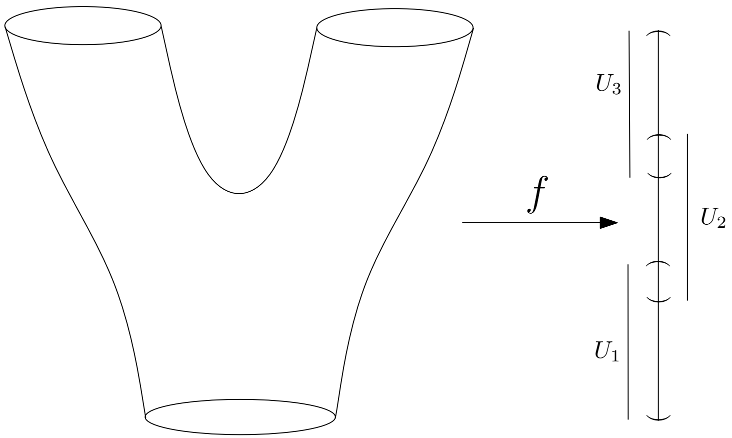

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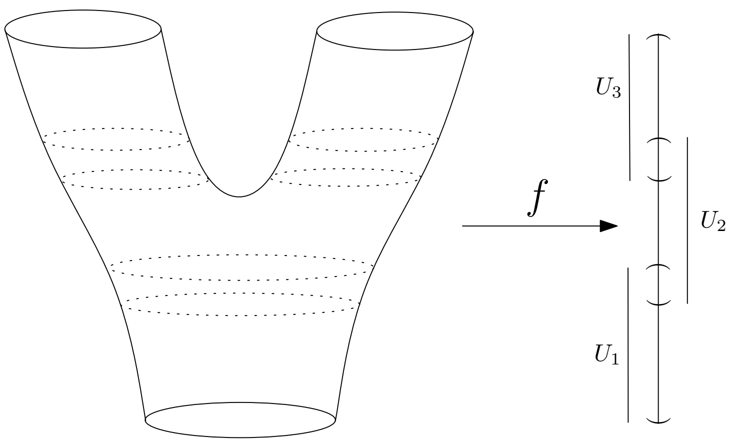

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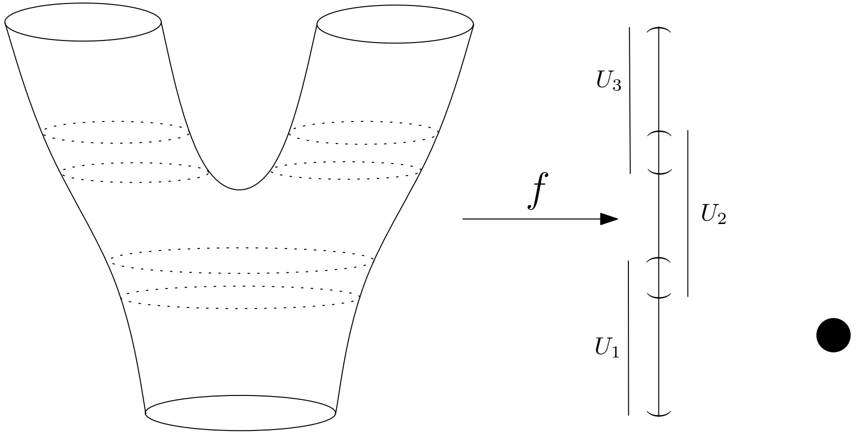

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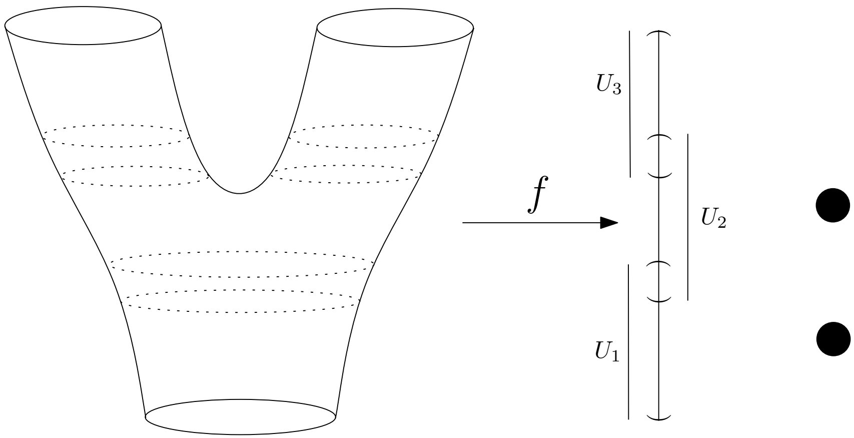

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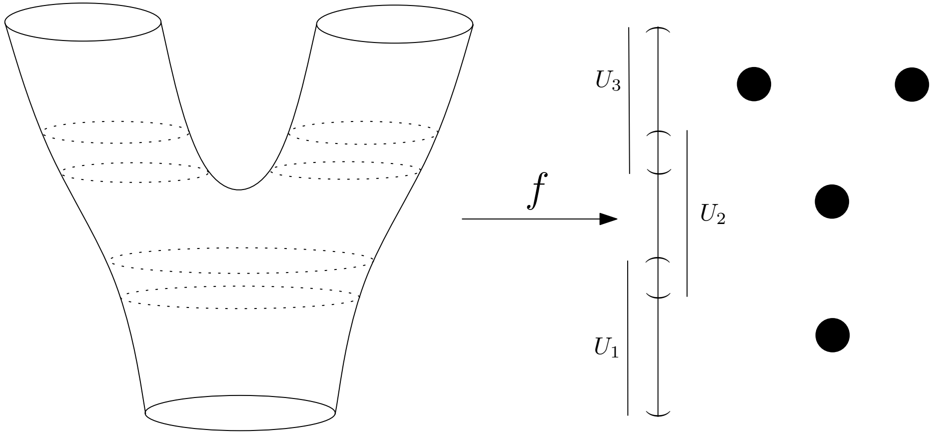

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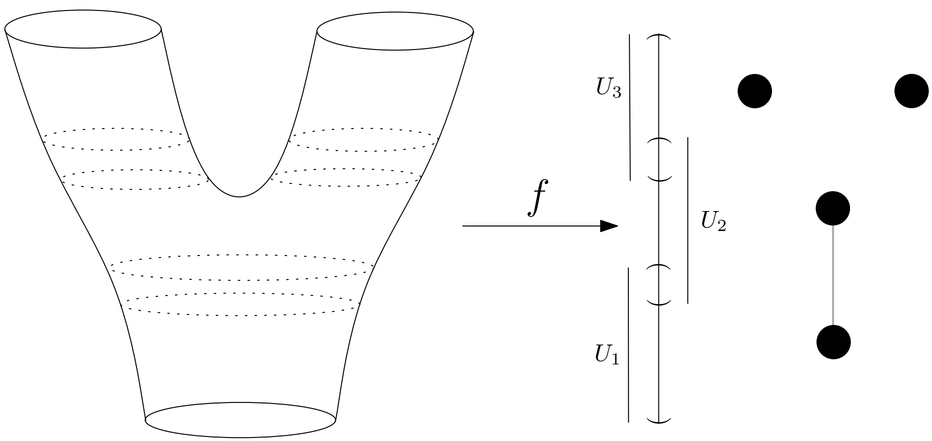
- Connect nodes when their corresponding sets intersect.



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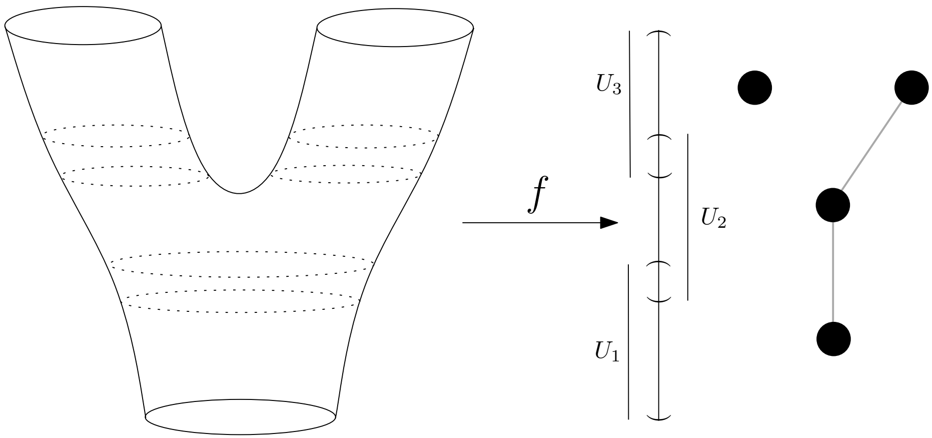

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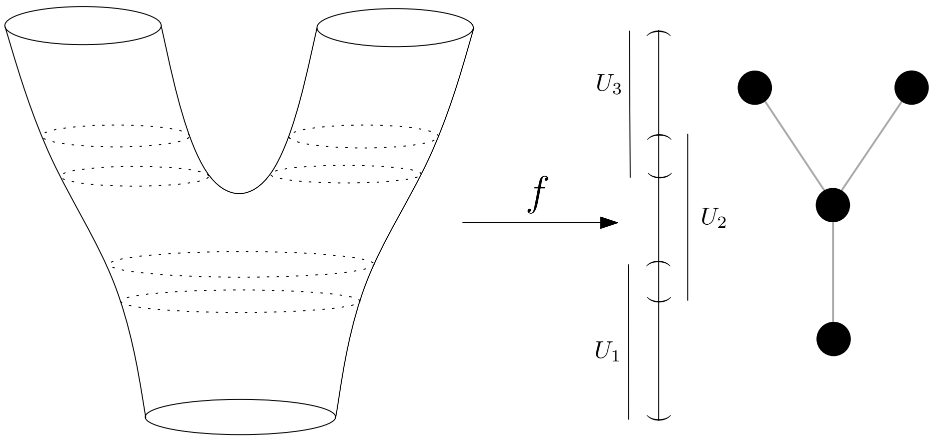

$\Rightarrow$ The output is now a graph.

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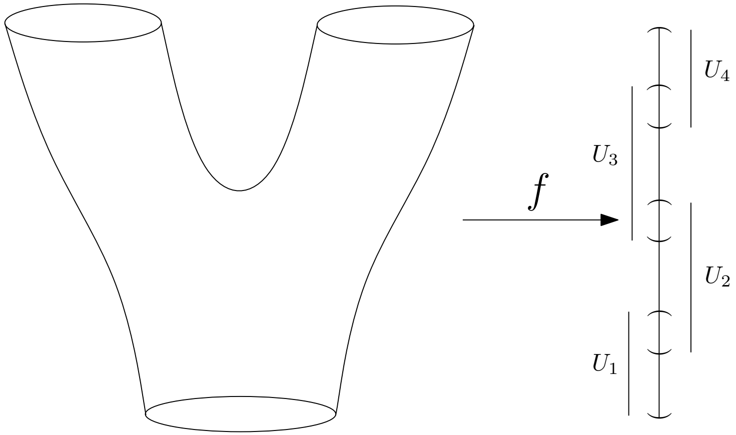
Roughly speaking, the resolution controls the number of nodes in the output and the 'size' of feature you can pick out, while the gain controls the number of edges and the 'tightness' of the graph.

Resolution: A closer look



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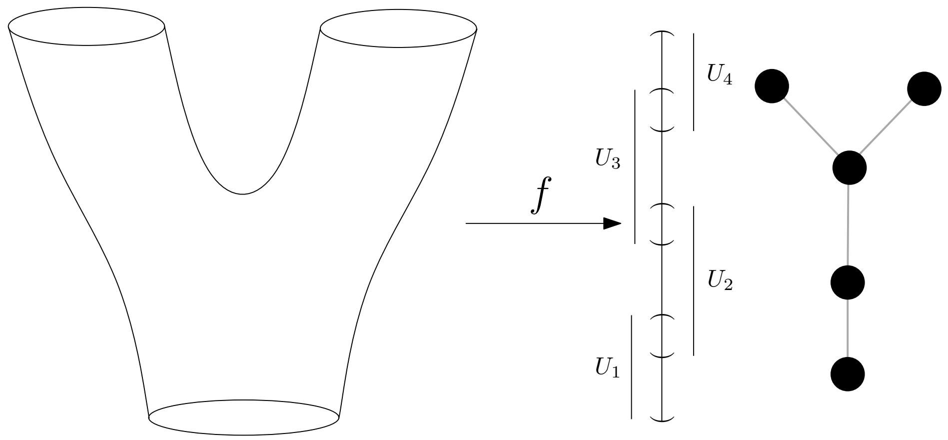

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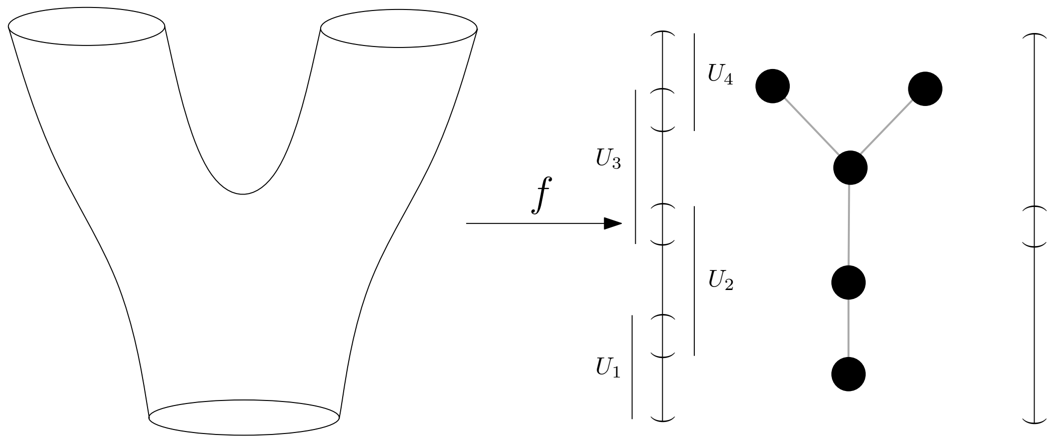

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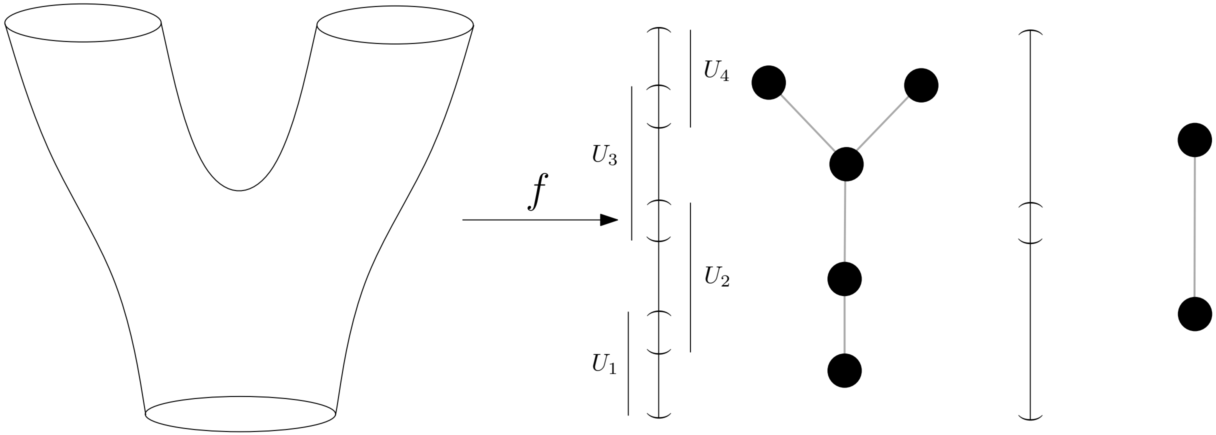

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- We replace "connected component of the inverse image" is with "*clusters* in the inverse image".
- We connect clusters (nodes) with an edge if they share points in common.

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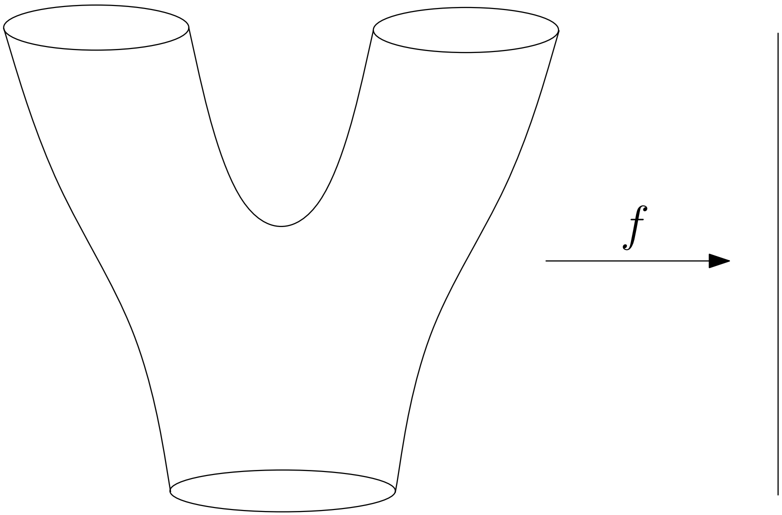

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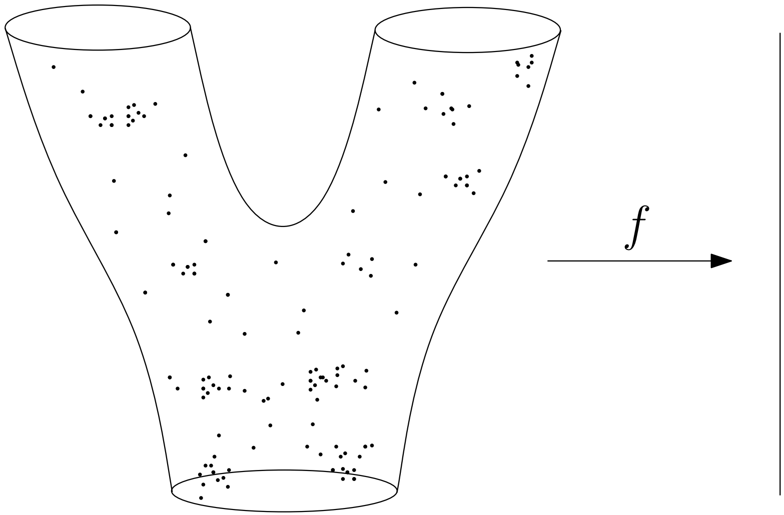

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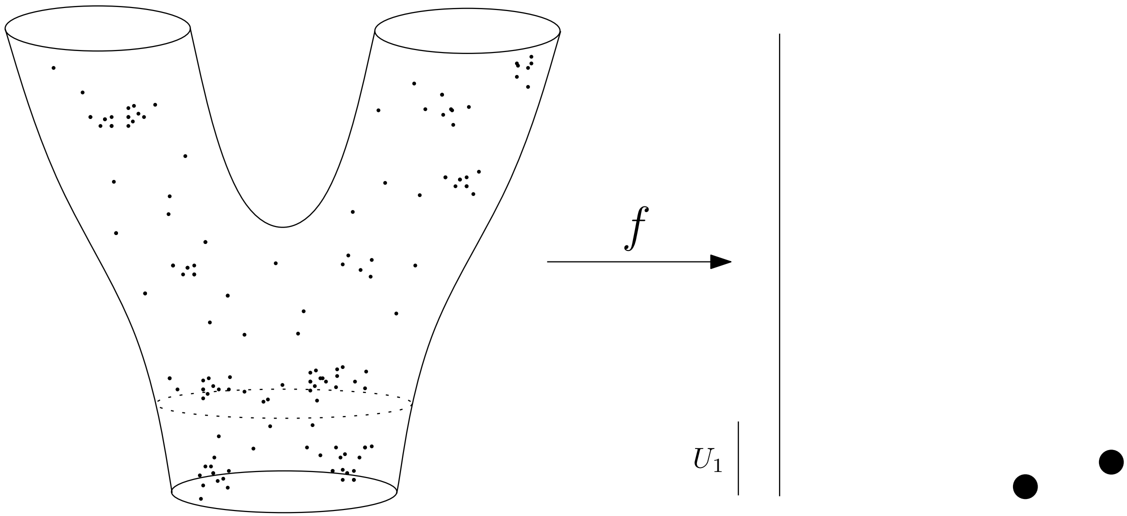

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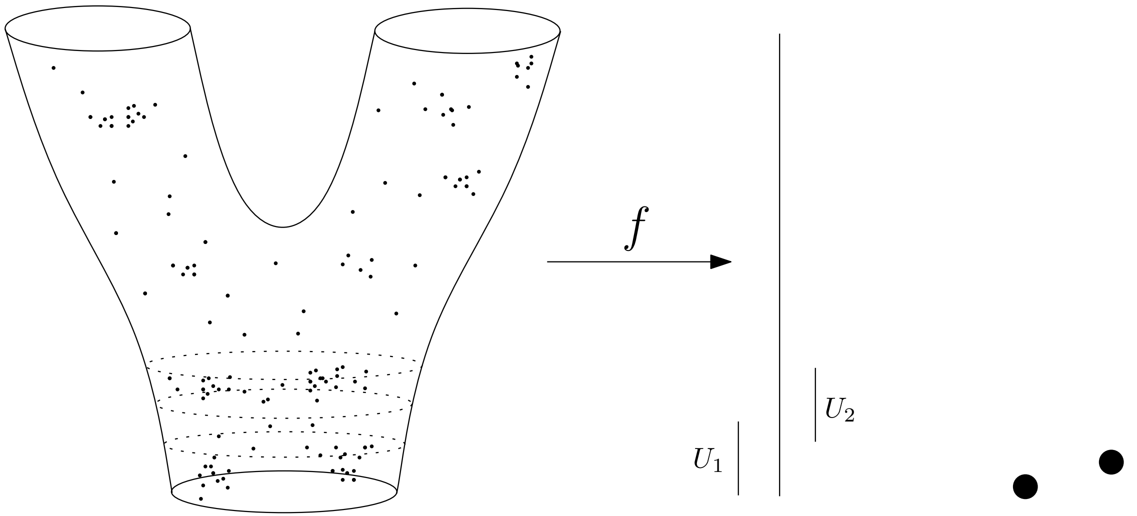

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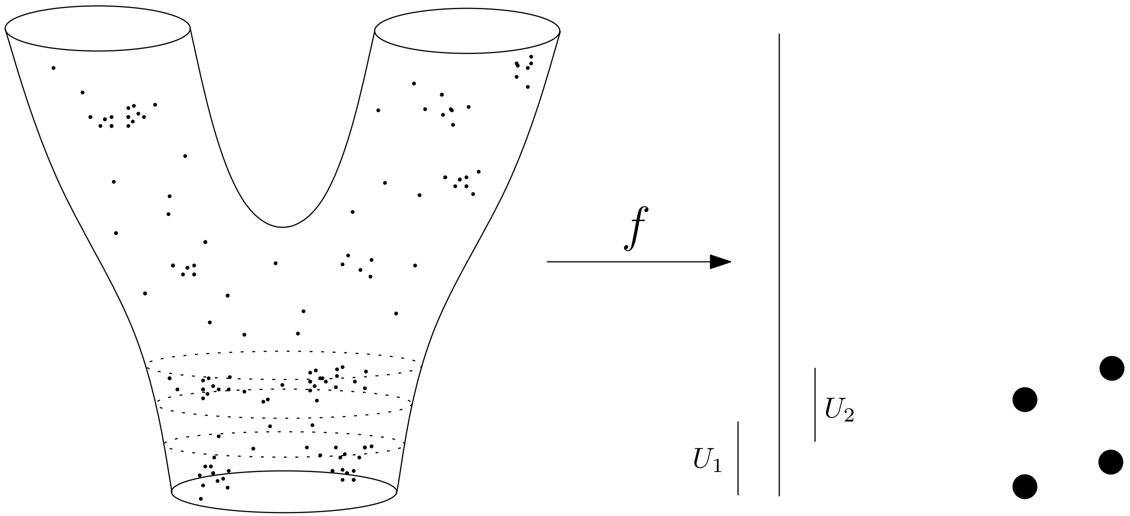

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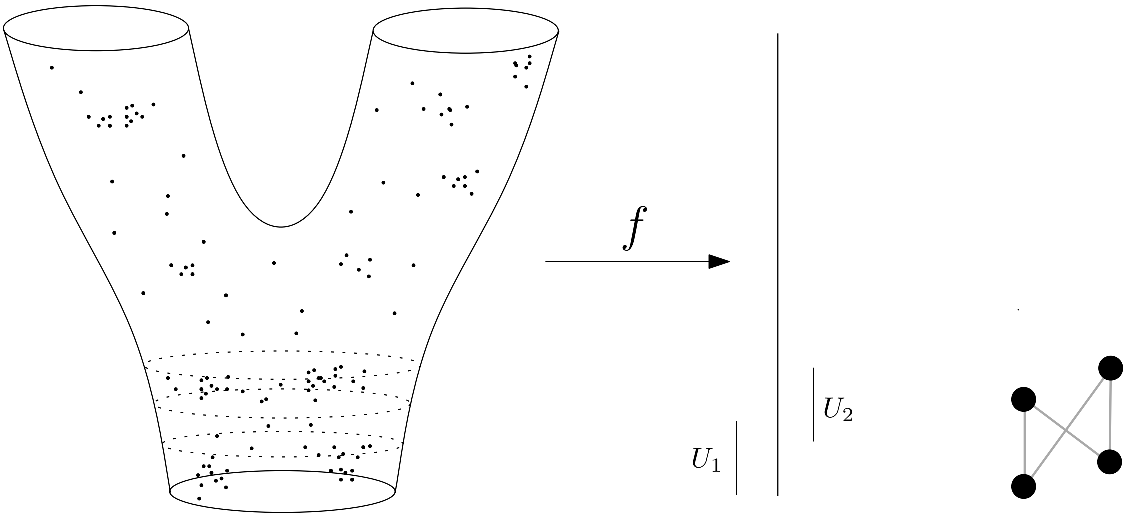

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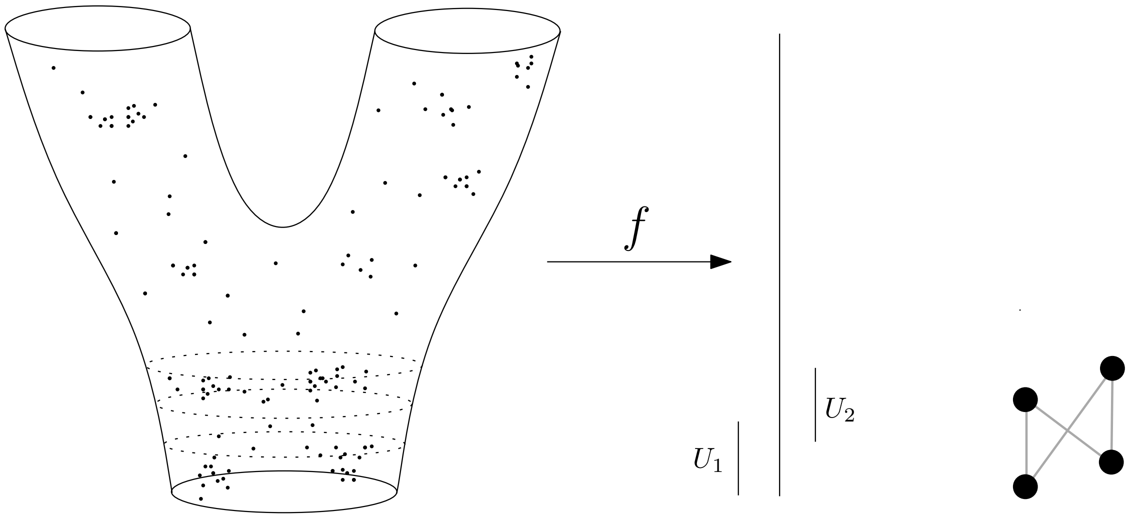
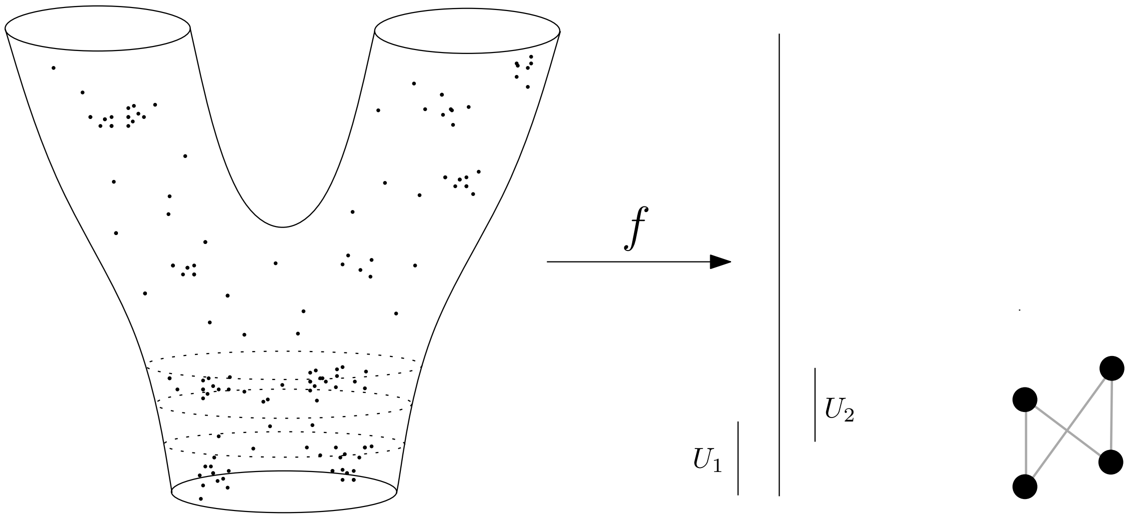


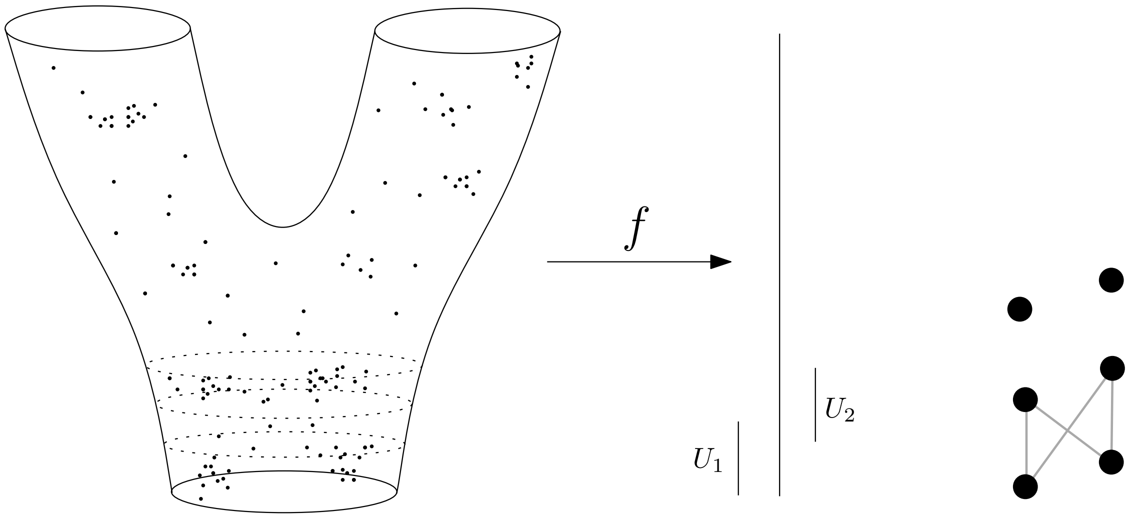
- Nodes are clusters of data points

Step 2: Clustering as π_0



- Nodes are clusters of data points
- Edges represent shared points between the clusters

Step 2: Clustering as π_0



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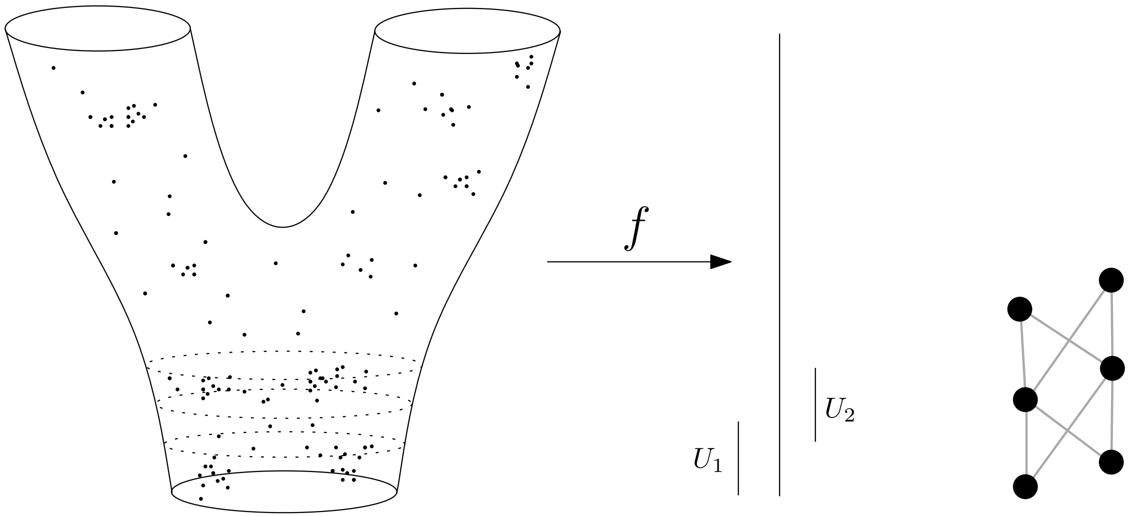

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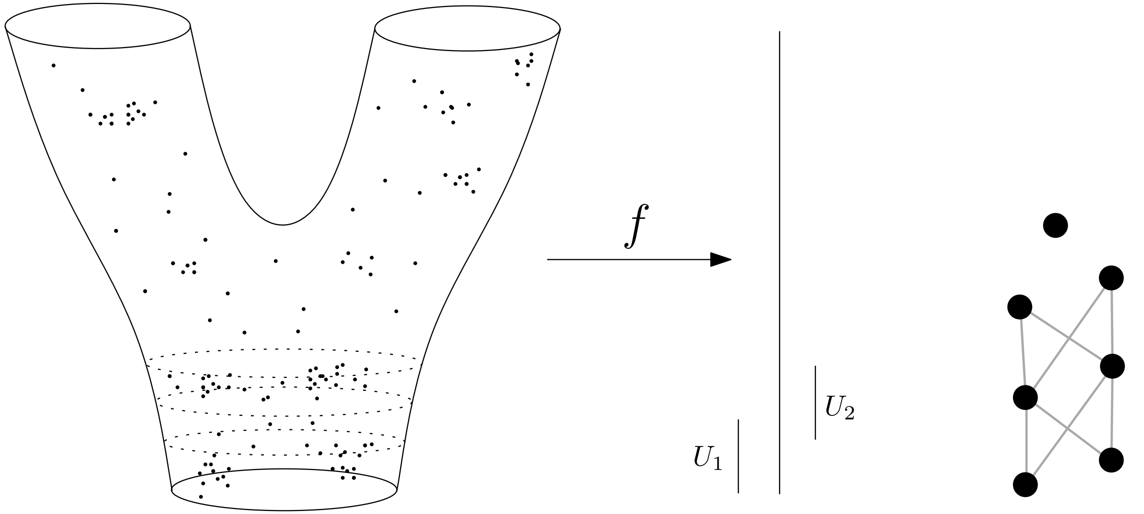

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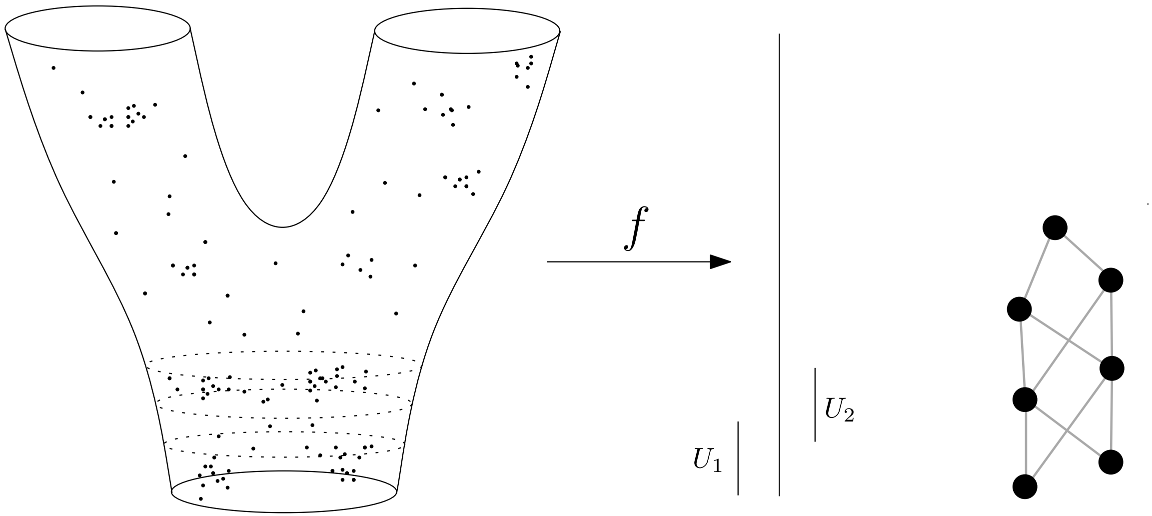

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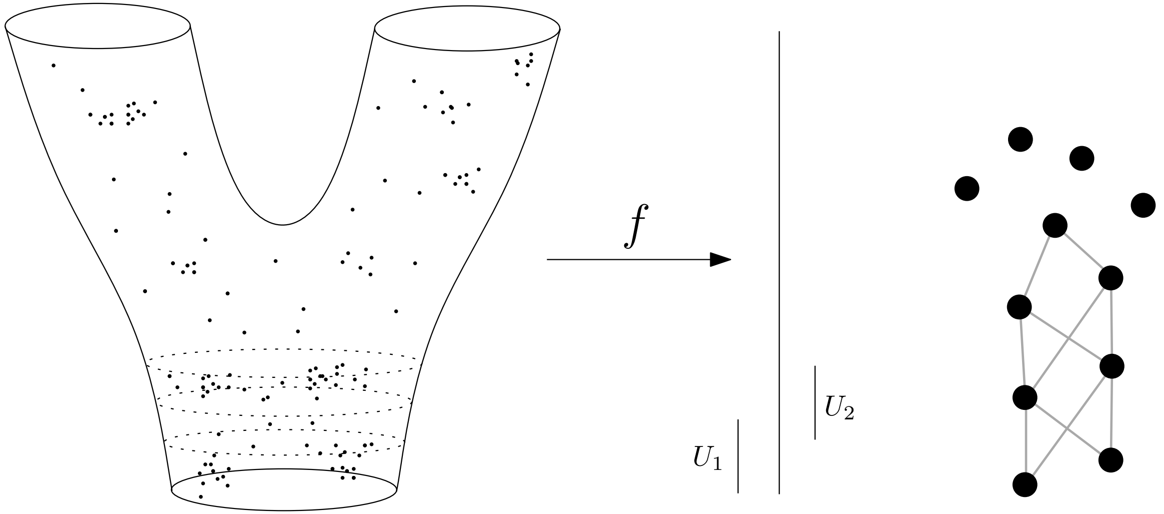

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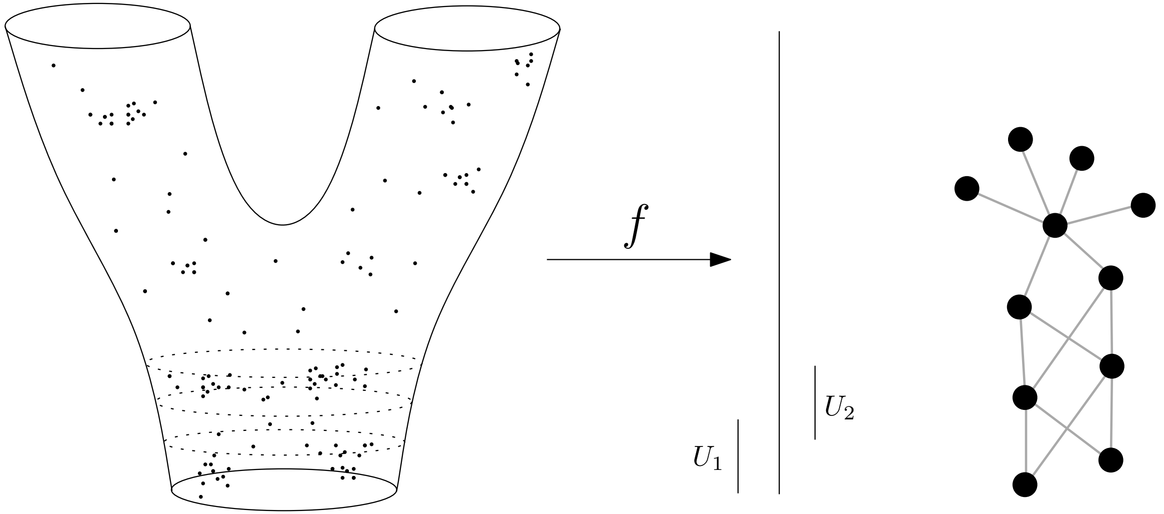

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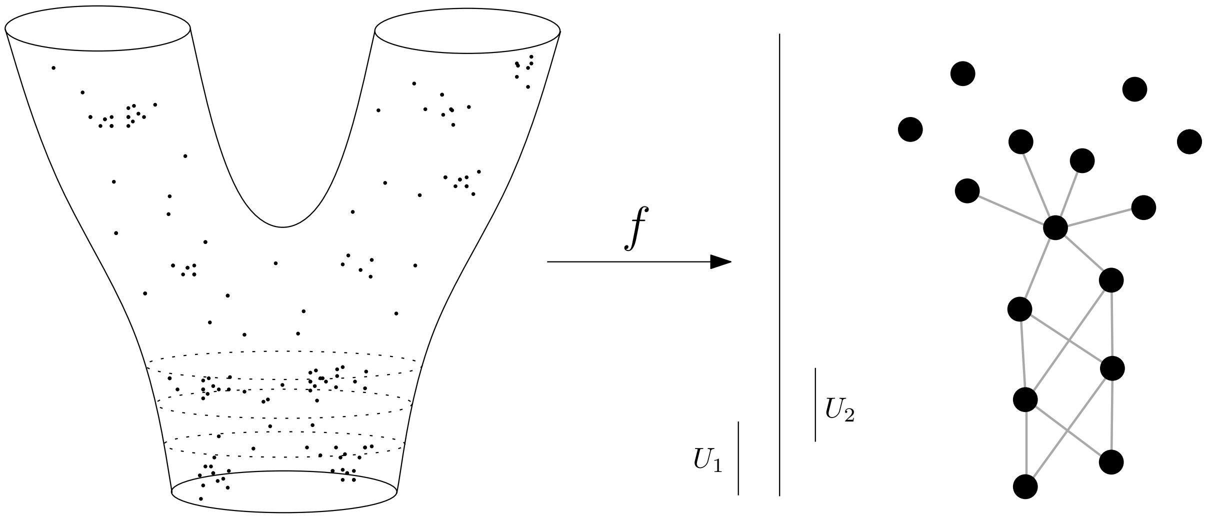

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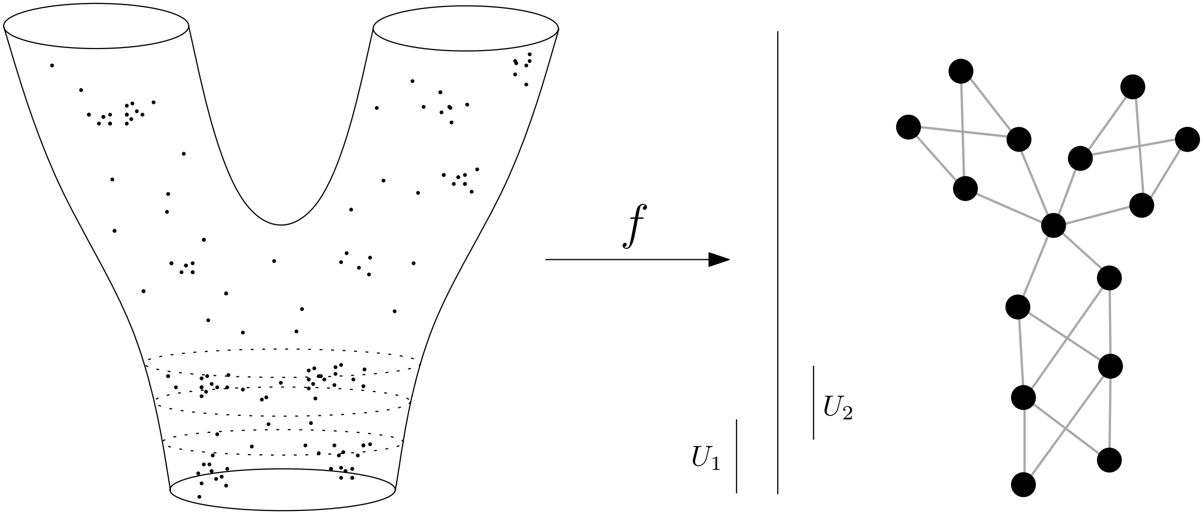

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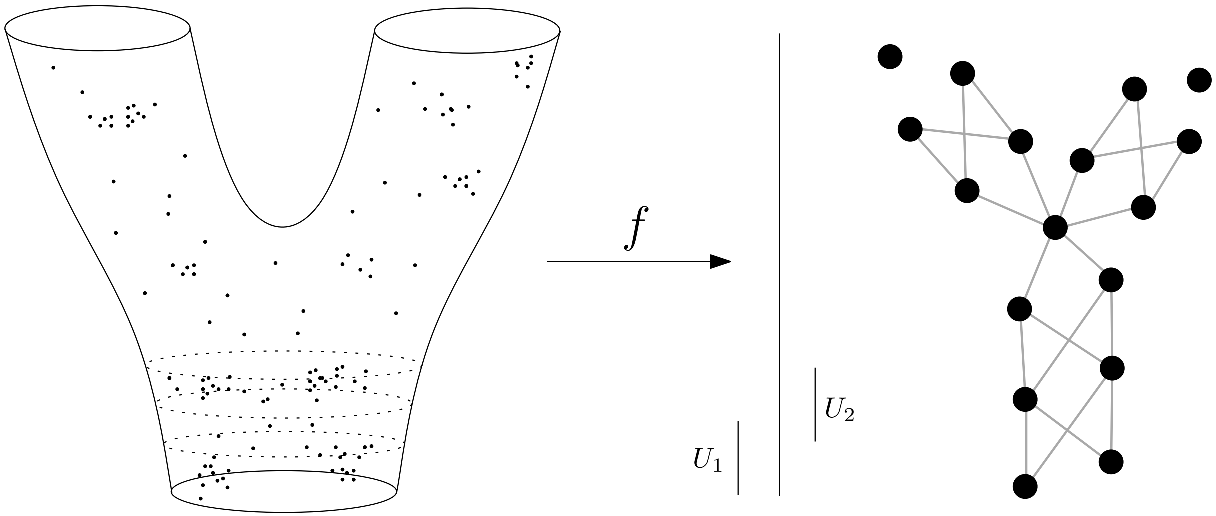

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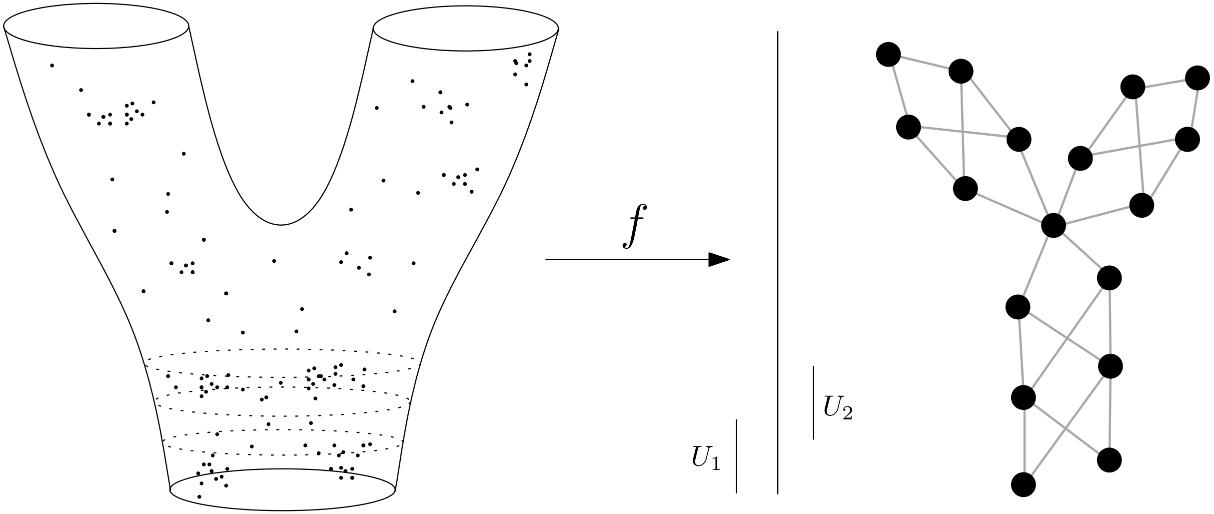

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- Edges represent shared points between the clusters

That’s It

That's It

Ok not quite...

Lenses: Where do they come from

The technique rests on finding good lenses.

Lenses: Where do they come from

The technique rests on finding good lenses.

$\Rightarrow$ Luckily lots of people have worked on this problem

Lenses: Where do they come from

A Non Exhaustive Table of Lenses

Lenses: Where do they come from

- Standard data analysis functions

A Non Exhaustive Table of Lenses

Statistics

Lenses: Where do they come from

- Standard data analysis functions

A Non Exhaustive Table of Lenses

Statistics
Mean/Max/Min

Lenses: Where do they come from

- Standard data analysis functions

A Non Exhaustive Table of Lenses

Statistics
Mean/Max/Min
Variance

Lenses: Where do they come from

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A Non Exhaustive Table of Lenses

Statistics
Mean/Max/Min
Variance
n-Moment

Lenses: Where do they come from

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A Non Exhaustive Table of Lenses

Statistics
Mean/Max/Min
Variance
n-Moment
Density

Lenses: Where do they come from

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A Non Exhaustive Table of Lenses

Statistics
Mean/Max/Min
Variance
n-Moment
Density
...

Lenses: Where do they come from

- Standard data analysis functions
- Geometry and Topology

A Non Exhaustive Table of Lenses

Statistics	Geometry
Mean/Max/Min	
Variance	
n-Moment	
Density	
...	

Lenses: Where do they come from

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A Non Exhaustive Table of Lenses

Statistics	Geometry
Mean/Max/Min	Centrality
Variance	
n-Moment	
Density	
...	

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Statistics	Geometry
Mean/Max/Min	Centrality
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...	

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Mean/Max/Min	Centrality
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n-Moment	Harmonic Cycles
Density	
...	

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Statistics	Geometry
Mean/Max/Min	Centrality
Variance	Curvature
n-Moment	Harmonic Cycles
Density	...
...	

Lenses: Where do they come from

- Standard data analysis functions
- Geometry and Topology
- Modern Statistics

A Non Exhaustive Table of Lenses

Statistics	Geometry	Machine Learning
Mean/Max/Min	Centrality	
Variance	Curvature	
n-Moment	Harmonic Cycles	
Density	...	
...		

Lenses: Where do they come from

- Standard data analysis functions
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A Non Exhaustive Table of Lenses

Statistics	Geometry	Machine Learning
Mean/Max/Min	Centrality	PCA/SVD
Variance	Curvature	
n-Moment	Harmonic Cycles	
Density	...	
...		

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Statistics	Geometry	Machine Learning
Mean/Max/Min	Centrality	PCA/SVD
Variance	Curvature	Autoencoders
n-Moment	Harmonic Cycles	
Density	...	
...		

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Mean/Max/Min	Centrality	PCA/SVD
Variance	Curvature	Autoencoders
n-Moment	Harmonic Cycles	Isomap/MDS/TSNE
Density	...	
...		

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Density	...	SVM Distance from Hyperplane
...		

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Density	...	SVM Distance from Hyperplane
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		...

Lenses: Where do they come from

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

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

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Variance	Curvature	Autoencoders	Dates
n-Moment	Harmonic Cycles	Isomap/MDS/TSNE	
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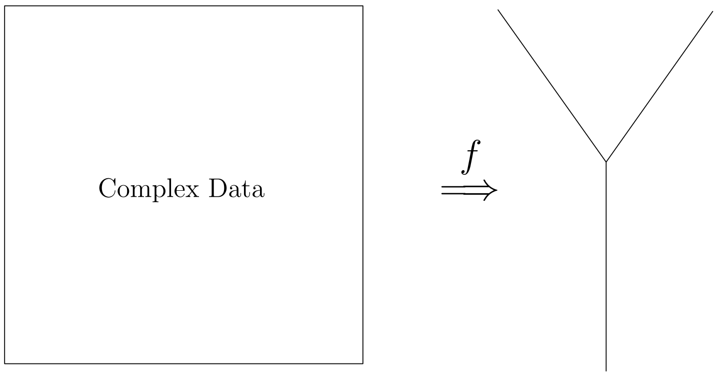
Density	...	SVM Distance from Hyperplane	
...		Error/Debugging Info	
		...	

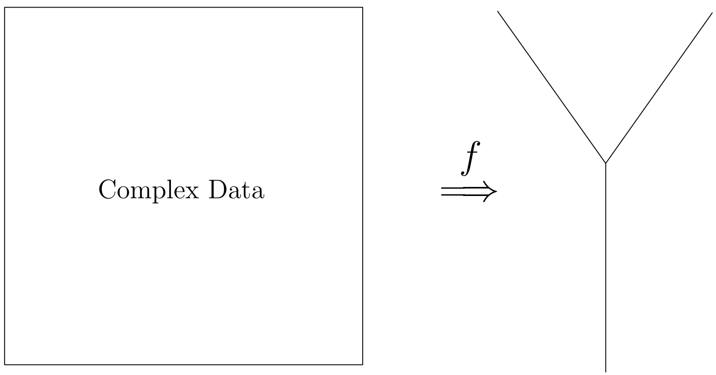
Interperability and Meaning

But what about insight? meaning?

Interperability and Meaning

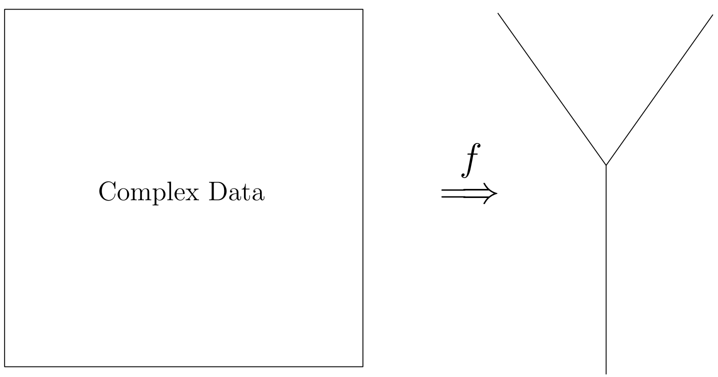


Interperability and Meaning



f is gaussian density

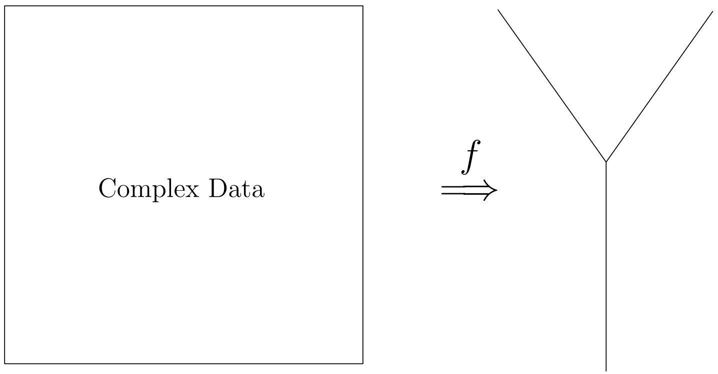
Interperability and Meaning



f is gaussian density

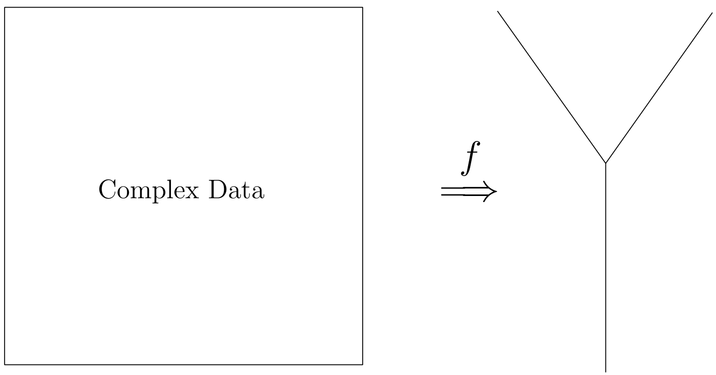
$\Rightarrow$ The data is bi-modal.

Interperability and Meaning



f is centrality

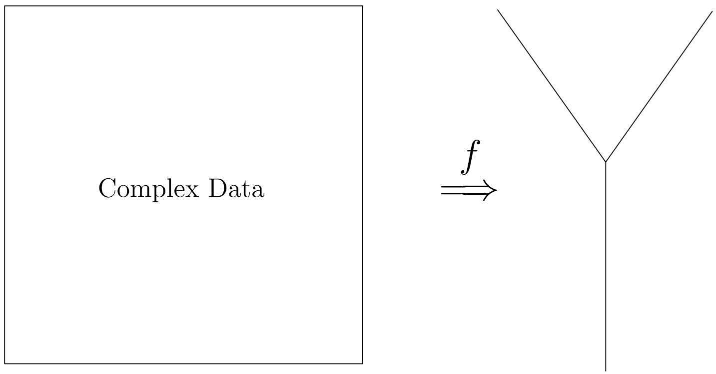
Interperability and Meaning



f is centrality

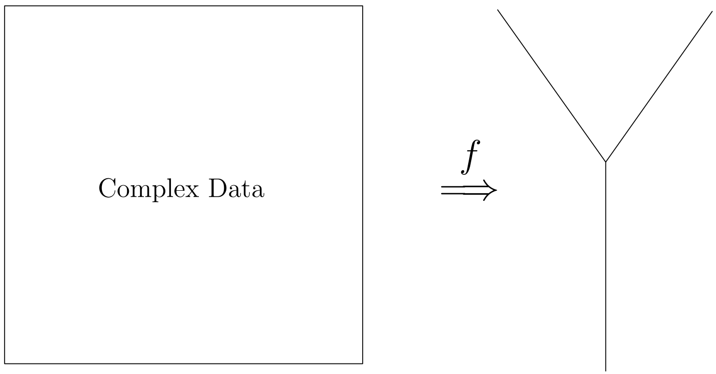
$\Rightarrow$ The data has two ways of being abnormal.

Interperability and Meaning



f is mean

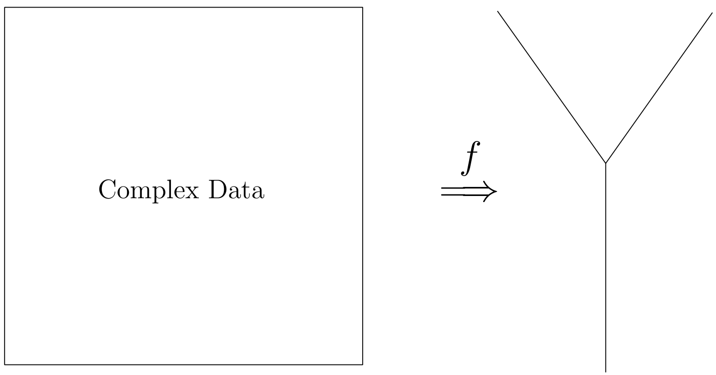
Interperability and Meaning



f is mean

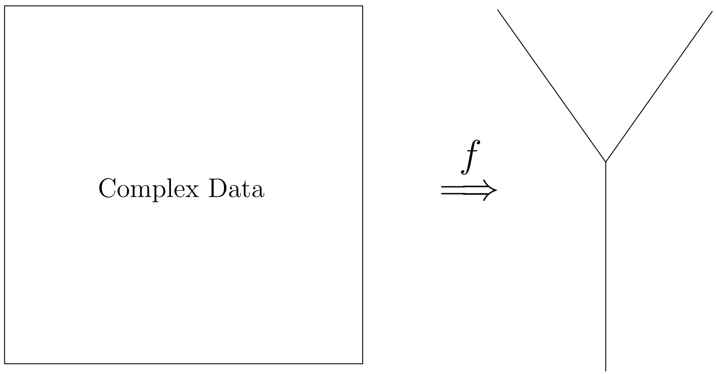
$\Rightarrow$ Two groups of high mean data.

Interperability and Meaning



f is error

Interperability and Meaning



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$\Rightarrow$ Two types of error.

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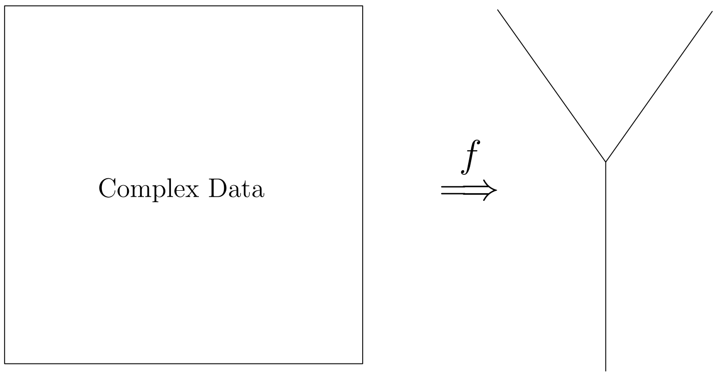

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The units on the lens give interperability/meaning to the topological summary.

Interperability and Meaning

Another way to think about lenses is as a kind of ’geometric query’.

Examples

Interperability and Meaning

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Examples

1. Heart disease study

Interperability and Meaning

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   - Stratification by age without making arbitrary cutoffs.

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2. Heavy machinery

Interperability and Meaning

Another way to think about lenses is as a kind of ’geometric query’.

Examples

1. Heart disease study
   - Stratification by age without making arbitrary cutoffs.
2. Heavy machinery
   - Use mean a variance as a lens to find what operating regimes lead to failure of mechanical components.

Some generalizations and extensions

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Metrics

Some generalizations and extensions

Metrics

- We don’t need a metric, just a notion of similarity - or perhaps a clustering mechanism.

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Output

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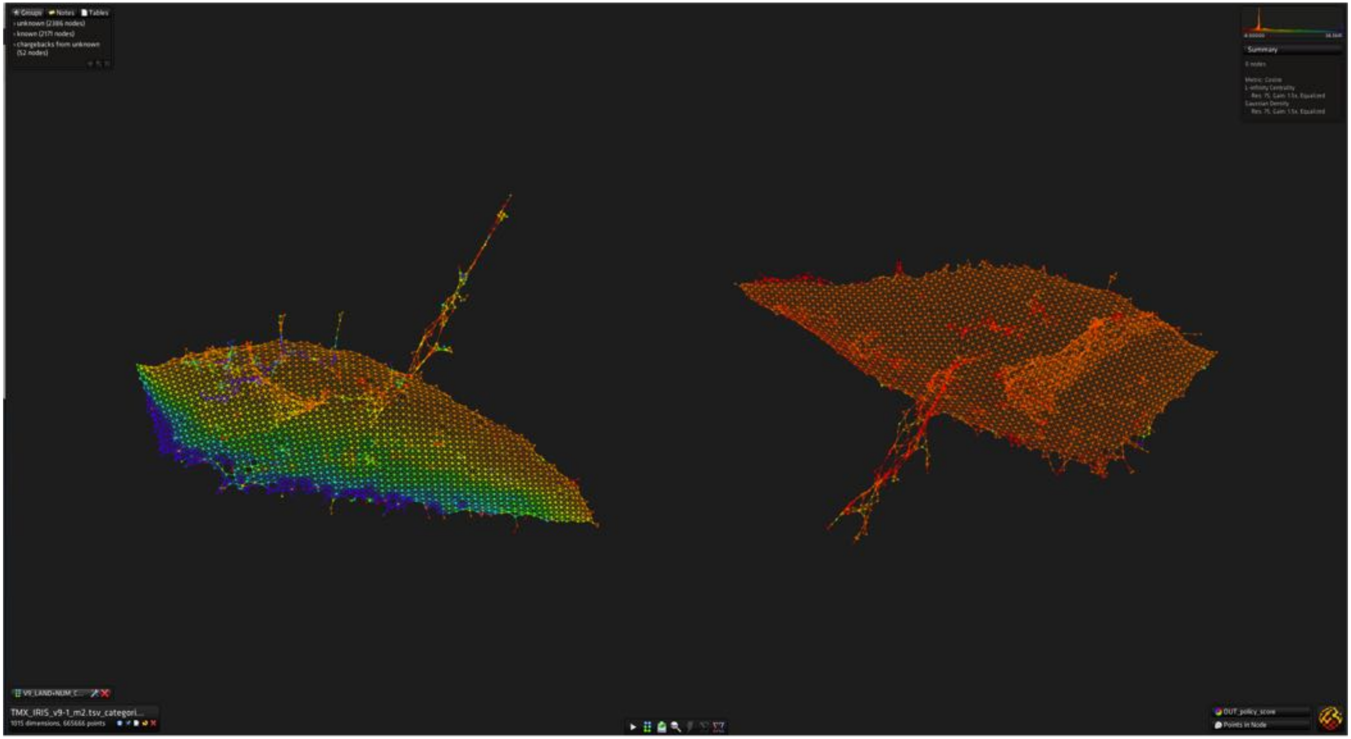
Output

- The output of the algorithm isn't just a graph but is an abstract simplicial complex (swept under the rug in this presentation).

Demo

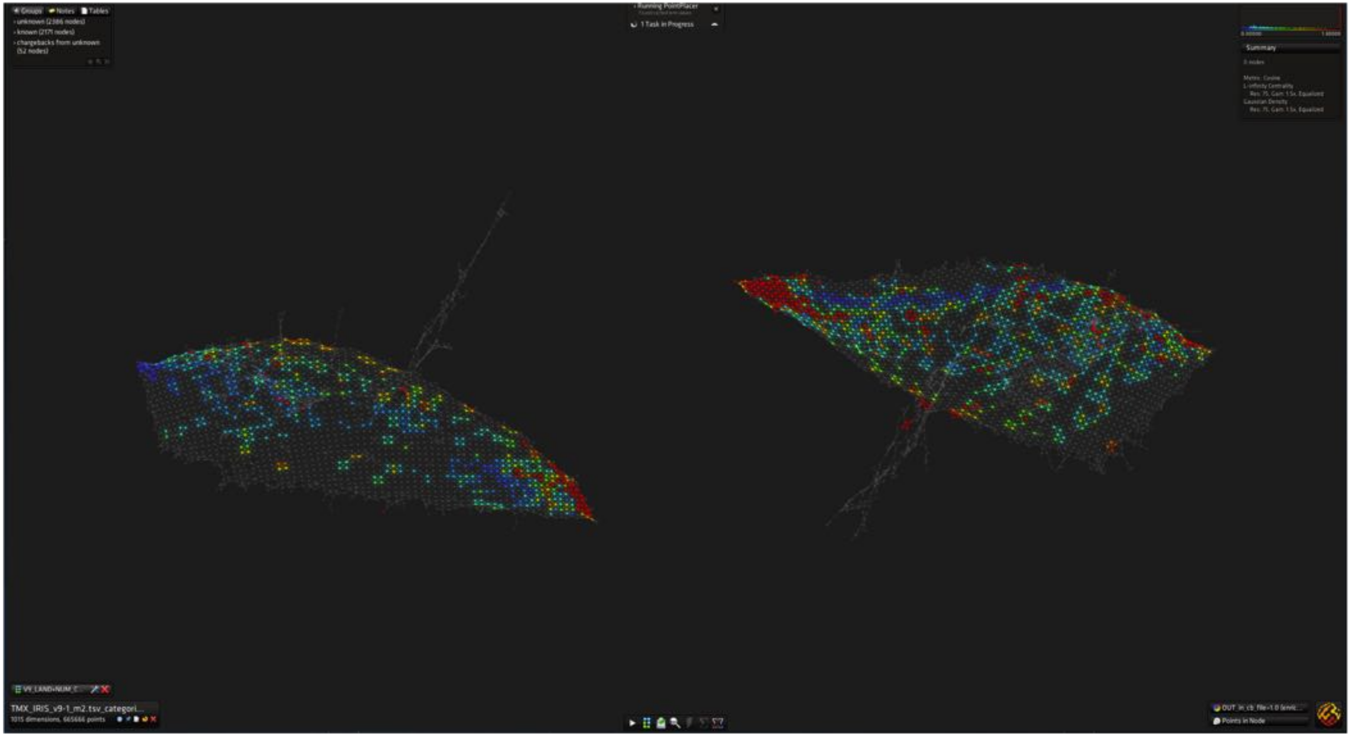
Online Fraud

Fraud Score



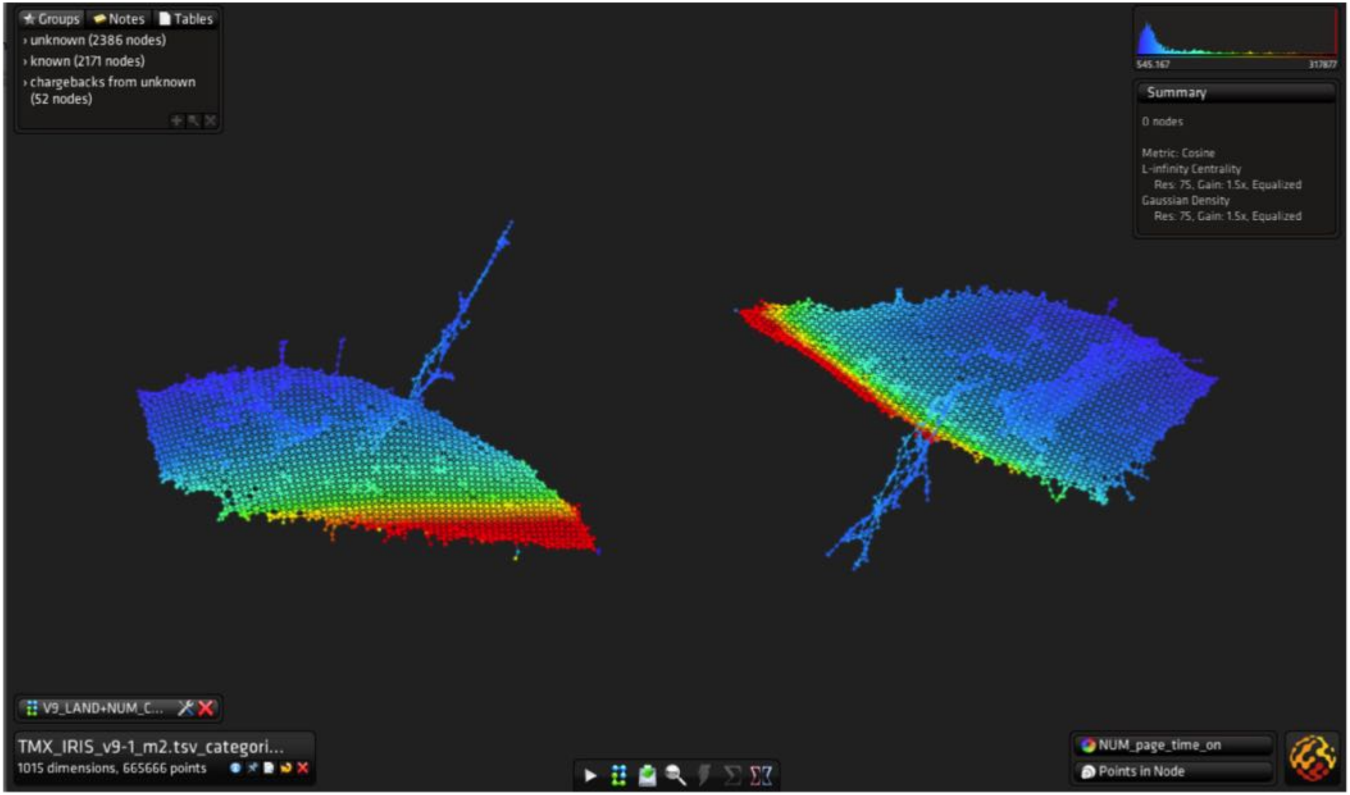
Online Fraud

Charge Back (Ground Truth)



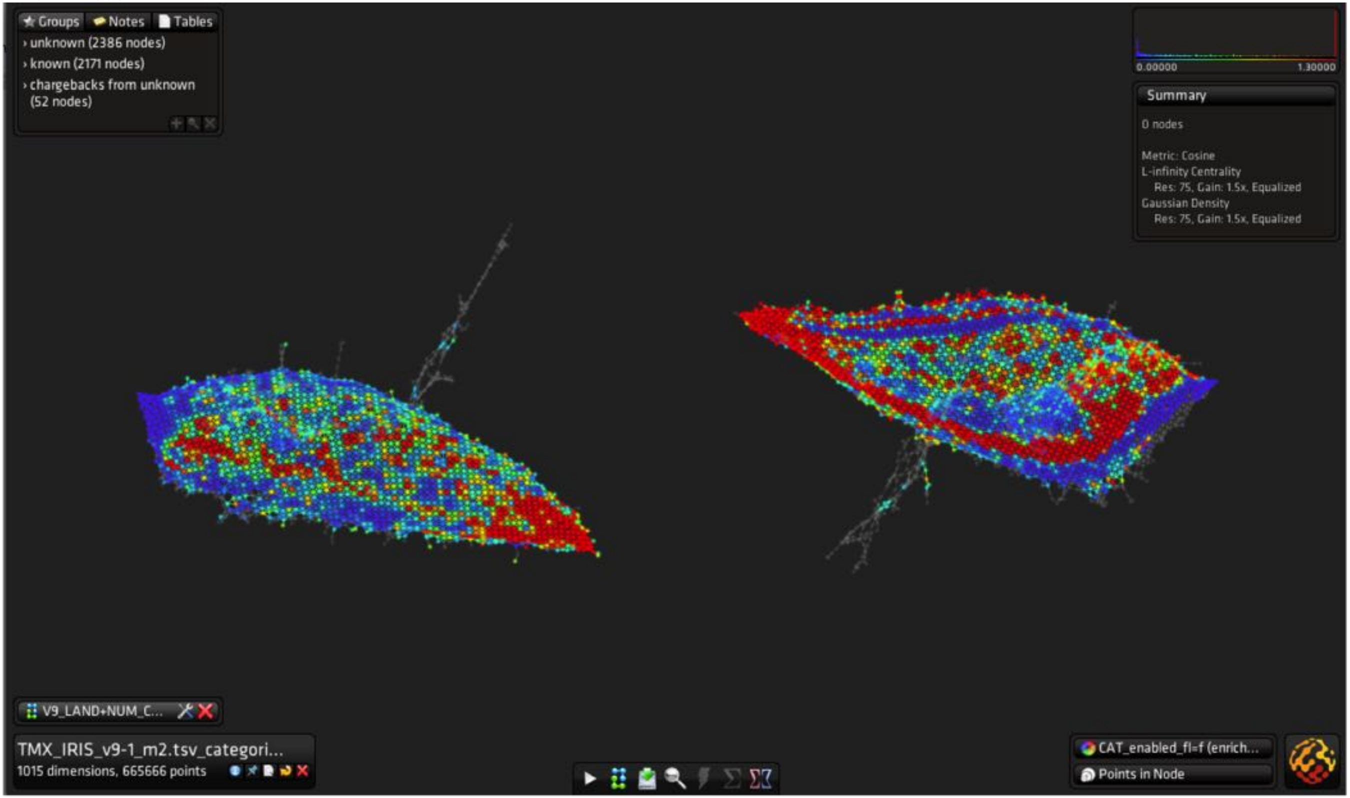
Online Fraud

Time On Page



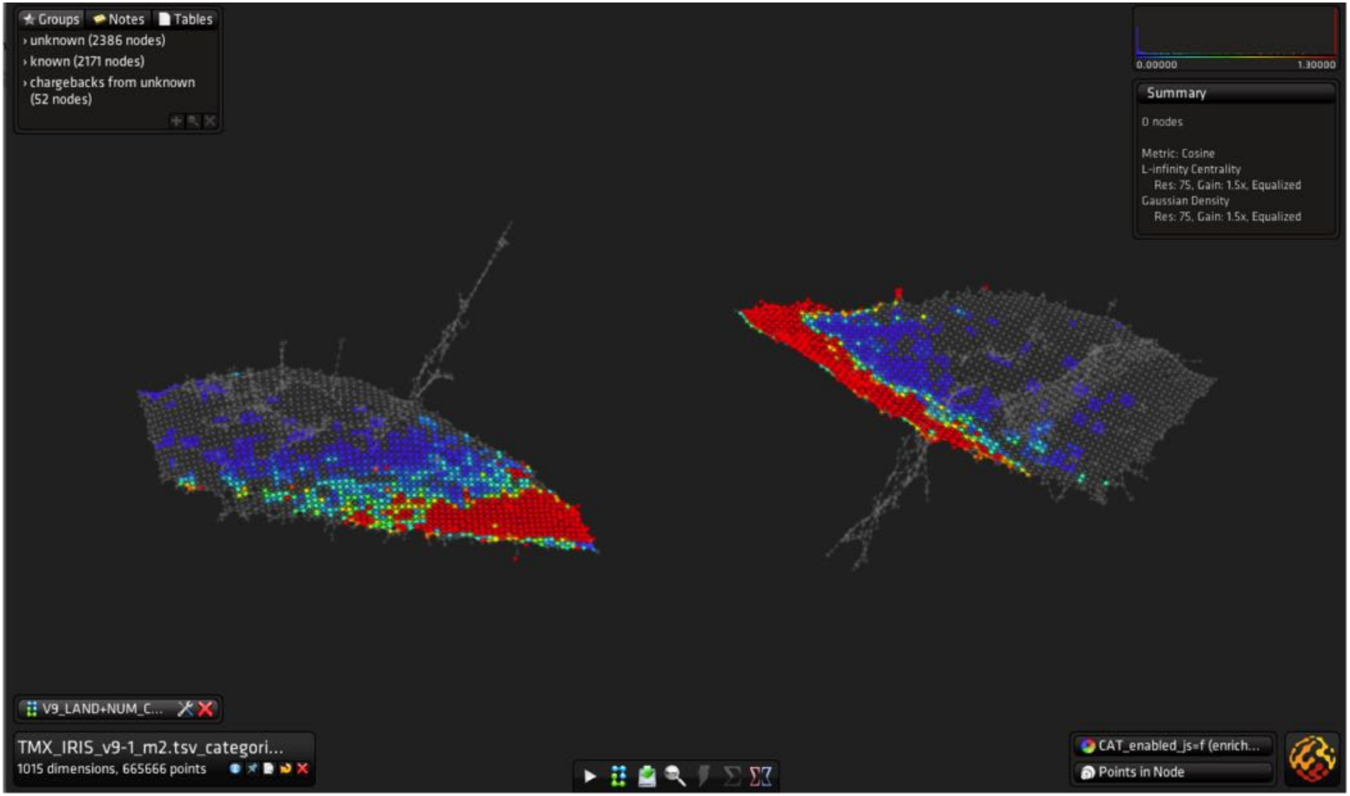
Online Fraud

No Flash



Online Fraud

No Javascript



Parkinson's Detection with Mobile Phone